

Path Integrals in Quantum Physics

Lectures given at ETH Zurich

R. Rosenfelder

Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Abstract

These lectures are intended for graduate students who want to acquire a working knowledge of path integral methods in a wide variety of fields in physics. In general the presentation is elementary and path integrals are developed in the usual heuristic, non-mathematical way for application in many diverse problems in quantum physics. Three main parts deal with path integrals in non-relativistic quantum mechanics, many-body physics and field theory and contain standard examples (quadratic Lagrangians, tunneling, description of bosons and fermions etc.) as well as specialized topics (scattering, dissipative systems, spin & color in the path integral, lattice methods etc.). In each part simple Fortran programs which can be run on a PC, illustrate the numerical evaluation of (Euclidean) path integrals by Monte-Carlo or variational methods. Also included are the set of problems which accompanied the lectures and their solutions.

0. Contents

First, an overview over the planned topics. The subsections marked by * are optional and may be left out if there is no time available whereas the chapters printed in blue deal with basic concepts. Problems from the optional chapters or referring to "Details" are marked by a * as well.

1. Path Integrals in Non-Relativistic Quantum Mechanics of a Single Particle

1. Action Principle and Sum over all Paths	6
2. Lagrange, Hamilton and other Path-Integral Formulations	10
3. Quadratic Lagrangians	22
4. Perturbation Theory *	26
5. Semiclassical Expansions	29
6. Potential Scattering and Eikonal Approximation *	33
7. Green Functions as Path Integrals	44
8. Symmetries and Conservation Laws *	53
9. Numerical Treatment of Path Integrals *	56
10. Tunneling and Instanton Solutions *	63

2. Path Integrals in Statistical Mechanics and Many-Body Physics

1. Partition Function	72
2. The Polaron	74
3. Dissipative Quantum Systems *	79
4. Particle Number Representation and Path Integrals over Coherent States	88
5. Description of Fermions: Grassmann Variables	95
6. Perturbation Theory and Diagrams *	98
7. Auxiliary Fields and Hartree Approximation *	105
8. Asymptotic Expansion of a Class of Path Integrals *	109

3. Path Integrals in Field Theory

1. Generating Functionals and Perturbation Theory	120
2. Effective Action *	135
3. Quantization of Gauge Theories	139
4. Worldlines and Spin in the Path Integral *	149
5. Anomalies *	157
6. Lattice Field Theories *	162

Additional Literature	175
Original Publications	176
Problems	180
Solutions	195

Literature:

There is a large number of text books which are dealing with path integrals either as a tool for specific problems or as basis for an unified treatment. In the following a small selection is presented in which my favorite books (whom I mostly follow ¹) are marked by the symbol ♣.

Section 1 :

- **R. P. Feynman and A. R. Hibbs:** *Quantum Mechanics and Path Integrals*, McGraw-Hill (1965).
- **L. S. Schulman:** *Techniques and Applications of Path Integration*, John Wiley (1981). ♣
- **J. Glimm and A. Jaffe:** *Quantum Physics: A Functional Point of View*, Springer (1987).
- **G. Roepstorff:** *Path Integral Approach to Quantum Physics*, Springer (1994).
- **G. W. Johnson and M. L. Lapidus:** *The Feynman Integral and Feynman's Operational Calculus*, Oxford University Press (2000).
- **J. Zinn-Justin:** *Path Integrals in Quantum Mechanics*, Oxford University Press (2006).

Section 2 :

- **R. P. Feynman:** *Statistical Mechanics*, Benjamin (1976).
- **V. N. Popov:** *Functional Integrals in Quantum Field Theory and Statistical Physics*, Reidel (1983).
- **J. W. Negele and H. Orland:** *Quantum Many-Particle Systems*, Addison-Wesley (1987). ♣
- **J. Zinn-Justin:** *Quantum Field Theory and Critical Phenomena*, 4th ed., Oxford U. Press (2002).
- **H. Kleinert:** *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 3rd ed., World Scientific (2004).

Section 3 :

- **C. Itzykson and J.-B. Zuber:** *Quantum Field Theory*, McGraw-Hill (1980), ch. 9.
- **T.-P. Cheng and L.-F. Li:** *Gauge Theory of Elementary Particle Physics*, Clarendon (1988).
- **R. J. Rivers:** *Path Integral Methods in Quantum Field Theory*, Cambridge University Press (1990).
- **M. E. Peskin and D. V. Schroeder:** *An Introduction to Quantum Field Theory*, Addison-Wesley (1995), ch. 9. ♣
- **V. Parameswaran Nair:** *Quantum Field Theory. A Modern Perspective*, Springer (2005). ♣
- **H. J. Rothe:** *Lattice Gauge Theories. An Introduction*, 3rd ed., World Scientific Lecture Notes in Physics, Vol. 74, World Scientific (2005).
- **A. Das:** *Field Theory. A Path Integral Approach*, 2nd ed., World Scientific Lecture Notes in Physics, Vol. 75, World Scientific (2006). ♣

¹"(My father used to say: 'If you steal from one book, you are condemned as a plagiarist, but if you steal from ten books, you are considered a scholar, and if you steal from thirty or forty books, a distinguished scholar.')" {Oz}, p.129.

Prerequisites:

Quantum Mechanics: A two-semester course, a little bit of Statistical Mechanics, basic concepts of Field Theory.

Practice Lessons:

Participation in the Practice Sessions is strongly recommended – according to the motto

不聞不若聞之聞之不
 若見之見之不若知之
 知之不若行之字至於
 行之而止矣

“I hear – and I forget,
 I see – and I remember,
 I do – and I understand !”

(Chinese proverb ²)

Remarks:

In order to find some orientation in the jungle of (over 1300 listed) equations, the most important equations are framed according to the following scheme

fundamental	(9 times)
very important	(24 times)
important	(101 times) ,

where, of course, my rating may be debatable ...

The “**Details**” in small print give more in-depth information or detailed derivations and can be omitted in a first study. Additional literature is referenced in the text in curly brackets, e.g. {Weiss} and is listed at the end in alphabetical order. Original publications are cited by consecutive numbers, e.g. [11], which are collected at the end of the text just before the **Problems**.

²Attributed to Xun Kuang (c. 310 - c. 235 BC) known as Xunzi (“Master Xun”), a Chinese Realist Confucian philosopher (see https://en.wikipedia.org/wiki/Xun_Kuang).

The following **abbreviations** are frequently used in the text:

w.r.t. : with respect to *i.e.* : (Latin: *id est*) that is *viz.* : (Latin: *videlicet*) namely
l.h.s. : left-hand side *r.h.s.* : right-hand side *e.g.* : (Latin: *exemplum gratum*) for example
cf. : (Latin: *confer*) compare *q.e.d.* : (Latin: *quod erat demonstrandum*) which was to be proved.

Despite the word "Integral" appearing in the title no knowledge of particular integrals is needed – the only integral which appears again and again in various (multi-dimensional) generalizations is the **Gaussian integral**

$$G(a) = \int_{-\infty}^{+\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \quad \text{Re } a > 0. \quad (0.1)$$

Proof: Evaluate

$$G^2(a) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \exp[-a(x^2 + y^2)] \quad (0.2a)$$

in polar coordinates $x = r \cos \phi, y = r \sin \phi, dx dy = r dr d\phi$. Then one obtains

$$G^2(a) = \int_0^{2\pi} d\phi \int_0^{\infty} dr r \exp(-ar^2) = 2\pi \int_0^{\infty} dr \left(-\frac{1}{2a} \frac{d}{dr}\right) \exp(-ar^2) = \frac{\pi}{a}. \quad (0.2b)$$

The constraint for the complex parameter a is needed for convergence of the integral or for vanishing of the integrated term at infinity, respectively.

Some Personal Words at the End of Section 0:

These notes have their origin in material handed over to students who attended my lectures. These I have given first at the universities of Mainz and Hannover in Germany and later for many years at the ETH Zurich in Switzerland.

Since a long time I have been fascinated by the elegance and versatility of this particular description of the quantum world and I hope that also these notes can convey both aspects – beauty and utility – to some of the readers. In addition to the "canonical" topics (which one has to deal with in a lecture on Path Integrals) I have added several chapters on themes in which I was particularly interested or to which I have added own contributions. In this way a rather personal collection of path integral methods in quantum physics³ has been created which may be attractive for some readers but obviously cannot replace a detailed text book.

Due to practical reasons (and insufficient knowledge) I have not tried to derive Feynman's path integral with strict mathematical rigor but I have chosen the usual heuristic and descriptive time-splitting approach. In order to show that one can use these functional integrals also for numerical work I have included small (and unsophisticated) FORTRAN programs in which Monte-Carlo methods play an important role.

I am indebted to all students asking "silly questions" which I could not answer immediately but which gave me (and hopefully them) a better understanding of the topic; of course, all remaining errors and deficiencies of these notes remain in my responsibility. Nadia Fettes and Mirko Birbaumer detected errors in the original lattice program which I hadn't seen. I would like to thank Qiang Li who unearthed the original chinese proverb for me when he was in the Theory Group of PSI. Valeri Markushin came to my rescue when my proven drawing program suddenly became obsolete ... With Julien Carron I had a very agreeable collaboration on complex Gaussian integrals and other curiosities. Thanks also to Matthias who gave me an important hint about the proper use of the German language ...

The present notes are (a rough) English version of the German text arXiv:1209.1315 v3 which includes many corrections and additions compared to the previous versions. In addition, (my) Solutions to the Problems are also attached. This is a good opportunity to thank Manfred Stingl for his constant support and encouragement and to appreciate Ingrid's skills for finding a particular, proper citation.

Villigen PSI, July 2017

Roland Rosenfelder

³I have left out applications in financial industry for obvious reasons

1. Path Integrals in Non-Relativistic Quantum Mechanics of a Single Particle

1.1 Action Principle and Sum over all Paths

There are essentially three formulations ⁴ of quantum mechanics:

- Matrix mechanics (Heisenberg 1925)
- Wave mechanics (Schrödinger 1926)
- Path integrals (**Feynman 1942/1948**)

The first two versions whose equivalence was shown very soon by Schrödinger, Dirac et al., are presented in every quantum mechanics course, or textbook; the last one is the subject of this lecture. It was developed by **Feynman** [2] and is based on a work of **Dirac** [3] (both reprinted in [4]). For a long time this formulation was considered as too difficult and useless for practical purposes, so that it was not included in a textbook. However, conceptually the Feynman path integral is easier to grasp and requires far less radical departure from the ideas of classical physics (to which we are all used) than the usual quantum mechanics with their operators and state vectors in a Hilbert space.

As for the practical side of the various formulations, it is undisputed that for many problems Schrödinger's wave mechanics is the fastest and easiest way to obtain result: For example, when calculating the stationary states of a particle in a given potential. But in many-particle problems the Schrödinger equation is of much less importance and Heisenberg's matrix mechanics of Heisenberg plays a much larger role (e.g. when diagonalization the Hamiltonian matrix in a certain subspace). Similarly, the method of the path integrals has become an indispensable tool in field theory: The Feynman rules for non-abelian gauge theories were first derived in this way and the attempts to treat numerically the field theory of the strong interaction are based directly on the (Euclidean) path integral representation of Quantum Chromodynamics.

Moreover, what this method distinguishes from the other formulations, is its applicability in many areas of physics. This “unification” of diverse fields not only helps in understanding, but also gives suggestions to apply new methods that have been successful in other areas.

One caveat: The Feynman path integral is not defined mathematically in a rigorous manner except for special cases (Euclidean formulation, i.e. for imaginary times \rightarrow Brownian motion \rightarrow Wiener integral). There are numerous attempts and formulations to provide a mathematically sound basis (see, e.g. **Johnson & Lapidus** in the list of textbooks or [5]). This will not worry us in the following – in most cases mathematical rigor is far behind physical intuition.

Feynman developed his formulation of quantum mechanics in close analogy to classical mechanics. First, therefore, a brief outline of the essential aspects of classical mechanics and quantum mechanics.

Classical Mechanics

A system (for simplicity: A point particle in one spatial dimension) with coordinate(s) $q(t)$ is described by the **Lagrangian**

$$L(q(t), \dot{q}(t), t) \tag{1.1}$$

Its dynamic development, that is, its trajectory (or “path”) from an initial point $q(t_a) = q_a$ to an end point $q(t_b) = q_b$ proceeds in such a way that among all possible paths the one is selected that makes the **action**

⁴The article [1] counts nine!

$$S = \int_{t_a}^{t_b} dt L(q(t), \dot{q}(t), t) \quad (1.2)$$

minimal (or more precisely: extremal):

$$\delta S = 0 \quad (1.3)$$

(Hamilton's principle or principle of "least" effect). From that the equations of motion (Euler-Lagrange equations) follow

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0. \quad (1.4)$$

An alternative formulation is the one which uses the **Hamiltonian** of the system: We define the conjugated momentum

$$p = \frac{\partial L}{\partial \dot{q}} \quad (1.5)$$

and define the Hamiltonian as

$$H(p(t), q(t), t) = [p \cdot \dot{q} - L(q, \dot{q}, t)]_{\dot{q}=\dot{q}(p)}. \quad (1.6)$$

Hamilton's equations

$$\begin{aligned} \dot{q}(t) &= \frac{\partial H}{\partial p} \\ \dot{p}(t) &= -\frac{\partial H}{\partial q} \end{aligned} \quad (1.7)$$

can also be obtained from an extremum of the action

$$\delta S = \delta \int_{t_a}^{t_b} dt [p \cdot \dot{q} - H(p(t), q(t), t)] = 0 \quad (1.8)$$

by independent variation of q and p .

Quantum Mechanics

In classical mechanics Nature seems to "compare" different paths and then to select the path of extremal action. This is also the case in optics, as long as the wavelength of light is much smaller than the typical dimensions of the system. However, if both sizes are comparable, we observe the typical interference behavior of waves, e.g. diffraction by a double slit as depicted in Fig. 1.

The different ways now play a crucial role, since the scattered wave is composed of two parts

$$\Phi \propto e^{ikl_1} + e^{ikl_2} \quad (1.9)$$

(k : wavenumber). The intensity at the detector (screen) is proportional to $|\Phi|^2$ and shows the typical diffraction minima and maxima.

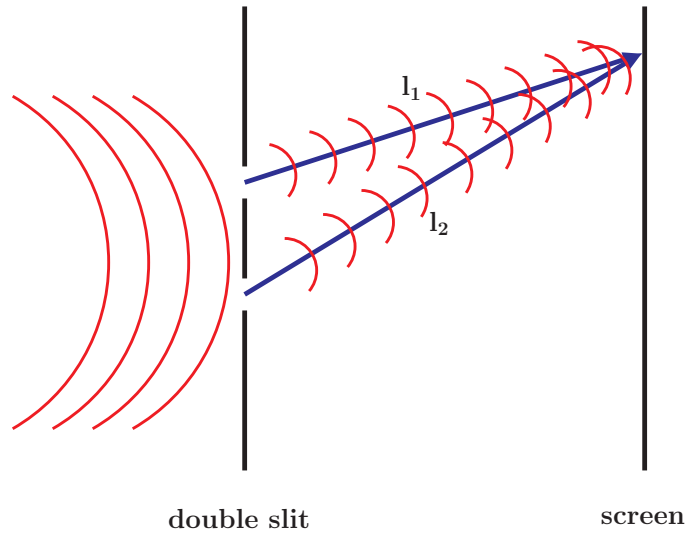


Fig. 1 : Diffraction of waves through a double slit.

It is now a crucial experimental fact that even matter particles (like electrons or neutrons) show diffraction effects when passing through slits or scatter from crystals. This happens when their de Broglie wavelength is comparable to the dimensions of the object to be imaged (for electrons, this was demonstrated for the first time by Davisson and Germer 1927).

The quantum mechanical description of this effect postulates a **probability amplitude** which is a superposition of the two possible amplitudes (for the passage through the respective slit):

$$\Phi = \Phi_1 + \Phi_2, \quad (1.10)$$

and the probability of finding the electron at the detector is,

$$W \sim |\Phi|^2. \quad (1.11)$$

In other words:

*One has to sum **coherently** over the various (unobserved) alternative ways an event can happen.*

Let us imagine that we now drill more and more holes in the screen – until it no longer exists – and that we put more and more screens in the space between source and detector which we also treat in the same way, then we have

$$\Phi(a, b) = \sum_{\text{all path from } a \text{ to } b} \Phi_i. \quad (1.12)$$

Of course, it remains to specify more precisely how this sum over “all paths from a to b ” has to be performed and with which weight each path contributes. The answer to the first question leads to **functional integrals**, which we will treat in the next chapter while the problem of the weighting is solved in a heuristic way: Since Planck’s constant \hbar has the dimension of an action and determines the quantum effects it is not surprising that the rule is:

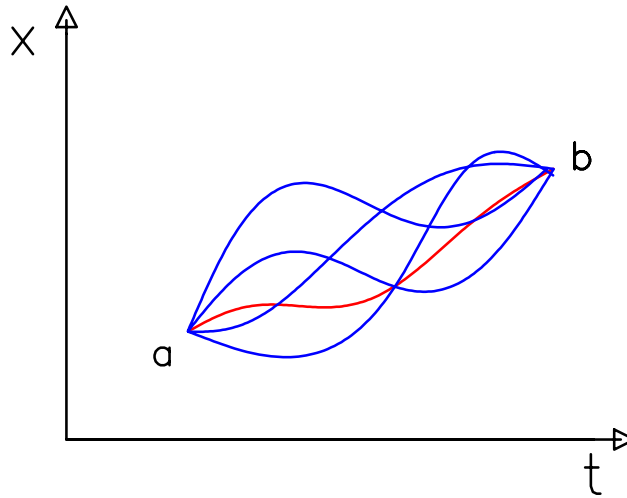


Fig. 2 : Quantum mechanical propagation of a particle from a to b . The classical path is indicated by a red line.

All paths contribute with the same absolute magnitude but with different phase: The phase of every path $x(t)$ is its classical action $S[x(t)]$ ⁵ divided by \hbar .

$$\Phi(a, b) = \sum_{\text{all path of } a \text{ to } b} \text{const. } e^{iS[x(t)]/\hbar} . \tag{1.13}$$

With this prescription the **classical limit** (formally: $\hbar \rightarrow 0$) can be performed immediately: If all actions $S \gg \hbar$ this leads to immense oscillations of the exponential function, that is, to each path with a positive contribution, there is an adjacent path which gives a negative contribution and therefore deletes it. There remains only the special path for which this doesn't happen, *viz.* whose phase is stationary

$$\delta S_{\text{classical}} = 0 \tag{1.14}$$

and only one trajectory, the classical trajectory, contributes to the sum over all paths.

Detail 1: Orders of Magnitude

It is instructive to estimate the magnitude of the action for two different systems by simple dimensional analysis: First, we take a mechanical watch, the moving parts of it having an approximate size $d \sim 10^{-4}$ m, mass $m \sim 10^{-4}$ kg and typical time $t \sim 1$ s. Then, the characteristic action of this system is

$$S_1 \sim m d^2 t^{-1} \sim 10^{-12} \text{ J} \sim 10^{22} \hbar . \tag{1.15a}$$

However, if we consider a microprocessor, the centerpiece of every computer, then we know that its integrated circuits typically are $d \sim 0.2 \mu\text{m} = 2 \times 10^{-7}$ m thick and that it operates with electrons ($m \sim 10^{-30}$ kg). With a clock frequency of 1 GHz, corresponding to an angular frequency of $\omega \sim 6$ GHz, the typical action then is

$$S_2 \sim m d^2 \omega \sim 2.4 \times 10^{-34} \text{ J} \sim 2 \hbar . \tag{1.15b}$$

Thus, although both systems possess comparable (outer) dimensions, the traditional watchmaker doesn't have to know anything about quantum theory while the developers of microprocessors definitely need it for their work.

Of course, the quantum mechanical description cannot be derived in this way from classical mechanics, the classical limit is only a necessary condition of the larger theory. Therefore, in the next chapter we will proceed in the opposite way and derive the path integral description from the usual quantum mechanical one. This will give us directly both the weighting of each path as well as the prescription how to do their summation.

⁵The notation means that S is a **functional** of the path $x(t)$, i.e. a number associated with each trajectory.

1.2 Lagrange, Hamilton and Other Formulations

In the following all quantum mechanical operators are denoted by an “hat”. We also assume that the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}, \quad \hat{V} = V(\hat{x}) \quad (1.16)$$

is time-independent and consider matrix elements of the **time-evolution operator** ⁶

$$U(x_b, t_b; x_a, t_a) = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle = \langle x_b | e^{-i(t_b - t_a)\hat{H}/\hbar} | x_a \rangle. \quad (1.17)$$

As we will see, the time-evolution operator contains all information about the system that we need.

Feynman’s Path Integral

The path integral representation of U is based on the decomposition of the time interval $t_b - t_a$ into N single, infinitesimal small intervals

$$\epsilon = \frac{t_b - t_a}{N}, \quad (1.18)$$

so that

$$\exp[-i(t_b - t_a)\hat{H}/\hbar] = \lim_{N \rightarrow \infty} \prod_{k=1}^N e^{-i\epsilon\hat{H}/\hbar}. \quad (1.19)$$

This is also called Trotter’s product formula. Now it is a fact that

$$\exp[-i\epsilon(\hat{T} + \hat{V})/\hbar] = \exp[-i\epsilon\hat{T}/\hbar] \cdot \exp[-i\epsilon\hat{V}/\hbar] + \mathcal{O}(\epsilon^2), \quad (1.20)$$

i.e. for infinitesimal times the non-commutativity of the the quantum mechanical operators can (**almost**) be neglected. If we use this expression in (1.19) and insert the identity operator

$$1 = \int_{-\infty}^{+\infty} dx_j |x_j\rangle \langle x_j| \quad j = 1, 2, \dots, (N-1) \quad (1.21)$$

between each factor, it is only a small step to obtain the path integral: Since for a local potential $V(\hat{x})|x\rangle = V(x)|x\rangle$ is valid, we obtain

$$\begin{aligned} U(x_b, t_b; x_a, t_a) &= \lim_{N \rightarrow \infty} \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1} \langle x_b | e^{-i\epsilon\hat{T}/\hbar} | x_{N-1} \rangle e^{-i\epsilon V(x_{N-1})/\hbar} \\ &\quad \cdot \langle x_{N-1} | e^{-i\epsilon\hat{T}/\hbar} | x_{N-2} \rangle e^{-i\epsilon V(x_{N-2})/\hbar} \\ &\quad \vdots \\ &\quad \cdot \langle x_1 | e^{-i\epsilon\hat{T}/\hbar} | x_a \rangle e^{-i\epsilon V(x_a)/\hbar}. \end{aligned} \quad (1.22)$$

We now need the matrix elements of $\exp(-i\epsilon\hat{T}/\hbar)$ between position eigenstates

$$\langle x_{j+1} | e^{-i\epsilon\hat{T}/\hbar} | x_j \rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_j \exp\left(-i\frac{\epsilon}{\hbar} \frac{p_j^2}{2m}\right) e^{ip_j \cdot (x_{j+1} - x_j)/\hbar}. \quad (1.23)$$

Here we have used that $\hat{T} = \hat{p}^2/(2m)$ is diagonal in momentum space. The integral in (1.23) is an extended Gaussian integral which can be derived from the basic integral (0.1) by completion of the square:

⁶Frequently the notation $\langle x_b, t_b | x_a, t_a \rangle$ is used for this matrix element.

$$\int_{-\infty}^{+\infty} dx \exp(-ax^2 + bx) = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}\right) , \quad a \neq 0 , \quad \text{Re } a \geq 0 . \quad (1.24)$$

Detail 2: Complex Gaussian Integrals

To be more precise the integral in Eq. (1.23) is an (extended) **Fresnel integral** which arises from the basic integral (0.1) through the limit $\text{Re } a \rightarrow 0$:

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{iax^2} &= \lim_{\delta \rightarrow 0^+} \int_{-\infty}^{+\infty} dx e^{-(\delta - ia)x^2} = \lim_{\delta \rightarrow 0^+} \sqrt{\frac{\pi}{\delta - ia}} \quad (a \text{ real}) \\ &= \sqrt{\frac{\pi}{|a|}} \exp\left[\frac{i}{2} \lim_{\delta \rightarrow 0^+} \arctan\left(\frac{a}{\delta}\right)\right] = \sqrt{\frac{\pi}{|a|}} \exp\left[i \frac{\pi}{4} \text{sgn}(a)\right] \\ &= \sqrt{\frac{\pi}{|a|}} \left[\frac{1}{\sqrt{2}} + i \frac{\text{sgn}(a)}{\sqrt{2}} \right] . \end{aligned} \quad (1.25a)$$

Note that the real parameters a can have any sign. Here and below we understand the root of a complex variable z as the **principal value**, i.e. the branch of the two-valued square-root function which has a positive real part (cf {Handbook}, eq. 3.7.26)

$$\sqrt{z} := \sqrt{|z|} \exp\left(\frac{1}{2} i \arg z\right) , \quad -\pi < \arg z \leq \pi . \quad (1.25b)$$

This value one already has to take in Eq. (0.1), as in the real case the above definition coincides with the positive root which one has take for a positive integrand. Therefore the Gaussian integral with complex parameters is to be understood as an **analytic continuation** of the result in the neighborhood of the real axis.

Another way to calculate the Fresnel integral with infinite limits is to regard it as the limit of finite Fresnel integrals:

$$\int_{-\infty}^{+\infty} dx e^{iax^2} = \lim_{R \rightarrow \infty} \int_{-R}^{+R} dx \left[\cos(ax^2) + i \sin(ax^2) \right] . \quad (1.25c)$$

The transformation $x = \sqrt{\pi/(2|a|)} t$ gives

$$\begin{aligned} \int_{-\infty}^{+\infty} dx e^{iax^2} &= 2\sqrt{\frac{\pi}{2|a|}} \lim_{T \rightarrow \infty} \left[\int_0^T dt \cos\left(\frac{\pi}{2} t^2\right) + i \text{sgn}(a) \int_0^T dt \sin\left(\frac{\pi}{2} t^2\right) \right] \\ &= 2\sqrt{\frac{\pi}{2|a|}} \lim_{T \rightarrow \infty} \left[C(T) - i \text{sgn}(a) S(T) \right] \end{aligned} \quad (1.25d)$$

where $T = R\sqrt{2|a|/\pi}$ and $C(T)$, $S(T)$ denote the standard Fresnel integrals as they are defined in **{Handbook}**, eq. (7.3.1) and (7.3.2). Since these tend to the asymptotic limit 1/2 for $T \rightarrow \infty$ (*ibid.*, eq. (7.3.20)) we obtain

$$\int_{-\infty}^{+\infty} dx e^{iax^2} = \sqrt{\frac{\pi}{2|a|}} \left[1 + i \text{sgn}(a) \right] , \quad (1.25e)$$

in agreement with Eq. (1.25a). The extended Fresnel integral (a, b reell)

$$\int_{-\infty}^{+\infty} dx e^{iax^2 + ibx} = \int_{-\infty}^{+\infty} dx \exp\left[ia \left(x + \frac{b}{2a} \right)^2 - i \frac{b^2}{4a} \right] \quad (1.25f)$$

follows from simple completion of the square

$$\int_{-\infty}^{+\infty} dx \exp(iax^2 + ibx) = \sqrt{\frac{\pi}{-ia}} \exp\left(-\frac{i}{4} b a^{-1} b\right) . \quad (1.25g)$$

Eq. (1.25g) has been written in mnemonic form ⁷ which makes the generalization to the multi- and infinite-dimensional case more obvious.

With this result we get

$$\left\langle x_{j+1} \left| e^{-i\epsilon\hat{T}/\hbar} \right| x_j \right\rangle = \sqrt{\frac{m}{2\pi i \epsilon \hbar}} \exp\left[\frac{im}{2\hbar} \frac{(x_{j+1} - x_j)^2}{\epsilon}\right] \quad (1.26)$$

and if, for notational simplification, we set

$$x_0 = x_a , \quad x_N = x_b \quad (1.27)$$

⁷see <https://en.wikipedia.org/wiki/Mnemonic>

we have

$$U(x_b, t_b; x_a, t_a) = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{N/2} \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1} \cdot \prod_{j=0}^{N-1} \exp \left[\frac{im}{2\epsilon \hbar} (x_{j+1} - x_j)^2 \right] \exp \left[\frac{-i\epsilon}{\hbar} V(x_j) \right]. \quad (1.28)$$

The product of exponential terms is the exponent of their sum and we obtain

$$U(x_b, t_b; x_a, t_a) = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{N/2} \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1} \cdot \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{j=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j) \right] \right\} \quad (1.29)$$

$$\equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t) e^{iS[x(t)]/\hbar}. \quad (1.30)$$

The last line is a *symbolic* shorthand for the limit

$$N \rightarrow \infty, \quad \epsilon \rightarrow 0, \quad \text{but } \epsilon N = t_b - t_a \quad \text{fixed} \quad (1.31)$$

of the $(N - 1)$ - dimensional integral. It is indeed the action which appears in the argument of the exponential function in this limit because the discrete sums approximate the Riemann integral

$$\begin{aligned} \epsilon \sum_{j=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j) \right] &\rightarrow \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{x}(t)^2 - V(x(t)) \right] \\ &= \int_{t_a}^{t_b} dt L(x(t), \dot{x}(t)) = S[x(t)]. \end{aligned} \quad (1.32)$$

Note that the short-time approximation

$$\exp \left[-i\epsilon(\hat{T} + \hat{V})/\hbar \right] = \exp \left[-i\epsilon\hat{V}/\hbar \right] \cdot \exp \left[-i\epsilon\hat{T}/\hbar \right] + \mathcal{O}(\epsilon^2) \quad (1.33)$$

leads to an action in which $V(x_{j+1})$ appears instead of $V(x_j)$. In a similar way the more symmetric form

$$\exp \left[-i\epsilon(\hat{T} + \hat{V})/\hbar \right] = \exp \left[-i\epsilon\hat{V}/(2\hbar) \right] \cdot \exp \left[-i\epsilon\hat{T}/\hbar \right] \cdot \exp \left[-i\epsilon\hat{V}/(2\hbar) \right] + \mathcal{O}(\epsilon^3), \quad (1.34)$$

would lead to a slightly different discrete action. In the simple case under discussion (one particle in a scalar potential) this does not lead to any consequence: The differences are of order ϵ and vanish in the continuum limit $\epsilon \rightarrow 0$. The situation is different if one considers velocity-dependent interactions because the velocity is represented by $(x_{j+1} - x_j)/\epsilon$. More on that under the heading “**Ordering Problem**”.

The expression (1.29) gives an exact prescription how to sum over “all paths from a to b ”: One discretizes the time and approximates each possible path from a to b by a **polygon path**. Integration over an intermediate point x_j corresponds to the summation over all paths from x_{j-1} to x_{j+1} , because with fixed x_{j-1}, x_{j+1} a new path is generated by a different value of x_j . There is no integration over the endpoints because they are fixed by the boundary conditions.

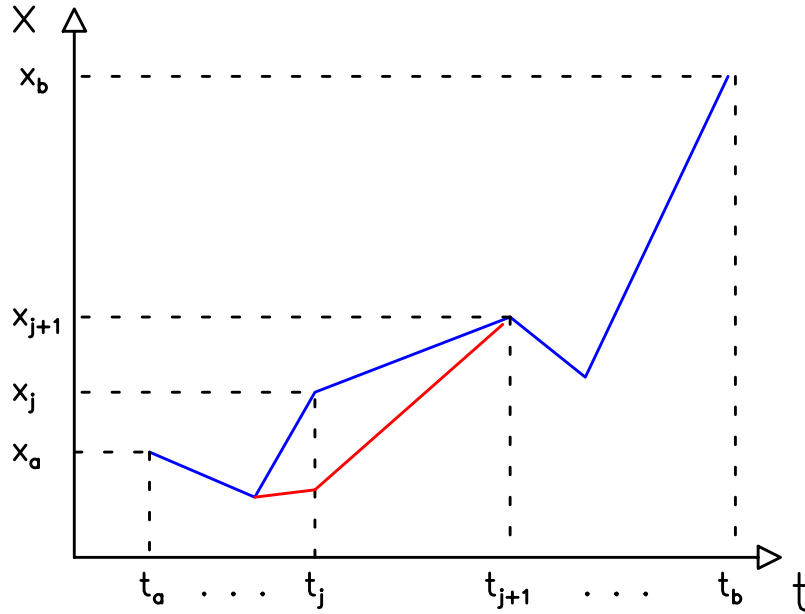


Fig. 3 : Discretization and summation over the quantum mechanical paths. The red path arises from a different value of x_j .

An extraordinary aspect of the path integrals is that they deal with **ordinary numbers** and not with non-commuting operators! This is an enormous advantage compared to the usual formulation of quantum mechanics. The price one has to pay for that is hidden in the complicated definition of the path integral: It is an infinite-dimensional integral, a so-called **functional integral**⁸.

It can be shown that the usual Schrödinger theory follows from Eq. (1.29). This proceeds in the following manner:

1. The wave function at an infinitesimal later time $T + \epsilon$ is obtained from the wave function at the time t by applying the time-evolution operator

$$\begin{aligned} \psi(x, t + \epsilon) &= \langle x | \hat{U}(t + \epsilon, t) | \psi \rangle = \int dy U(x, \epsilon; y, 0) \psi(y, t) \\ &= \int_{-\infty}^{+\infty} dy \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{1/2} \exp \left\{ \frac{i\epsilon}{\hbar} \left[\frac{m}{2} \frac{(x - y)^2}{\epsilon^2} - V(y) \right] \right\} \psi(y, t), \end{aligned} \quad (1.35)$$

where in the last line the discretized form (1.29) for the time-evolution operator has been employed with $N = 1$.

2. Now we substitute $\xi = y - x$ in the integral (1.35) and obtain

$$\psi(x, t + \epsilon) = \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{1/2} \int_{-\infty}^{+\infty} d\xi \exp \left(\frac{im\xi^2}{2\epsilon\hbar} \right) \exp \left[-\frac{i\epsilon}{\hbar} V(x + \xi) \right] \psi(x + \xi, t). \quad (1.36)$$

Due to the Gaussian factor in the integral, which restricts the values of ξ to $\mathcal{O}(\epsilon^{1/2})$, we can expand in

⁸Other notations for it are $\int [dx]$ or $\int Dx$.

powers of ξ and ϵ :

$$\begin{aligned} \psi(x, t + \epsilon) = & \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{1/2} \int_{-\infty}^{+\infty} d\xi \exp\left(\frac{im\xi^2}{2\epsilon\hbar}\right) \left[1 - \frac{i\epsilon}{\hbar} V(x) - \frac{i\epsilon}{\hbar} \xi \frac{\partial}{\partial x} V(x) + \mathcal{O}(\epsilon^2, \epsilon\xi^2) \right] \\ & \cdot \left[\psi(x, t) + \xi \frac{\partial}{\partial x} \psi(x, t) + \frac{1}{2} \xi^2 \frac{\partial^2}{\partial x^2} \psi(x, t) + \mathcal{O}(\xi^3) \right]. \end{aligned} \quad (1.37)$$

3. We now perform the Gaussian integrals: The ones over odd powers vanish whereas the integrals over even powers of ξ lead to

$$\int_{-\infty}^{+\infty} d\xi \exp\left(\frac{im\xi^2}{2\epsilon\hbar}\right) = \left(\frac{2\pi i \epsilon \hbar}{m}\right)^{1/2}, \quad \int_{-\infty}^{+\infty} d\xi \xi^2 \exp\left(\frac{im\xi^2}{2\epsilon\hbar}\right) = \frac{i\epsilon\hbar}{m} \left(\frac{2\pi i \epsilon \hbar}{m}\right)^{1/2} \quad (1.38)$$

(the last integral is easily obtained by differentiation of the Gaussian integral (0.1) with respect to the parameter a). This gives

$$\psi(x, t + \epsilon) = \psi(x, t) - \frac{i\epsilon}{\hbar} V(x) \psi(x, t) + \frac{i\epsilon\hbar}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + \mathcal{O}(\epsilon^2). \quad (1.39)$$

The neglected terms come from higher powers of $\epsilon V(x)$, higher terms in the expansion of $V(x + \xi)$ and from the Gaussian integral over the fourth power of ξ . It is now seen that **all** short-time approximations (1.20, 1.33, 1.34) only differ by higher-order terms and thus lead to the same result in the limit $\epsilon \rightarrow 0$.

4. If we now multiply by $i\hbar/\epsilon$ we obtain

$$i\hbar \frac{\psi(x, t + \epsilon) - \psi(x, t)}{\epsilon} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t) + \mathcal{O}(\epsilon). \quad (1.40)$$

In the limit $\epsilon \rightarrow 0$ this gives exactly **Schrödinger's equation**

$$\boxed{i\hbar \dot{\psi}(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t)} \quad (1.41)$$

for a particle in the potential $V(x)$. As mentioned before one must be more cautious when dealing with velocity-dependent interactions: For example, the interaction of a charged particle in a magnetic field contains a term $\mathbf{A}(\mathbf{x}) \cdot \dot{\mathbf{x}}$ (where $\mathbf{A}(\mathbf{x})$ is the corresponding vector potential) and it is now essential which discrete form of the path integral is used in the above derivation:

$$\begin{aligned} & \mathbf{A}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{y})/\epsilon, \quad \text{or} \\ & [\mathbf{A}(\mathbf{x}) + \mathbf{A}(\mathbf{y})] \cdot (\mathbf{x} - \mathbf{y})/(2\epsilon), \quad \text{or} \\ & \mathbf{A}((\mathbf{x} + \mathbf{y})/2) \cdot (\mathbf{x} - \mathbf{y})/\epsilon \quad ? \quad (\text{see **Problem 7**}). \end{aligned}$$

Some other properties of the time-evolution operator can be obtained from the path integral form (1.29). For example, the law for consecutive events can be derived in the following way: Let t_c be an intermediate time with $t_a < t_c < t_b$. If we divide the intervals $t_c - t_a = L\epsilon$, $t_b - t_c = M\epsilon$ we get

$$\begin{aligned} U(x_b, t_b; x_a, t_a) = & \lim_{L \rightarrow \infty} \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{L/2} \int_{-\infty}^{+\infty} dx_1 \dots dx_{L-1} \int_{-\infty}^{+\infty} dx_L \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{j=0}^{L-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j) \right] \right\} \\ & \cdot \lim_{M \rightarrow \infty} \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{M/2} \int_{-\infty}^{+\infty} dx_{L+1} \dots dx_{L+M-1} \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{k=L}^{L+M-1} \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\epsilon} \right)^2 - V(x_k) \right] \right\} \\ & \equiv \int_{-\infty}^{+\infty} dx_c U(x_b, t_b; x_c, t_c) U(x_c, t_c; x_a, t_a), \end{aligned} \quad (1.42)$$

where we have set $x_c \equiv x_L$. This is the **composition law** of the time-evolution operator which, of course, is quite obvious in the operator form (1.17). A special case is the unitarity of the time evolution operator

$$\hat{U}(t', t) \hat{U}^\dagger(t', t) = \hat{U}(t', t) \hat{U}(t, t') = \hat{1}. \quad (1.43)$$

The above example illustrates that path-integral methods can be more complicated and intransparent than operator methods when it comes to proving such properties. However, “*nobody is perfect*”!

Furthermore, one can show that the path-integral representation (1.29) remains valid also for time-dependent potentials $V(x, t)$ if at each time step the corresponding value of the potential is taken (**Problem 3**). This is again a simplification compared to the operator form of quantum mechanics : As is well known, there one has to order the operators chronologically to get a formal solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t'} \hat{U}(t', t) = \hat{H}(t') \hat{U}(t', t) \quad (1.44)$$

for a time-dependent Hamiltonian .

Phase Space Path Integral

We obtain another form of the path integral if the p -integration of the Gaussian integral is not performed:

$$\begin{aligned}
 U(x_b, t_b; x_a, t_a) &= \lim_{N \rightarrow \infty} \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1} \int_{-\infty}^{+\infty} \frac{dp_1}{2\pi\hbar} \frac{dp_2}{2\pi\hbar} \dots \frac{dp_N}{2\pi\hbar} \\
 &\cdot \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{j=1}^N \left[p_j \cdot \frac{x_j - x_{j-1}}{\epsilon} - \frac{p_j^2}{2m} - V(x_{j-1}) \right] \right\} \\
 &\equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \frac{\mathcal{D}'x(t) \mathcal{D}p(t)}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt [p(t) \cdot \dot{x}(t) - H(p(t), x(t))] \right\}.
 \end{aligned}
 \quad (1.45)$$

$$\quad (1.46)$$

Some comments about the “phase space” or Hamiltonian formulation:

1. The argument of the exponential is again the classical action divided by the action quantum, but this time formulated in coordinates and canonical momenta (see. Eq. (1.8)).
2. The “integration measure” $dx_j dp_j / (2\pi\hbar)$ is different from the Lagrangian formulation; for distinction we therefore use the notation $\mathcal{D}'x(t)$. This is descriptive and easily remembered as dividing the phase space into cells of the size $h = 2\pi\hbar$ (as in statistical mechanics).
3. There is an **additional integration** over dp_N and **no** boundary conditions for the momenta.
4. The interpretation is more difficult: Is this a sum over trajectories in phase space? Classically, however, a single **point** in phase space determines the trajectory.

5. While in the Lagrangian formulation the paths are continuous and only the velocities are discontinuous (see Fig. 3), in the phase-space path integral the paths are discontinuous as well. Therefore caution is needed when performing canonical transformations and other manipulations (an instructive example is given in [Schulman](#), p. 306-309).
6. Klauder [6] has shown that by introducing a regularizing factor

$$\lim_{\nu \rightarrow \infty} \int \mathcal{D}x \mathcal{D}p \exp \left\{ \frac{i}{\hbar} S[x, p] \right\} \cdot \exp \left[-\frac{1}{2\nu\hbar} \int_{t_a}^{t_b} dt \left(m^2 \dot{x}^2 + \frac{\dot{p}^2}{m^2} \right) \right] \quad (1.47)$$

the phase space path integral can be defined unambiguously.

An Example: The Free Particle

We now want to calculate explicitly the path integral for the propagator of the free particle using the Hamiltonian formulation. We write the discretized action in Eq. (1.45) as

$$S[x, p] = \sum_{j=1}^{N-1} (p_j - p_{j+1}) \cdot x_j + p_N \cdot x_N - p_1 \cdot x_0 - \epsilon \sum_{j=1}^N \frac{p_j^2}{2m}, \quad (1.48)$$

and first perform the x_j integrations. This gives $(N-1)$ δ -functions which allow to perform the p_j integrations ($j = 1, 2, \dots, N-1$): $p_1 = p_2 = \dots = p_{N-1} = p_N$. There remains

$$U_0(x_b, t_b; x_a, t_a) = \lim_{N \rightarrow \infty} \int_{-\infty}^{+\infty} \frac{dp_N}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left(p_N \cdot (x_b - x_a) - \epsilon N \frac{p_N^2}{2m} \right) \right]. \quad (1.49)$$

Since $\epsilon N = t_b - t_a$, the limit can be performed trivially and we obtain

$$U_0(x_b, t_b; x_a, t_a) = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left(p \cdot (x_b - x_a) - \frac{p^2}{2m} T \right) \right] \quad (1.50)$$

$$= \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left[\frac{im}{2\hbar T} (x_b - x_a)^2 \right] \quad (1.51)$$

where the abbreviation $T = t_b - t_a$ has been used.

Discussion:

1. Comparing Eq. (1.50) with the [spectral representation](#)⁹ of the time-evolution operator

$$U(x_b, t_b; x_a, t_a) = \left\langle x_b \left| \sum_n |\psi_n\rangle \langle \psi_n| e^{-i\hat{H}T/\hbar} \right| x_a \right\rangle = \sum_n \psi_n(x_b) e^{-iE_n T/\hbar} \psi_n^*(x_a) \quad (1.52)$$

⁹Of course, here the spectrum is completely continuous and the summation over discrete states ψ_n has to be replaced by an integral over the continuous parameter p .

allows to read off the normalized eigenfunctions

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ip \cdot x/\hbar} \tag{1.53}$$

and eigenenergies

$$E_p = \frac{p^2}{2m} . \tag{1.54}$$

This is, of course, the expected result.

- 2. For a free particle the classical action is $S_{kl}/\hbar = m(x_b - x_a)^2/(2\hbar T)$ (**Problem 2 a**) which agrees with the phase of Eq. (1.51). We will see that this is no coincidence, but is valid for all actions which are quadratic in coordinates and momenta.

The Ordering Problem

If a classical Hamiltonian is given, in which products of coordinates and momenta occur, the question arises how to quantize such forms:

*“Aucune règle basée sur la correspondance avec la Mécanique Classique ne peut résoudre de telles ambiguïtés, puisque ces dernières proviennent de la **non-commutativité** des opérateurs, elle-même liée au caractère fini et non nul de \hbar ... Dans tout les cas d'intérêt pratique, il faut se conformer aux prescriptions suivantes: ... la fonction de Hamilton étant mise sous ... la forme $\sum_i p_i f_i(q_1...q_n)$... , on y remplace le dernier term de la somme par l'expression **<<symétrisée>>** $\frac{1}{2} \sum_i [\hat{p}_i \hat{f}_i + \hat{f}_i \hat{p}_i]$...*

({Messiah}, p. 59) ¹⁰

How do these ambiguities show up in the path integral? Obviously not in the symbolic notation as used in Eq. (1.30) and (1.46)! Actually, they appear in the innocent-looking problem how the Hamilton function is treated in the discretized form of the path integral, e.g.

- a) outer averaging: $\frac{1}{2} [H(p_j, x_j) + H(p_j, x_{j-1})]$
- b) inner averaging: $H\left(p_j, \frac{x_j + x_{j-1}}{2}\right)$
- c) right hand: $H(p_j, x_j)$
- d) left hand: $H(p_j, x_{j-1})$.

If there are no products of x and p in the Hamiltonian, then - as discussed before - the various procedures give identical results and one can chose the simplest formulation. In the general case one can show that for the treatment of products of the form

$$A := p^m x^n \tag{1.55}$$

in the Hamilton function, there exists the following correspondence between the above path integral prescriptions and the operator ordering:

¹⁰ "No rule based on the correspondence with Classical Mechanics can resolve such ambiguities, since the latter arise from the **non-commutability** of operators, which in turn is tied to the finite and non-zero character of \hbar ... In all cases of practical interest, one must conform to the following prescriptions: ... Having put the Hamiltonian function into the form $\sum_i p_i f_i(q_1...q_n)$ one replaces... (this) term... by the **symmetrized** expression $\frac{1}{2} \sum_i [\hat{p}_i \hat{f}_i + \hat{f}_i \hat{p}_i]$ " {Messiah 1}, p. 70

- a) $\frac{1}{2} [\hat{p}^m \hat{x}^n + \hat{x}^n \hat{p}^m]$
 b) $\frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} \hat{x}^k \hat{p}^m \hat{x}^{n-k}$
 c) $\hat{x}^n \hat{p}^m$
 d) $\hat{p}^m \hat{x}^n$.

Since \hat{x}, \hat{p} are hermitean operators, only the symmetric forms a) and b) also give hermitean operators. Rule b) is called **Weyl's quantization rule** or "**mid-point rule**" and is obtained automatically if Eq. (1.55) is considered as **Wigner transform**

$$A \equiv A_W(x, p) = \int_{-\infty}^{+\infty} dy \left\langle x - \frac{y}{2} \left| \hat{A} \right| x + \frac{y}{2} \right\rangle e^{ip \cdot y / \hbar} \quad (1.56)$$

of the corresponding quantum mechanical operator \hat{A} . The reverse transform is (**Problem 5**)

$$\langle x \left| \hat{A} \right| x' \rangle = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} A_W \left(\frac{x+x'}{2}, p \right) e^{ip \cdot (x-x') / \hbar}. \quad (1.57)$$

If we apply this to each factor in Trotter's product formula, we obtain

$$\begin{aligned} \langle x_{j+1} \left| e^{-i\epsilon \hat{H} / \hbar} \right| x_j \rangle &= \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \underbrace{\left(e^{-i\epsilon \hat{H} / \hbar} \right)_W \left(\frac{x_{j+1} + x_j}{2}, p_j \right)}_{=1 - i\epsilon H_W((x_{j+1} + x_j)/2, p_j) / \hbar + \dots} e^{ip_j \cdot (x_{j+1} - x_j) / \hbar} \\ &\simeq \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \exp \left[-\frac{i\epsilon}{\hbar} H_W \left(\frac{x_{j+1} + x_j}{2}, p_j \right) \right] e^{ip_j \cdot (x_{j+1} - x_j) / \hbar}, \end{aligned} \quad (1.58)$$

which leads to a generalization of Eq. (1.45) for arbitrary Hamilton functions and which contains the mid-point rule.

The ordering prescription becomes important for curvi-linear coordinates or for quantization in curved spaces. A less exotic application is the case of a charged particle in a magnetic field because the minimal substitution for the electromagnetic field leads to the velocity-dependent Lorentz force (**Problem 7**).

Fourier Path Integral

In the following we will determine the propagator for the harmonic oscillator, i.e. for the potential

$$V(x) = \frac{1}{2} m \omega^2 x^2 \quad (1.59)$$

by a method that illustrates how to integrate functionally over paths which are parametrized by **Fourier series** and not by polygon paths. At the same time we want to use the symbolic notation for the path integrals more frequently, but will return to the discretized form when required or in case of doubt. First, in the path integral

$$U(x_b, t_b; x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t) \exp \left[\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left(\frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2 \right) \right] \quad (1.60)$$

we introduce a new integration variable

$$y(t) = x(t) - x_{cl}(t) \quad (1.61)$$

where $x_{\text{cl}}(t)$ is the **classical path**. It fulfills the equation of motion $\ddot{x}_{\text{cl}} + \omega^2 x_{\text{cl}} = 0$ with the boundary conditions $x_{\text{cl}}(t_a) = x_a$ and $x_{\text{cl}}(t_b) = x_b$. The Jacobi determinant of the transformation is 1, since in any x_i -integral only a shift takes place.

Detail 3: Jacobi Determinant and Functional Derivative

If in a n -dimensional integral $I = \int_V dx_1 \dots dx_n f(x_1, \dots, x_n)$ a substitution of variables is performed $x_i = x_i(\xi_1, \dots, \xi_n)$, $i = 1 \dots n$ then

$$I = \int_{V'} d\xi_1 \dots d\xi_n |\mathcal{J}| f(\xi_1, \dots, \xi_n), \quad \mathcal{J} = \det_n \frac{\partial x_i}{\partial \xi_j} \quad (1.62a)$$

where \mathcal{J} denotes **Jacobi determinant** (or Jacobian) and V' is the transformed integration region expressed in the new variables.

The **functional derivative** is the generalization of the partial derivative of a function of several variables to the case of infinitely many variables. It can be defined by

$$\int d\sigma \frac{\delta S[x]}{\delta x(\sigma)} \eta(\sigma) = \lim_{\epsilon \rightarrow 0} \frac{S[x + \epsilon \eta] - S[x]}{\epsilon} \quad (1.62b)$$

where $\eta(\sigma)$ is an arbitrary test function. In the physical literature one can also find the expression

$$\frac{\delta S[x]}{\delta x(\sigma)} := \lim_{\epsilon \rightarrow 0} \frac{S[x + \epsilon \delta(\sigma)] - S[x]}{\epsilon} \quad (1.62c)$$

which resembles the definition of the ordinary derivative of a function. From these definitions it immediately follows that

$$\frac{\delta x(t)}{\delta x(\sigma)} = \delta(t - \sigma) \quad (1.62d)$$

(cf. $\partial x_i / \partial x_j = \delta_{ij}$ in the finite-dimensional case). Keeping this property in mind all usual rules of differentiation like product rule or chain rule are valid (see **Problem 4**).

In the new integration variables the action is

$$\begin{aligned} S[x(t)] = S[x_{\text{cl}}(t) + y(t)] &= S[x_{\text{cl}}(t)] + \int_{-\infty}^{+\infty} d\sigma \frac{\delta S}{\delta x_{\text{cl}}(\sigma)} y(\sigma) \\ &+ \frac{1}{2} \int_{-\infty}^{+\infty} d\sigma \int_{-\infty}^{+\infty} d\sigma' \frac{\delta^2 S}{\delta x_{\text{cl}}(\sigma) \delta x_{\text{cl}}(\sigma')} y(\sigma) y(\sigma'). \end{aligned} \quad (1.63)$$

In our case the (functional) Taylor expansion stops after the second term since the action is quadratic. The first term in Eq. (1.63) is the classical action of the harmonic oscillator, for which one finds

$$S_{\text{cl}}^{\text{h.O.}} = \frac{m}{2} \frac{\omega}{\sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2x_a \cdot x_b \right] \quad (1.64)$$

(**Problem 2 b**). Here again $T = t_b - t_a$ is the time difference. The second term in Eq. (1.63) vanishes since we have expanded around the classical path which is determined by $\delta S_{\text{cl}} = 0$. One easily finds (**Problem 4 b**)

$$\frac{1}{2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\sigma d\sigma' \frac{\delta^2 S}{\delta x_{\text{cl}}(\sigma) \delta x_{\text{cl}}(\sigma')} y(\sigma) y(\sigma') = \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{y}^2(t) - \frac{m}{2} \omega^2 y^2(t) \right]. \quad (1.65)$$

After these steps the calculation of the harmonic oscillator propagator

$$U(x_b, t_b; x_a, t_a) = F(t_b, t_a) e^{iS_{\text{cl}}/\hbar} \quad (1.66)$$

is reduced to the calculation of the simpler path integral

$$F(t_b, t_a) = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp \left[\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left(\frac{m}{2} \dot{y}^2 - \frac{m}{2} \omega^2 y^2 \right) \right]. \quad (1.67)$$

Of course, due to time translation invariance the prefactor can only depend on the difference $T = t_b - t_a$.

Since all paths $y(t)$ start at the point 0 at $t = t_a$ and end at the point 0 at $t = t_b$ they also can be written as a Fourier sine series:

$$y(t) = \sum_{k=1}^{N-1} b_k \sin\left(\frac{k\pi(t-t_a)}{T}\right), \quad (1.68)$$

Detail 4: Mathematical Background

Note that this is **not** the usual (well-known) Fourier series of a function $f(t)$ which reads

$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\left(\frac{2k\pi t}{T}\right) + \sum_{k=1}^{\infty} b_k \sin\left(\frac{2k\pi t}{T}\right) = \sum_{k=-\infty}^{+\infty} c_k \exp\left(\frac{2k\pi i t}{T}\right) \quad (1.69a)$$

and which represents the (periodic) function in the interval $0 < t < T$. Due to this periodicity different function values at the endpoints are not possible. However, since the fluctuations around the classical path vanish at the endpoints and therefore the function $y(t)$ indeed is periodic, one also could use the *ansatz*

$$y(t) = \sum_{k=1}^{\infty} a_k \left[\cos\left(\frac{2k\pi t}{T}\right) - 1 \right] + \sum_{k=1}^{\infty} b_k \sin\left(\frac{2k\pi t}{T}\right). \quad (1.69b)$$

Less known ¹¹ are the Fourier series with double period

$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\left(\frac{k\pi t}{T}\right), \quad (1.69c)$$

which represents a function in the full interval $0 \leq t \leq T$ and

$$f(t) = \sum_{k=1}^{\infty} b_k \sin\left(\frac{k\pi t}{T}\right), \quad (1.69d)$$

which is valid for an arbitrary function in the interval $0 < t < T$, i.e. except the endpoints. Since the fluctuations vanish at the endpoints, the last form is most convenient for our purposes as this behaviour is already built in.

Instead of integrating over the intermediate points y_j , $j = 1 \dots (N-1)$ in the discretized path integral we may integrate over the Fourier coefficients b_k , $k = 1 \dots (N-1)$. Indeed, this is a linear transformation whose Jacobian is constant and independent of ω , m and \hbar . In this calculation, however, we keep the action as **full** time integral and do not use its approximation as Riemann sum as before – the difference is of higher order and disappears in the continuum limit $N \rightarrow \infty, \epsilon \rightarrow 0$. By using the orthogonality relations of the trigonometric functions in the interval $[0, T]$ one finds for the kinetic energy

$$\int_{t_a}^{t_b} dt \frac{m}{2} \dot{y}^2(t) = \frac{m}{4} T \sum_k \left(\frac{k\pi}{T}\right)^2 b_k^2, \quad (1.70)$$

and for the potential energy

$$\int_{t_a}^{t_b} dt \frac{m}{2} \omega^2 y^2(t) = \frac{m}{4} \omega^2 T \sum_k b_k^2. \quad (1.71)$$

Therefore

$$F(T) = \text{const.} \int_{-\infty}^{+\infty} db_1 db_2 \dots db_{N-1} \exp\left\{ \frac{imT}{4\hbar} \sum_{k=1}^{N-1} \left[\left(\frac{k\pi}{T}\right)^2 - \omega^2 \right] b_k^2 \right\}. \quad (1.72)$$

This simply is the $(N-1)$ -fold product of a Gaussian integral so that we obtain

$$F(T) = \text{const}' \cdot \left[\prod_{k=1}^{N-1} \left(1 - \frac{\omega^2 T^2}{k^2 \pi^2} \right) \right]^{-1/2} \xrightarrow{N \rightarrow \infty} \text{const}' \cdot \left(\frac{\omega T}{\sin \omega T} \right)^{1/2}. \quad (1.73)$$

¹¹See, e.g., {Bronstein-Semendjajew}, S. 475

In the last step we have used a product representation of $\sin x/x$ which is due to Euler **{Euler}**. The constant is determined by requiring that for $\omega = 0$ the result (1.51) for the free particle should follow. Therefore we have

$$F^{\text{h.o.}}(T) = \left(\frac{m\omega}{2\pi i \hbar \sin \omega T} \right)^{1/2}. \quad (1.74)$$

However, this only holds for $T < \pi/\omega$: In this case all factors in the product are positive. For $\pi/\omega < T < 2\pi/\omega$, $F(T)$ acquires an additional factor $(-1)^{-1/2} = -i$, as the $k = 1$ term of the produkt has become negative ¹²; for $2\pi/\omega < T < 3\pi/\omega$ a factor $(-i)^2$ etc. In general, Eq. (1.74) is multiplied by the **Maslov correction**

$$e^{-in\frac{\pi}{2}} \quad (1.75)$$

where n counts how many times the trajectory has passed through a **focal point** where the prefactor diverges [7]. At these points the quantum mechanical probability amplitude becomes singular which in real systems is prevented by anharmonic terms, so that the intensity only becomes maximal. The spatial accumulation of such points is called a **caustic**, a phenomenon frequently encountered in optics (e.g. when a water glass is illuminated by sunlight (see [https://en.wikipedia.org/wiki/Caustic_\(optics\)](https://en.wikipedia.org/wiki/Caustic_(optics))). The Maslov correction is a result of the so-called index theorem and we will encounter it again when studying semi-classical approximations.

From the result in Eqs. (1.66, 1.64) and (1.74) we can again extract the energy eigenvalues and eigenfunctions of the (one-dimensional) system: Using

$$\cos \omega T = \frac{1}{2} e^{i\omega T} (1 + e^{-2i\omega T}), \quad i \sin \omega T = \frac{1}{2} e^{i\omega T} (1 - e^{-2i\omega T})$$

one obtains

$$\begin{aligned} U^{\text{h.o.}} &= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-i\omega T/2} (1 - e^{-2i\omega T})^{-1/2} \exp \left\{ -\frac{m\omega}{2\hbar} \left[(x_a^2 + x_b^2) \frac{1 + e^{-2i\omega T}}{1 - e^{-2i\omega T}} - 4x_a \cdot x_b \frac{e^{-i\omega T}}{1 - e^{-2i\omega T}} \right] \right\} \\ &= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-i\omega T/2} \left(1 + \frac{1}{2} e^{-2i\omega T} + \dots \right) \exp \left[-\frac{m\omega}{2\hbar} (x_a^2 + x_b^2) (1 + 2e^{-2i\omega T}) \right] \\ &\quad \cdot \exp \left[\frac{2m\omega}{\hbar} x_a \cdot x_b e^{-i\omega T} (1 + \dots) \right] \end{aligned}$$

and the comparison with the spectral representation (1.52) yields

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp \left(-\frac{m\omega}{2\hbar} x^2 \right), \quad E_0 = \frac{1}{2} \hbar\omega \quad (1.76a)$$

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x \exp \left(-\frac{m\omega}{2\hbar} x^2 \right), \quad E_1 = \frac{3}{2} \hbar\omega. \quad (1.76b)$$

Since we are expanding in powers of $e^{-i\omega T}$ and an additional factor $e^{-i\omega T/2}$ is always coming from the prefactor, it is obvious that the general rule for the energies is

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega, \quad n = 0, 1, \dots \quad (1.77)$$

Note that **zero-point energy** $\frac{1}{2} \hbar\omega$ arises from the prefactor, i.e. from the quadratic fluctuations around the classical path.

¹²Another possibility to prove that is by using the composition law of the time-evolution operator, see **Problem 9**.

Detail 5: All Eigenfunctions

The general form of the eigenfunctions can be derived from Mehler's formula (**Bateman Proj. 2**, ch. 10.13, eq. (22)) for the Hermite polynomials

$$\sum_{n=0}^{\infty} \frac{(z/2)^n}{n!} H_n(\xi) H_n(\eta) = (1 - z^2)^{-1/2} \exp \left[\frac{2\xi\eta z - (\xi^2 + \eta^2)z^2}{1 - z^2} \right] \quad (1.78a)$$

If one sets $\xi = x_a/b$, $\eta = x_b/b$, ($b = \hbar/(m\omega)$ is the oscillator length), $z = \exp(-i\omega T)$ and multiplies both sides of Mehler's formula by $\exp[-(\xi^2 + \eta^2)/2]$ then one finds by comparing with the spectral representation (1.52)

$$\psi_n(x) = \left(\sqrt{\pi b} 2^n n! \right)^{-1/2} H_n \left(\frac{x}{b} \right) \exp \left(-\frac{x^2}{2b^2} \right), \quad (1.78b)$$

which is in agreement with **Messiah 1**, eq. (B.70).

1.3 Quadratic Lagrangians

We now consider the general¹³ quadratic Lagrangian

$$L = \frac{1}{2} m \dot{x}^2 + b(t) x \cdot \dot{x} - \frac{1}{2} c(t) x^2 + d(t) \dot{x} - e(t) x. \quad (1.79)$$

Without restriction of generality one may omit the terms with the coefficient functions $b(t)$ and $d(t)$ since they may be added to the terms $c(t)$ and $e(t)$, respectively, after an integration by parts in the action. Thus we only need to consider

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} c(t) x^2 - e(t) x. \quad (1.80)$$

Special cases are the free particle ($c = e = 0$), the harmonic oscillator ($e = 0$, $c = m\omega^2$) or the forced harmonic oscillator ($c = m\omega^2$, $e \neq 0$). As in the treatment of the harmonic oscillator in the last chapter we introduce the deviation from the classical path

$$y(t) = x(t) - x_{\text{cl}}(t) \quad (1.81)$$

as integration variable. $x_{\text{cl}}(t)$ is solution of the classical equation of motion

$$m\ddot{x}_{\text{cl}} + c(t)x_{\text{cl}} + e(t) = 0 \quad (1.82)$$

with boundary conditions

$$x_{\text{cl}}(t_a) = x_a \quad x_{\text{cl}}(t_b) = x_b. \quad (1.83)$$

Functional expansion of the action $S[x(t)] = S[x_{\text{cl}}(t) + y(t)]$ gives again

$$U(x_b, t_b; x_a, t_a) = e^{iS_{\text{cl}}/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{y}^2 - \frac{1}{2} c(t) y^2 \right] \right\} = e^{iS_{\text{cl}}/\hbar} F(t_b, t_a). \quad (1.84)$$

The prefactor explicitly reads

$$F(t_b, t_a) = \lim_{N \rightarrow \infty} \mathcal{N}_\epsilon^{N+1} \int dy_1 dy_2 \dots dy_N \exp \left\{ \frac{i}{\hbar} \sum_{j=1}^{N+1} \left[\frac{m}{2\epsilon} (y_j - y_{j-1})^2 - \frac{1}{2} \epsilon c_j y_j^2 \right] \right\}, \quad (1.85)$$

where (to simplify the notation) we have replaced N by $N + 1$ in the discretized path integral. In addition,

$$\mathcal{N}_\epsilon = \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{1/2} \quad (1.86)$$

¹³Except for requiring a constant mass. General time-dependent quadratic Hamiltonian system are treated, for example, in [8].

is the normalization factor of the Lagrange path integral and $c_j = c(t_j) = c(t_a + j\epsilon)$. Eq. (1.85) is again a Gaussian integral of the type

$$F(t_b, t_a) = \lim_{N \rightarrow \infty} \mathcal{N}_\epsilon^{N+1} \int dy_1 dy_2 \dots dy_N e^{i\mathbf{y}^t \mathbb{B}_N \mathbf{y}}, \quad (1.87)$$

where \mathbf{y}^t denotes the row vector $(y_1 \dots y_N)$, \mathbf{y} the corresponding column vector and

$$\mathbb{B}_N = \frac{m}{2\epsilon\hbar} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix} - \frac{\epsilon}{2\hbar} \begin{pmatrix} c_1 & 0 & 0 & \dots & 0 \\ 0 & c_2 & 0 & \dots & 0 \\ 0 & 0 & c_3 & \dots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \dots & c_N \end{pmatrix}. \quad (1.88)$$

In contrast to previous applications this integral does not factorize into individual integrals of the type of Eq. (0.1). This only happens if we have diagonalized the real, symmetric matrix \mathbb{B}_N by an orthogonal transformation. The product of eigenvalues in the denominator of the square-root expression of Eq. (0.1) then yields the determinant of the matrix.

In general, the **Gaussian integral for a real, symmetric matrix** \mathbb{A} therefore is

$$G_N(\mathbb{A}) := \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_N e^{-\mathbf{x}^t \mathbb{A} \mathbf{x}} = \frac{\pi^{N/2}}{\sqrt{\det \mathbb{A}}}. \quad (1.89)$$

In addition, the matrix A has to be **positive definite**¹⁴ in order that the integral converges. In the present Fresnel-like case where $\mathbb{A} = 0^+ I - i\mathbb{B}_N$ the sign of the eigenvalues of \mathbb{B}_N is again irrelevant. The prefactor then is

$$F(t_b, t_a) = \lim_{N \rightarrow \infty} \frac{\pi^{N/2} \mathcal{N}_\epsilon^{N+1}}{\sqrt{\det(-i\mathbb{B}_N)}} = \sqrt{\frac{m}{2\pi i \hbar} \frac{1}{f(t_b, t_a)}} \quad (1.90)$$

with

$$f(t_b, t_a) = \lim_{N \rightarrow \infty} \epsilon \left(\frac{2\hbar\epsilon}{m} \right)^N \det \mathbb{B}_N. \quad (1.91)$$

There remains the problem to evaluate the determinant of the matrix \mathbb{B}_N and to perform the limit $N \rightarrow \infty, \epsilon \rightarrow 0$. **Gel'fand and Yaglom** [9] have shown that this is possible by solving a differential equation: We have to calculate the determinant

$$p_N = \left(\frac{2\hbar\epsilon}{m} \right)^N \det \mathbb{B}_N = \det \left\{ \begin{pmatrix} 2 & -1 & \dots & 0 & 0 \\ -1 & 2 & \dots & 0 & 0 \\ 0 & -1 & \dots & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & \dots & -1 & 2 \end{pmatrix} - \frac{\epsilon^2}{m} \begin{pmatrix} c_1 & 0 & 0 & \dots & 0 \\ 0 & c_2 & 0 & \dots & 0 \\ 0 & 0 & c_3 & \dots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \dots & c_N \end{pmatrix} \right\} \quad (1.92)$$

This is done by expanding p_{j+1} with respect to the $(j+1)^{\text{th}}$ column. The remaining determinant is then expanded with respect to j^{th} row. In this way one obtains the recursion relation

$$p_{j+1} = \left(2 - \frac{\epsilon^2}{m} c_{j+1} \right) p_j - p_{j-1}, \quad j = 2, 3 \dots N-1, \quad (1.93)$$

¹⁴i.e., all eigenvalues are > 0 . More about positive definite matrices, see, e.g., **{Horn-Johnson}**, ch. 7.

which is also valid for $j = 1$ if the convention $p_0 = 1$ is adopted. If we write Eq. (1.93) as

$$\frac{p_{j+1} - 2p_j + p_{j-1}}{\epsilon^2} = -\frac{c_{j+1}}{m} p_j, \quad (1.94)$$

then we see that in the limit $\epsilon \rightarrow 0$ the desired function $\epsilon p_j \rightarrow f(t, t_a)$ is given by the solution of the differential equation

$$\boxed{\frac{\partial^2 f_{\text{GY}}(t, t_a)}{\partial t^2} = -\frac{c(t)}{m} f_{\text{GY}}(t, t_a)}. \quad (1.95)$$

The initial conditions are

$$\begin{aligned} f_{\text{GY}}(t_a, t_a) &= \epsilon p_0 = \epsilon \rightarrow 0 \\ \left. \frac{\partial f_{\text{GY}}(t, t_a)}{\partial t} \right|_{t=t_a} &= \epsilon \frac{p_1 - p_0}{\epsilon} = 2 - \frac{\epsilon^2}{m} c_1 - 1 \rightarrow 1. \end{aligned} \quad (1.96)$$

Examples :

1. As a test we consider the harmonic oscillator, i.e. $c = m\omega^2$. Gel'fand-Yaglom's differential equation (1.95) then simply is a free wave equation with the general solution $f_{\text{GY}}(t, t_a) = C \sin(\omega(t - t_a) + \gamma)$. The initial conditions (1.96) give $\gamma = 0$, $\omega C = 1$ for the integration constants. Using that we indeed obtain the correct result

$$f_{\text{GY}}^{h.o.}(t_b, t_a) = \frac{1}{\omega} \sin(\omega T). \quad (1.97)$$

2. The forced harmonic oscillator ($c = m\omega^2$, $e(t)$ arbitrary) may be treated in the same way. Its classical action is (**Problem 4 c**)

$$\boxed{S_{\text{cl}} = \frac{m\omega}{2 \sin \omega T} \left\{ (x_b^2 + x_a^2) \cos \omega T - 2x_a \cdot x_b - \frac{2x_b}{m\omega} \int_{t_a}^{t_b} dt e(t) \sin \omega(t - t_a) \right.} \\ \left. - \frac{2x_a}{m\omega} \int_{t_a}^{t_b} dt e(t) \sin \omega(t_b - t) - \frac{2}{m^2 \omega^2} \int_{t_a}^{t_b} dt \int_{t_a}^t dt' e(t) e(t') \sin \omega(t_b - t) \sin \omega(t' - t_a) \right\}. \quad (1.98)$$

The function $f_{\text{GY}}(t_b, t_a)$ and thus the prefactor remain the same as for the free harmonic oscillator since $e(t)$ does not appear in the Gel'fand-Yaglom equation. In this way the problem has been solved completely by "quadrature", i.e. by evaluating ordinary integrals!

A further simplification results from the fact that there is no need to solve the Gel'fand-Yaglom equation if one already knows the classical action. That is because one can show (**Problem 8**) that

$$\frac{1}{f_{\text{GY}}(t_b, t_a)} = -\frac{1}{m} \frac{\partial^2 S_{\text{cl}}}{\partial x_a \partial x_b} \quad (1.99)$$

holds – meaning that the time-evolution operator for a quadratic Lagrangian is completely determined by the classical action! If the classical trajectory goes through a **focal point** in which $f_{\text{GY}}(t_b, t_a)$ vanishes an additional phase is generated – as for the simple harmonic oscillator. Therefore we have the result

$$U(x_b, t_b; x_a, t_a) = \sqrt{\frac{1}{2\pi i \hbar} \left| \frac{\partial^2 S_{\text{cl}}}{\partial x_a \partial x_b} \right|} \exp \left\{ i \left[S_{\text{cl}}(x_b, x_a) / \hbar - n \frac{\pi}{2} \right] \right\}, \quad (1.100)$$

where n is the number of focal points (including their multiplicity).

It is instructive to evaluate the prefactor in the symbolic notation for the path integral:

$$F(t_b, t_a) = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y \exp \left[\frac{i}{2\hbar} \int dt dt' y(t) \frac{\delta^2 S}{\delta x(t) \delta x(t')} \Big|_{\text{cl}} y(t') \right] = \frac{\text{const}}{\sqrt{\text{Det } \delta^2 S_{\text{cl}}}}. \quad (1.101)$$

Here $\text{Det } \delta^2 S$ is the **functional determinant** of the operator

$$\delta^2 S_{\text{cl}} \equiv \frac{\delta^2 S}{\delta x(t) \delta x(t')} \Big|_{\text{cl}} = \left[-\frac{m}{2} \frac{\partial^2}{\partial t^2} - \frac{1}{2} c(t) \right] \delta(t - t'), \quad (1.102)$$

i.e. the product of its eigenvalues. Therefore n can be understood as **number of negative eigenvalues** of the operator $\delta^2 S_{\text{cl}}$ (Morse's index theorem).

Detail 6: Evaluation of Functional Determinants

One has to calculate the eigenvalues of $\delta^2 S_{\text{cl}}$ in the space of functions which fulfill the boundary conditions for the path integral, i.e. in the present case functions which vanish at t_a as well as at t_b . As an example we take the simple case $c(t) = m\omega^2$ for which the eigenvalue equation reads

$$-\frac{m}{2} \ddot{f}(t) - \frac{m}{2} \omega^2 f(t) = \lambda f(t) \quad (1.103a)$$

The eigenfunction, which vanishes at t_a , obviously is

$$f(t) = C \cdot \sin \left[\left(2\frac{\lambda}{m} + \omega^2 \right)^{1/2} (t - t_a) \right]. \quad (1.103b)$$

The boundary condition at $t = t_b$ gives as eigenvalues

$$\begin{aligned} \left(2\frac{\lambda}{m} + \omega^2 \right)^{1/2} T &= k\pi, \quad k = 1, 2, \dots \\ \Rightarrow \lambda_k(\omega) &= \frac{m}{2} \frac{k^2 \pi^2}{T^2} \left[1 - \left(\frac{\omega T}{k\pi} \right)^2 \right] = \lambda_k(\omega = 0) \cdot \left[1 - \left(\frac{\omega T}{k\pi} \right)^2 \right], \end{aligned} \quad (1.103c)$$

which immediately leads to the product representation (1.73) for the prefactor of the harmonic oscillator. In the general case this infinite product of eigenvalues has to be calculated without Euler's help ... While this method to evaluate functional determinants is quite general, it obviously is much more difficult than the Gel'fand-Yaglom method which, however, is only applicable for one-dimensional systems. To calculate functional determinants for radial operators see [10].

It is easy to generalize Eq. (1.100) to any space dimension d : For each dimension the quadratic fluctuations give a prefactor in the form of a root expression and the second derivative of the classical action w.r.t. the endpoints is replaced by the **van-Vleck-Pauli-Morette determinant**

$$\frac{\partial^2 S_{\text{cl}}}{\partial x_a \partial x_b} \longrightarrow \det \frac{\partial^2 S_{\text{cl}}}{\partial \mathbf{x}_a \partial \mathbf{x}_b} \quad (1.104)$$

Note that this is an ordinary $d \times d$ -determinant and not a functional determinant (which we write as Det). Therefore the result is

$$U(x_b, t_b; x_a, t_a) = \left(\frac{1}{2\pi i \hbar} \right)^{d/2} \sqrt{\left| \det \frac{\partial^2 S_{\text{cl}}}{\partial \mathbf{x}_a \partial \mathbf{x}_b} \right|} \exp \left\{ i \left[S_{\text{cl}}(\mathbf{x}_b, \mathbf{x}_a) / \hbar - n d \frac{\pi}{2} \right] \right\}. \quad (1.105)$$

1.4 Perturbation Theory

We now consider the (for simplicity again: one-dimensional) motion of a particle in a general potential $V(x)$, i.e. Lagrange functions of the form

$$L = \frac{m}{2}\dot{x}^2 - V(x). \quad (1.106)$$

In general the path integral cannot be evaluated anymore¹⁵. A widely used method for weak interactions (potentials) is perturbation theory, which we may obtain from the phase space formula (1.46) by expansion in powers of the potential:

$$\begin{aligned} U(x', t'; x, t) &= \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \int_t^{t'} d\sigma \left(p\dot{x} - \frac{p^2}{2m} \right) \right] \sum_{j=0}^{\infty} \left(-\frac{i}{\hbar} \right)^j \frac{1}{j!} \left(\int_t^{t'} d\tau V(x(\tau)) \right)^j \\ &=: \sum_{j=0}^{\infty} \left(-\frac{i}{\hbar} \right)^j U_j(x', t'; x, t). \end{aligned} \quad (1.107)$$

The first term is the free propagator which we already have determined in Eq. (1.51):

$$U_0(x', t'; x, t) = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[p(x' - x) - \frac{p^2}{2m}(t' - t) \right] \right\}. \quad (1.108)$$

Let us now consider the next term of the perturbation expansion

$$U_1(x', t'; x, t) = \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \int_t^{t'} d\sigma \left(p\dot{x} - \frac{p^2}{2m} \right) \right] \int_t^{t'} d\tau V(x(\tau)). \quad (1.109)$$

In the discretized form the last factor is

$$\int_t^{t'} d\tau V(x(\tau)) = \epsilon \sum_{j=1}^N V(x_j), \quad \text{with } \epsilon = \frac{t' - t}{N} \quad (1.110)$$

and thus

$$U_1(x', t'; x, t) = \lim_{N \rightarrow \infty} \epsilon \sum_{j=1}^N \prod_{k=1}^{N-1} \left(\int_{-\infty}^{+\infty} \frac{dx_k dp_k}{2\pi\hbar} \right) \int_{-\infty}^{+\infty} \frac{dp_N}{2\pi\hbar} V(x_j) \exp \left\{ \frac{i}{\hbar} \sum_{l=1}^N \left[p_l(x_l - x_{l-1}) - \epsilon \frac{p_l^2}{2m} \right] \right\}. \quad (1.111)$$

Similarly as in the evaluation of the free propagator we write the exponent as

$$\frac{i}{\hbar} \left[\sum_{l=1}^{N-1} (p_l - p_{l+1}) x_l + p_N x' - p_1 x - \epsilon \sum_{l=1}^N \frac{p_l^2}{2m} \right] \quad (1.112)$$

and perform all x_k -integrations (except x_j). This gives $(N-2)$ momentum δ -functions

$$\begin{aligned} U_1(x', t'; x, t) &= \lim_{N \rightarrow \infty} \epsilon \sum_{j=1}^N \int_{-\infty}^{+\infty} dx_j V(x_j) \prod_{k=1}^N \left(\int_{-\infty}^{+\infty} \frac{dp_k}{2\pi\hbar} \right) (2\pi\hbar)^{N-2} \\ &\quad \cdot \delta(p_1 - p_2) \delta(p_2 - p_3) \dots \delta(p_{j-1} - p_j) \delta(p_{j+1} - p_{j+2}) \dots \delta(p_{N-1} - p_N) \\ &\quad \cdot \exp \left\{ \frac{i}{\hbar} [(p_j - p_{j+1})x_j + p_N x' - p_1 x] - \epsilon \sum_{l=1}^N \frac{p_l^2}{2m} \right\}. \end{aligned} \quad (1.113)$$

¹⁵For some cases, such as the Coulomb potential, special methods have been found to obtain the (already known) solutions from the path integral formalism, see, e.g. [11]. However, these methods do not help in the general case.

These enforce $p_1 = p_2 = \dots p_{j-1} = p_j$ and $p_{j+1} = p_{j+2} = \dots p_{N-1} = p_N$, so that we obtain

$$U_1(x', t'; x, t) = \lim_{N \rightarrow \infty} \epsilon \sum_{j=1}^N \int_{-\infty}^{+\infty} dx_j V(x_j) \int_{-\infty}^{+\infty} \frac{dp_j dp_N}{(2\pi\hbar)^2} \exp \left\{ \frac{i}{\hbar} [(p_j - p_N)x_j + p_N x' - p_j x] \right\} \cdot \exp \left[-\frac{i}{\hbar} \epsilon \left(\frac{p_j^2}{2m} j + \frac{p_N^2}{2m} (N - j) \right) \right]. \quad (1.114)$$

If we now write $\xi = x_j$, $p = p_j$ and $p' = p_N$, the result is

$$U_1(x', t'; x, t) = \lim_{N \rightarrow \infty} \epsilon \sum_{j=1}^N \int_{-\infty}^{+\infty} d\xi V(\xi) \underbrace{\int_{-\infty}^{+\infty} \frac{dp'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[(x' - \xi)p' - \frac{p'^2}{2m} \epsilon(N - j) \right] \right\}}_{=U_0(x', t'; \xi, t + j\epsilon)} \cdot \underbrace{\int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[(\xi - x)p - \frac{p^2}{2m} j\epsilon \right] \right\}}_{=U_0(\xi, t + j\epsilon; x, t)}. \quad (1.115)$$

It is now possible to perform the limit which gives a Riemannian integral over the intermediate time τ , ($\tau_j = t + j\epsilon$)

$$U_1(x', t'; x, t) = \int_t^{t'} d\tau \int_{-\infty}^{+\infty} d\xi U_0(x', t'; \xi, \tau) V(\xi) U_0(\xi, \tau; x, t). \quad (1.116)$$

Read from right to left this contribution to the perturbative expansion can be depicted as a **Feynman diagram** as shown in Fig. 4a .

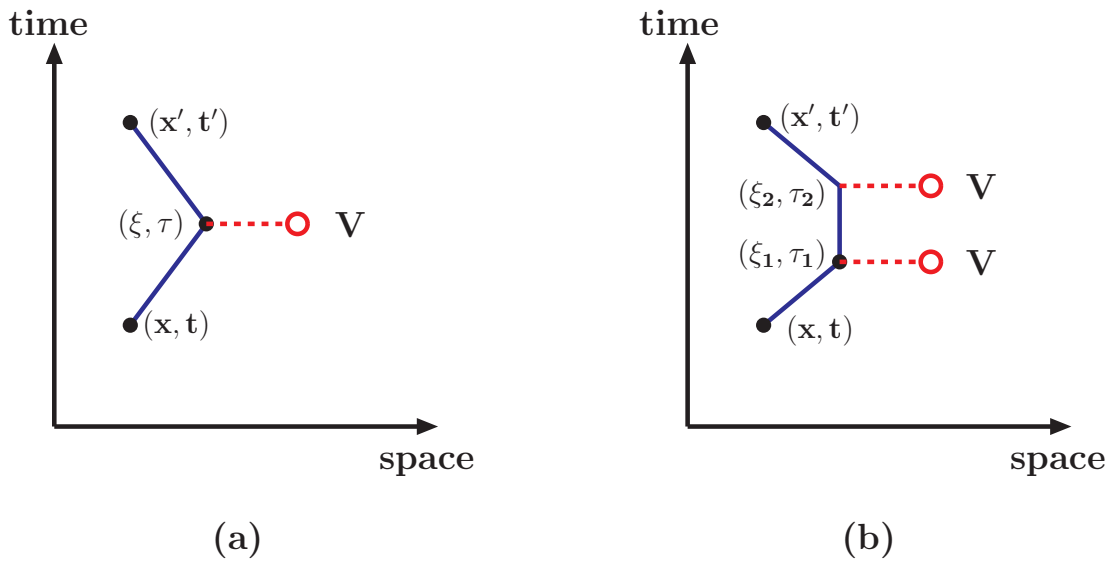


Fig. 4 : (a) Feynman diagram in 1st order perturbation theory for the time-evolution operator in Eq. (1.116). The solid blue lines represent the free propagator between two space-time points, the dashed red line the interaction of the potential V . Intermediate points are to be integrated over. (b) Feynman diagram for the 2nd order, see Eq. (1.120).

Similarly one proceeds in higher orders

$$U_j(x', t'; x, t) = \frac{1}{j!} \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \int_t^{t'} d\sigma \left(p\dot{x} - \frac{p^2}{2m} \right) \right] \left(\int_t^{t'} d\tau V(x(\tau)) \right)^j . \quad (1.117)$$

By induction one can prove that

$$\left(\int_t^{t'} d\tau V(x(\tau)) \right)^j = j! \int_t^{t'} d\tau_1 \int_t^{\tau_1} d\tau_2 \dots \int_t^{\tau_{j-1}} d\tau_j V(x(\tau_1)) V(x(\tau_2)) \dots V(x(\tau_j)) \quad (1.118)$$

which – with a similar calculation – leads to

$$U_j(x', t'; x, t) = \int_t^{t'} d\tau \int_{-\infty}^{+\infty} d\xi U_0(x', t'; \xi, \tau) V(\xi) U_{j-1}(\xi, \tau; x, t) , \quad j = 1, 2, \dots \quad (1.119)$$

The graphical representation for $j = 2$

$$\begin{aligned} U_2(x', t'; x, t) &= \int_t^{t'} d\tau_2 \int_{-\infty}^{+\infty} d\xi_2 U_0(x', t'; \xi_2, \tau_2) V(\xi_2) \\ &\quad \cdot \int_t^{\tau_2} d\tau_1 \int_{-\infty}^{+\infty} d\xi_1 U_0(\xi_2, \tau_2; \xi_1, \tau_1) V(\xi_1) U_0(\xi_1, \tau_1; x, t) \end{aligned} \quad (1.120)$$

is shown in Fig. 4b . Insertion of the recursion relation (1.119) into Eq. (1.107) gives an integral equation for the time-evolution operator

$$U(x', t'; x, t) = U_0(x', t'; x, t) - \frac{i}{\hbar} \int_t^{t'} d\tau \int_{-\infty}^{+\infty} d\xi U_0(x', t'; \xi, \tau) V(\xi) U(\xi, \tau; x, t) . \quad (1.121)$$

This is the usual equation for the time-evolution operator in the **interaction picture** as one can see if one writes Eq. (1.121) in operator form

$$\hat{U}(t', t) = \hat{U}_0(t', t) - \frac{i}{\hbar} \int_t^{t'} d\tau \hat{U}_0(t', \tau) \hat{V} \hat{U}(\tau, t) . \quad (1.122)$$

Defining

$$\hat{U}(t', t) =: \hat{U}_0(t', t) \hat{U}_I(t', t) , \quad (1.123)$$

one obtains

$$\hat{U}_0(t', t) \hat{U}_I(t', t) = \hat{U}_0(t', t) - \frac{i}{\hbar} \int_t^{t'} d\tau \underbrace{\hat{U}_0(t', \tau)}_{=\hat{U}_0(t', t)\hat{U}_0(t, \tau)=\hat{U}_0(t', t)\hat{U}_0^\dagger(\tau, t)} \hat{V} \hat{U}(\tau, t) . \quad (1.124)$$

Here the composition law for the free propagator \hat{U}_0 has been used. Multiplying from the left with $\hat{U}_0^{-1}(t', t)$ one obtains

$$\hat{U}_I(t', t) = 1 - \frac{i}{\hbar} \int_t^{t'} d\tau \underbrace{\hat{U}_0^\dagger(\tau, t) \hat{V} \hat{U}_0(\tau, t)}_{=: \hat{V}_I(t', t)} \hat{U}_I(\tau, t) , \quad (1.125)$$

which is identical with the equation of motion for the time-evolution operators in the interaction picture ¹⁶.

From the derivation of Eq. (1.121) it is clear that this equation is also valid for time-dependent potentials. However, if the potential is **time-independent** then the integral term on the right side of Eq. (1.122) is a

¹⁶See, e.g., {Messiah 2}, p. 723 .

convolution integral, since the evolution operators then only depend on the time difference. According to well-known theorems for the Fourier transformation we then immediately obtain for the time-independent Green function

$$\hat{G}(E) = \int_{-\infty}^{+\infty} dt \hat{G}(t) e^{iEt/\hbar}, \quad \text{with} \quad \hat{G}(t) := -\frac{i}{\hbar} \Theta(t) \hat{U}(t, 0) \quad (1.126)$$

the **Lippmann-Schwinger equation**

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E) \hat{V} \hat{G}(E), \quad (1.127)$$

which simply is the operator identity

$$\frac{1}{E - \hat{H} + i0^+} = \frac{1}{E - \hat{H}_0 + i0^+} + \frac{1}{E - \hat{H}_0 + i0^+} \hat{V} \frac{1}{E - \hat{H} + i0^+}. \quad (1.128)$$

The prescription that the singularity in these operators has to be regularized by adding $+i \times$ an infinitesimal positive quantity in the denominator follows from the definition (1.126) in which the energy E must have a small, positive imaginary part in order that the time integral converges¹⁷.

Finally it should be mentioned that, of course, one can derive other perturbative expansions; e.g. one may write $V = V_0 + (V - V_0)$ to obtain

$$U(x', t'; x, t) = \sum_{j=0}^{\infty} \frac{1}{j!} \left(-\frac{i}{\hbar}\right)^j \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \left\{ \int_t^{t'} d\tau [V(x(\tau)) - V_0(x(\tau))] \right\}^j \cdot \exp \left\{ \frac{i}{\hbar} \int_t^{t'} d\sigma \left[p(\sigma) \dot{x}(\sigma) - \frac{p^2(\sigma)}{2m} - V_0(x(\sigma)) \right] \right\}. \quad (1.129)$$

This only makes sense if the time-evolution operator for the potential V_0 can be evaluated.

1.5 Semi-classical Expansions

It is possible to evaluate the path integral for a particle in an arbitrary potential in an approximate way for those situations where the classical description gives the main contribution. Path integrals are the natural starting point for such semi-classical approximations because the notion of a trajectory and the classical limit are "built in".

The obvious method is to take into account only the **quadratic fluctuations** around the classical path. This corresponds to the generalization of the well-known **saddle point approximation** or **stationary phase method** from ordinary integrals to functional integrals.

Detail 7: Asymptotic Expansion of Integrals

A (real) integral of the form

$$I = \int_a^b dt \exp[-f(t)/\epsilon] \quad (1.130a)$$

can be evaluated in the limit $\epsilon \rightarrow 0$ by **Laplace's method**: Find the **minimum** of the function $f(t)$ at the point $t_0 \in [a, b]$ and expand the function in a Taylor series around this minimum up to 2nd order. This gives

$$I \simeq \exp[-f(t_0)/\epsilon] \int_a^b dt \exp \left[-\frac{1}{2\epsilon} f''(t_0) (t - t_0)^2 \right]. \quad (1.130b)$$

¹⁷Obviously only propagation with increasing time ($t \geq 0$) is possible, i.e. we deal here with the **advanced** Green function which frequently is denoted by $\hat{G}^{(+)}(E)$.

Since $f''(t_0) > 0$ we can substitute $s = \sqrt{f''(t_0)/(2\epsilon)}(t - t_0)$ as new integration variable. For $\epsilon \rightarrow 0$ the limits of the s -Integrals become $-\infty, +\infty$, if t_0 is between a, b and $-\infty, 0$, or $0, +\infty$ if t_0 happens to coincide with one of the integration limits. After performing the s -integration we therefore have

$$I \simeq \exp[-f(t_0)/\epsilon] \sqrt{\frac{2\pi\epsilon}{f''(t_0)}} \cdot A, \quad (1.130c)$$

in which the factor A takes the value $A = 1$ if the minimum is within the integration interval and $A = 1/2$ if the minimum occurs at the boundary. If one writes in Eq. (1.130c) $\epsilon^{1/2} = \exp(\frac{1}{2} \ln \epsilon)$ then one sees that the quadratic expansion around the minimum is subdominant compared to the leading term $(-f(t_0)/\epsilon)$: $\ln \epsilon$ diverges weaker than $1/\epsilon$. Eq. (1.130c) can be seen as the beginning of a systematic (asymptotic) expansion of the integral I which can be obtained by higher terms in the Taylor expansion of $f(t)$ around the minimum. The standard example for such an expansion is Euler's integral representation of the Gamma function

$$\Gamma(x+1) = \int_0^\infty dt t^x e^{-t} \quad (1.130d)$$

in which $f(t) = t - x \ln t$. The minimum of this function occurs at $t_0 = x$ and we have $f''(t_0) = 1/x$ so that Stirling's formula is obtained for large positive x :

$$x! \equiv \Gamma(x+1) \xrightarrow{x \rightarrow \infty} \sqrt{2\pi} x^{x+1/2} e^{-x}. \quad (1.130e)$$

A generalization of this method to (complex) integrals of the form

$$I = \int_C dz g(z) \exp[f(z)/\epsilon], \quad (1.130f)$$

has been developed by P. Debye. Here $f(z), g(z)$ are analytic functions in a region of the complex plane which contains the path of integration C . The crucial idea is to deform C in such a way that on a part C_0 of C the following conditions are fulfilled: (1) Along C_0 $\text{Im} f(z)$ is constant, (2) C_0 goes through a saddle point z_0 where $df(z)/dz = 0$, and (3) at $z = z_0$ $\text{Re} f(z)$ goes through a relative maximum, that is C_0 is the path of **steepest descent**. If one writes $f(z) = f(z_0) - \tau^2$, expands the product $g(z(\tau)) dz(\tau)/d\tau = \sum_m c_m \tau^m$ in a power series and integrates term by term then one can derive the asymptotic expansion¹⁸

$$I \simeq \exp[f(z_0)/\epsilon] \sqrt{\epsilon} \sum_{m=0}^{\infty} c_m \Gamma(m+1/2) \epsilon^m. \quad (1.130g)$$

From the Taylor expansion of $f(z), g(z)$ around $z = z_0$ it is easy to find the lowest coefficient as

$$c_0 = \frac{g(z_0)}{\sqrt{-f''(z_0)/2}}. \quad (1.130h)$$

The classical path obeys the equation of motion

$$m\ddot{x}_{\text{cl}}(t) + V'(x_{\text{cl}}(t)) = 0, \quad x_{\text{cl}}(t_a) = x_a, \quad x_{\text{cl}}(t_b) = x_b. \quad (1.131)$$

With $y(t) = x(t) - x_{\text{cl}}(t)$ we obtain

$$\begin{aligned} U(x_b, t_b; x_a, t_a) &= e^{iS_{\text{cl}}/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp \left\{ \frac{i}{\hbar} (S[x_{\text{cl}} + y] - S[x_{\text{cl}}]) \right\} \\ &\simeq e^{iS_{\text{cl}}/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp \left\{ \frac{i}{2\hbar} \int d\sigma d\sigma' \frac{\delta^2 S}{\delta x_{\text{cl}}(\sigma) \delta x_{\text{cl}}(\sigma')} y(\sigma) y(\sigma') \right\}, \end{aligned} \quad (1.132)$$

if we stop the functional Taylor expansion after the quadratic term. A simple calculation (**problem 4 b**) gives

$$\frac{1}{2} \int d\sigma d\sigma' \frac{\delta^2 S}{\delta x_{\text{cl}}(\sigma) \delta x_{\text{cl}}(\sigma')} y(\sigma) y(\sigma') = \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{y}^2(t) - \frac{1}{2} V''(x_{\text{cl}}(t)) y^2(t) \right], \quad (1.133)$$

i.e. the action of a harmonic oscillator with a time-dependent oscillator constant

$$\omega^2(t) = \frac{1}{m} V''(x_{\text{cl}}(t)). \quad (1.134)$$

Employing the results from the previous chapter we immediately can write down the result

$$U(x_b, t_b; x_a, t_a) = \sqrt{\frac{m}{2\pi i \hbar} \left| f(t_b, t_a) \right|^{-1}} \exp \left\{ i \left[S_{\text{cl}}(x_b, t_b; x_a, t_a)/\hbar - n \frac{\pi}{2} \right] \right\}, \quad (1.135)$$

¹⁸An excellent and particularly clear account can be found in **{Dennery-Krzywicki}**, ch. I.31.

in which $f(t_b, t_a)$ fulfills the Gel'fand-Yaglom equation ¹⁹

$$m \frac{\partial^2 f(t, t_a)}{\partial t^2} + V''(x_{cl}(t)) f(t, t_a) = 0, \quad \text{with } f(t_a, t_a) = 0, \quad \left. \frac{\partial f(t, t_a)}{\partial t} \right|_{t=t_a} = 1 \quad (1.136)$$

Of course, it is also possible to express the prefactor of the propagator by the second derivative of the classical action with respect to the boundary points, i.e. by the van-Vleck determinant (see Eq. (1.99)).

If there are several stationary points in the functional integral (sufficiently far apart) their contributions must be summed up:

$$U(x_b, t_b; x_a, t_a) \simeq \sum_k \left(\frac{1}{2\pi i \hbar} \left| \frac{\partial^2 S_k}{\partial x_a \partial x_b} \right| \right)^{1/2} \exp \left\{ i \left[S_k / \hbar - n_k \frac{\pi}{2} \right] \right\}. \quad (1.137)$$

We now want to determine the energy eigenvalues of possible bound states of the system using the semi-classical result (1.137). In principle, this would be possible again by comparing the semi-classical result with the spectral representation of the time-evolution operator. However, it is generally not possible to solve the classical equation of motion (1.131) in closed form and thereby to determine the classical action. Instead, we look at the time-independent Green function

$$G(x_b, x_a; E) = \int_0^\infty d(t_b - t_a) \left(-\frac{i}{\hbar} \right) U(x_b t_b; x_a t_a) e^{iE(t_b - t_a)/\hbar} = \sum_n \frac{\psi_n(x_b) \psi_n^*(x_a)}{E - E_n + i0^+}, \quad (1.138)$$

the poles of which give us the energy eigenvalues and the residues give us the eigenfunctions. If we are not interested in the latter ones, the simplest quantity to study is

$$\text{tr } G(E) = \int_{-\infty}^{+\infty} dx G(x, x; E) = \sum_n \frac{1}{E - E_n + i0^+}. \quad (1.139)$$

The Fourier transform will be performed again by using the stationary phase method. The stationary points of the time integral obey

$$\frac{\partial}{\partial T} \left[S_{cl}(xT, x0) + ET \right] = 0, \quad (1.140)$$

which is a well-known relation for the energy of a classical trajectory. In the same way we can evaluate the integral over x (i.e. the trace) by this method. Since the derivative of the action with respect to the endpoints gives us the momentum of the particle at these points (**Problem 6**) we find the relation

$$p(T) - p(0) = 0. \quad (1.141)$$

In other words: We search for classical trajectories with energy E , which are periodic both in the coordinates x as well in the momenta p . Eq. (1.139) then becomes

$$\text{tr } G(E) \simeq \text{const.} \sum_k A_k e^{iW(T_k)/\hbar} \quad (1.142)$$

in which

$$W(T) = ET + S_{cl}(T) = ET + \int_0^T dt (p \cdot \dot{x} - H) = \int_0^T dt p \cdot \dot{x}. \quad (1.143)$$

The factor A_k contains all pre-factors arising from the semi-classical approximation and the quadratic fluctuations around the stationary points. The result (1.142) is particularly simple for a potential with a single minimum as sketched in Fig. 5.

¹⁹In the calculus of variations this equation is also known as **Jacobi equation**. It determines that displacement of the path that makes $\delta^2 S$ minimal. If this minimum is positive, we know that for all displacements the classical path is a minimum, not only an extremal value of the action. It can be shown (e.g. **Schulman**, p. 81 - 83), that for sufficiently small $T = t_b - t_a$ the classical path indeed is a minimum but that the second functional derivative of the action changes sign ($\delta^2 S < 0$) as the particle passes through a focal point. This means that the classical path in general is only an extremum of the action.

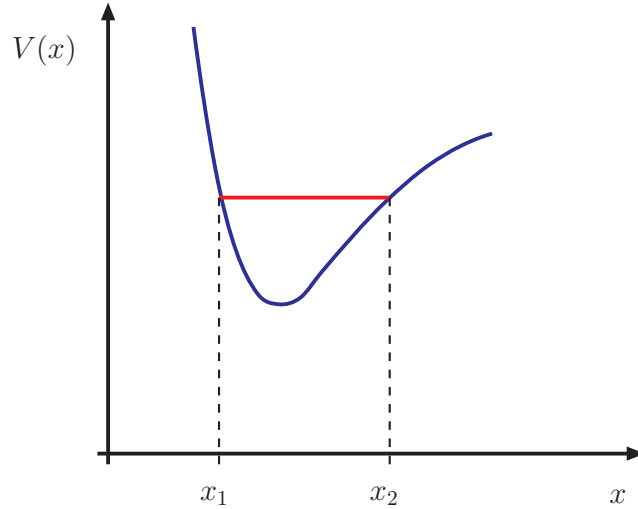


Fig. 5 : A potential with two turning points.

The particle then executes a periodic classical motion between the **turning points** x_1 and x_2 ; as derived from energy conservation $m\dot{x}^2/2 + V(x) = E$, one obtains for the period

$$T(E) = 2 \int_{x_1}^{x_2} dx \sqrt{\frac{m}{2[E - V(x)]}}. \quad (1.144)$$

Any multiple value of $T(E)$ also fulfills the stationary condition (1.140) so that $T_k(E) = kT(E)$ holds. The exponent in Eq. (1.142) can then be written as a multiple value of $W[T(E)]/\hbar$. If the prefactor A_k is ignored then one obtains

$$\text{tr}G(E) = \text{const.} \sum_{k=1}^{\infty} \left(e^{iW[T(E)]/\hbar} \right)^k = \text{const.} \frac{\exp(iW[T(E)]/\hbar)}{1 - \exp(iW[T(E)]/\hbar)}. \quad (1.145)$$

This expression has poles at energies which fulfill the quantization condition

$$W[T(E)] = \oint p dx = 2\pi n \hbar. \quad (1.146)$$

It can be shown (**Schulman**, ch. 18) that prefactors which have been neglected up to now give a phase $\pi/2$ each. This means that the minus sign in the denominator of Eq. (1.145) is converted into a plus sign and that, finally, we have obtained the old **Bohr-Sommerfeld quantization rule**

$$\boxed{\oint p dx = 2 \int_{x_1}^{x_2} dx \sqrt{2m[E - V(x)]} = \pi(2n + 1) \hbar} \quad (1.147)$$

1.6 Potential Scattering and Eikonal Approximation

We now want to consider scattering in a local potential

$$\hat{V} = V(\hat{\mathbf{r}}) \quad (1.148)$$

which leads to a continuous spectrum of the Hamiltonian if it falls off (sufficiently fast) for large values of \mathbf{r} . Let the initial momentum of the particle be \mathbf{k}_i ($\hbar = 1$) and the final one \mathbf{k}_f . Time-dependent scattering is formulated in the **interaction picture** in which the free propagation of the particle has been removed. The S matrix then simply is the matrix element of the time-evolution operator in the interaction picture $\hat{U}_I(t_b, t_a) = \exp(i\hat{H}_0 t_b) \hat{U}(t_b, t_a) \exp(-i\hat{H}_0 t_a)$ between the scattering states and evaluated at asymptotic times:

$$S_{i \rightarrow f} = \lim_{T \rightarrow \infty} \langle \mathbf{k}_f | \hat{U}_I(T, -T) | \mathbf{k}_i \rangle = \lim_{T \rightarrow \infty} e^{i(E_i + E_f)T} \langle \mathbf{k}_f | \hat{U}(T, -T) | \mathbf{k}_i \rangle \quad (1.149)$$

$$=: (2\pi)^3 \delta^{(3)}(\mathbf{k}_i - \mathbf{k}_f) - 2\pi i \delta(E_i - E_f) T_{i \rightarrow f}. \quad (1.150)$$

The second line defines the T matrix in which the energy-conserving δ -function²⁰ has been removed. It is customary to define a scattering amplitude

$$f(\Omega) = -\frac{m}{2\pi} T_{i \rightarrow f} \quad (1.151)$$

so that the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2. \quad (1.152)$$

Here Ω is the solid angle of the outgoing particle. For a spherically symmetric potential the scattering amplitude is only a function of the polar angle θ .

We now want to find a path-integral representation of the T matrix²¹. We start from the formulation (1.30) for the time-evolution operator $U(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)$ and use a trick to switch to an **integration over velocities**: We multiply the path integral with the following "One"

$$1 = \prod_{k=1}^N \int d^3 v_k \delta\left(\frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} - \mathbf{v}_k\right) = \epsilon^{3N} \prod_{k=1}^N \int d^3 v_k \delta(\mathbf{x}_k - \mathbf{x}_{k-1} - \epsilon \mathbf{v}_k). \quad (1.153)$$

Now we can perform the \mathbf{x}_k -integrations ($k = 1, \dots, N-1$) This gives $\mathbf{x}_j = \mathbf{x}_0 + \epsilon \sum_{i=1}^j \mathbf{v}_i$, or in the continuous notation the trajectory $\mathbf{x}_B(t) = \mathbf{x}_a + \int_{t_a}^t dt' \mathbf{v}(t')$, in which the boundary condition at $t = t_a$ was used. The boundary condition at $t = t_b$ gives $x_b = x_a + \int_{t_a}^{t_b} dt' \mathbf{v}(t')$, which – after addition of the resulting expressions for $\mathbf{x}_B(t)$ and dividing by two – leads to the symmetric form

$$\mathbf{x}_B(t) = \frac{x_a + x_b}{2} + \frac{1}{2} \left[\int_{t_a}^t dt' \mathbf{v}(t') - \int_t^{t_b} dt' \mathbf{v}(t') \right] =: \frac{x_a + x_b}{2} + \mathbf{x}_v(t). \quad (1.154)$$

However, when integrating over \mathbf{x}_k there remains one δ -function so that we obtain

²⁰Since the scattering potential is not translationally invariant there is only energy and not momentum conservation: $E_i = \mathbf{k}_i^2/(2m) = E_f = \mathbf{k}_f^2/(2m)$. The scattering states are normalized as $\langle \mathbf{k}_f | \mathbf{k}_i \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k}_f - \mathbf{k}_i)$.

²¹This derivation follows Ref. [12].

$$\begin{aligned}
U(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) &= \lim_{N \rightarrow \infty} \left(\frac{\epsilon m}{2\pi i} \right)^{\frac{3N}{2}} \int d^3 v_1 \dots d^3 v_N \delta^{(3)} \left(\mathbf{x}_b - \mathbf{x}_a - \epsilon \sum_{j=1}^N \mathbf{v}_j \right) \\
&\quad \cdot \exp \left\{ i\epsilon \sum_{j=1}^N \left[\frac{m}{2} \mathbf{v}_j^2 - V \left(\mathbf{x}_j = \mathbf{x}_a + \epsilon \sum_{i=1}^j \mathbf{v}_i \right) \right] \right\} \quad (1.155) \\
&\equiv \int \mathcal{D}^3 v(t) \delta^{(3)} \left(\mathbf{x}_b - \mathbf{x}_a - \int_{t_a}^{t_b} dt \mathbf{v}(t) \right) \exp \left\{ i \int_{t_a}^{t_b} dt \left[\frac{m}{2} \mathbf{v}^2(t) - V(\mathbf{x}_B(t)) \right] \right\}. \quad (1.156)
\end{aligned}$$

Here the "measure" $\mathcal{D}\mathbf{v}$ is defined in such a way that the Gaussian integral yields unity

$$\int \mathcal{D}^3 v(t) \exp \left\{ i \int_{t_a}^{t_b} dt \frac{m}{2} \mathbf{v}^2(t) \right\} = 1, \quad (1.157)$$

as may be seen from the discretized form. Of course, for a general potential this path-integral representation of the time-evolution operator is analytically as unsolvable as the original form. However, because of the physical interpretation of the auxiliary variable \mathbf{v} as velocity Eq. (1.156) is a good starting point for approximations, especially in the high-energy case. Note that the functional integral over \mathbf{v} has no boundary conditions since they are all contained in the remaining δ -function and the path $\mathbf{x}_B(t)$.

We now write Eq. (1.149) as

$$S_{i \rightarrow f} = \lim_{T \rightarrow \infty} e^{i(E_i + E_f)T} \int d^3 x d^3 y e^{-i\mathbf{k}_f \cdot \mathbf{x}} U(\mathbf{x}, T; \mathbf{y}, -T) e^{i\mathbf{k}_i \cdot \mathbf{y}} \quad (1.158)$$

and insert the representation (1.155). If we use the coordinates $\mathbf{r} = (\mathbf{x} + \mathbf{y})/2$, $\mathbf{s} = \mathbf{x} - \mathbf{y}$, then we obtain

$$\begin{aligned}
S_{i \rightarrow f} &= \lim_{T \rightarrow \infty} \exp[i(E_i + E_f)T] \int d^3 r e^{-i\mathbf{q} \cdot \mathbf{r}} \int \mathcal{D}^3 \mathbf{v} \exp \left\{ i \int_{-T}^{+T} dt \left[\frac{m}{2} \mathbf{v}^2(t) - \mathbf{K} \cdot \mathbf{v}(t) \right] \right\} \\
&\quad \cdot \exp \left\{ -i \int_{-T}^{+T} dt V(\mathbf{r} + \mathbf{x}_v(t)) \right\}, \quad (1.159)
\end{aligned}$$

since the relative coordinate \mathbf{s} is fixed by the δ -function in Eq. (1.155). Here we have introduced the momentum transfer and the average momentum

$$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i, \quad \mathbf{K} = \frac{1}{2}(\mathbf{k}_i + \mathbf{k}_f). \quad (1.160)$$

In addition, the sign function $\text{sgn}(x) = x/|x|$ has been used to write the argument of the potential compactly as

$$\mathbf{x}_v(t) := \frac{1}{2} \int_{-T}^{+T} dt' \text{sgn}(t - t') \mathbf{v}(t'). \quad (1.161)$$

($\mathbf{x}_v(t)$ is the deviation of the trajectory from the mean position, see Eq. (1.154)). The shift

$$\mathbf{v}(t) \longrightarrow \mathbf{v}(t) + \frac{\mathbf{K}}{m} \quad (1.162)$$

eliminates the linear term in the exponent of the functional integral. Since $\int_{-T}^{+T} dt' \text{sgn}(t - t') = 2t$ and $E_i + E_f - \mathbf{K}^2/m = \mathbf{q}^2/(4m)$ the result is

$$\begin{aligned}
S_{i \rightarrow f} &= \lim_{T \rightarrow \infty} \exp \left(i \frac{\mathbf{q}^2}{4m} T \right) \int d^3 r e^{-i\mathbf{q} \cdot \mathbf{r}} \int \mathcal{D}^3 v \exp \left[i \int_{-T}^{+T} dt \frac{m}{2} \mathbf{v}^2(t) \right] \\
&\quad \cdot \exp \left\{ -i \int_{-T}^{+T} dt V \left(\mathbf{r} + \frac{\mathbf{K}}{m} t + \mathbf{x}_v(t) \right) \right\}. \quad (1.163)
\end{aligned}$$

If the interaction is weak one can expand in powers of the potential. In zeroth order one has

$$S^{(0)} = \lim_{T \rightarrow \infty} \exp\left(i \frac{\mathbf{q}^2}{4m} T\right) \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} = (2\pi)^3 \delta^{(3)}(\mathbf{k}_i - \mathbf{k}_f) \quad (1.164)$$

and thus we may write

$$(S-1)_{i \rightarrow f} = \lim_{T \rightarrow \infty} \exp\left(i \frac{\mathbf{q}^2}{4m} T\right) \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \int \mathcal{D}^3v \exp\left[i \int_{-T}^{+T} dt \frac{m}{2} \mathbf{v}^2(t)\right] \cdot \left\{ \exp\left[-i \int_{-T}^{+T} dt V\left(\mathbf{r} + \frac{\mathbf{K}}{m}t + \mathbf{x}_v(t)\right)\right] - 1 \right\}. \quad (1.165)$$

The path-integral representation (1.165) has the disadvantage that a phase $\mathbf{q}^2 T/(4m)$ appears which in the limit $T \rightarrow \infty$ seems to diverge. Of course, in each order of perturbation theory this phase cancels so that the limit $T \rightarrow \infty$ actually exists but one would like to have a formulation where this property is explicitly built in. This can be achieved in the following manner: First one uses the fact that any power of \mathbf{q}^2 in the \mathbf{r} -integral can be generated by applying the Laplace operator $-\Delta$ on $\exp(i\mathbf{q}\cdot\mathbf{r})$. In other words:

$$\exp\left(i \frac{\mathbf{q}^2}{4m} T\right) e^{-i\mathbf{q}\cdot\mathbf{r}} = \exp\left(-i \frac{\Delta}{4m} T\right) e^{-i\mathbf{q}\cdot\mathbf{r}}. \quad (1.166)$$

An integration by parts (which doesn't produce any boundary terms if the potential falls off rapidly enough) leads to the exponential function with the Laplace operator acting to the right, i.e. on the potential term.

Finally, we use a trick which goes under the name [undoing the square](#)²² and which linearizes the square (of an operator) in the exponent. In the simplest case of an ordinary integral this simply is the identity

$$e^{-iax^2} = \sqrt{\frac{i}{4\pi a}} \int_{-\infty}^{+\infty} dy \exp\left(-\frac{i}{4a}y^2\right) e^{-xy} \quad (a \text{ real}), \quad (1.167)$$

which can be proved by completing the square. This can be extended to path integrals and one may write

$$\exp\left(-\frac{i}{4m} T \Delta\right) = \int \mathcal{D}^3w(t) \exp\left[-i \int_{-T}^{+T} dt \frac{m}{2} \mathbf{w}^2(t) - \int_{-T}^{+T} dt f(t) \mathbf{w}(t) \cdot \nabla\right], \quad (1.168)$$

where the "measure" has again been chosen such that the Gaussian integral is normalized to one.

The arbitrary function $f(t)$ only has to fulfill $\int_{-T}^{+T} dt f^2(t) = T/2$ and we chose it as $f(t) = \text{sgn}(t)/2$. Our representation now reads

$$\exp\left(-\frac{i}{4m} T \Delta\right) = \int \mathcal{D}^3w(t) \exp\left[-i \int_{-T}^{+T} dt \frac{m}{2} \mathbf{w}^2(t) - \mathbf{x}_w(0) \cdot \nabla\right]. \quad (1.169)$$

Note that the sign of the quadratic \mathbf{w} -term in Eq. (1.169) necessarily is negative – therefore we may call the 3-dimensional auxiliary variable $\mathbf{w}(t)$ an "**anti-velocity**"²³.

The advantage of linearizing the exponent is that we now have a differential operator which simply shifts the argument of the potential function by $-\mathbf{x}_w(0)$ (that is nothing else than Taylor's theorem $\exp(a \frac{d}{dx})f(x) = f(x+a)$). The result of these manipulations is therefore the expression

$$(S-1)_{i \rightarrow f} = i \lim_{T \rightarrow \infty} \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \int \mathcal{D}^3v \mathcal{D}^3w \exp\left\{i \frac{m}{2} \int_{-\infty}^{+\infty} dt [\mathbf{v}^2(t) - \mathbf{w}^2(t)]\right\} \cdot \left\{ \exp\left[i \int_{-T}^{+T} dt V\left(\mathbf{r} + \frac{\mathbf{K}}{m}t + \mathbf{x}_v(t) - \mathbf{x}_w(0)\right)\right] - 1 \right\}. \quad (1.170)$$

²²In many-body physics this is called the "Hubbard-Stratonovich" transformation, see [chapter 2.7](#).

²³Formulations of potential scattering [without](#) anti-velocity can be found in Refs. [13], [14].

That is free of the "dangerous" phase which allows us to perform formally the limit $T \rightarrow \infty$. The price to pay is an additional (functional) integration over the "anti-velocity".

However, we have not yet displayed the energy-conserving δ -function to obtain the T matrix according to Eq. (1.150). One can check that this is achieved when Eq. (1.165) is expanded in powers of the interaction: In each term of this perturbative expansion we find such an energy-conserving δ -function.

How to achieve this without expanding in powers of the interaction? For that purpose one may use a trick which [Faddeev and Popov](#) have introduced in field theory to quantize non-abelian gauge theories (see [chapter 3.3](#)). We first note that in the limit $T \rightarrow \infty$ the action in the path integral (1.163) is invariant under the transformation

$$t = \bar{t} + \tau, \quad \mathbf{r} = \bar{\mathbf{r}} - \frac{\mathbf{K}}{m}\tau, \quad \mathbf{v}(t) = \bar{\mathbf{v}}(\bar{t}) \quad (1.171)$$

since

$$\int_{-T}^{+T} dt V \left(\mathbf{r} + \frac{\mathbf{K}}{m}t + \mathbf{x}_v(t) \right) = \int_{-T-\tau}^{T-\tau} d\bar{t} V \left(\bar{\mathbf{r}} + \frac{\mathbf{K}}{m}\bar{t} + \frac{1}{2} \int_{-T-\tau}^{T-\tau} d\bar{t}' \bar{\mathbf{v}}(\bar{t}') \operatorname{sgn}(\bar{t} - \bar{t}') \right). \quad (1.172)$$

For finite τ and $T \rightarrow \infty$ the change of the integration limits is irrelevant and the action remains invariant under the transformation (1.171) ²⁴.

However, this means that the component of the vector \mathbf{r} which is parallel to \mathbf{K} is not fixed leading to a singularity when we integrate over this component, This singularity is just the energy-conserving δ -function we are looking for. We can it extract, if we first fix the longitudinal component and then integrate over all possible values – that is, we multiply the path integral (1.165), for example with the following "one"

$$1 = \frac{|\mathbf{K}|}{m} \int_{-\infty}^{+\infty} d\tau \delta \left(\hat{\mathbf{K}} \cdot \left[\mathbf{r} + \frac{\mathbf{K}}{m}\tau \right] \right) \quad (1.173)$$

Now we perform the transformation (1.171) in the path integral and obtain

$$\begin{aligned} (S-1)_{i \rightarrow f} &= \frac{|\mathbf{K}|}{m} \lim_{T \rightarrow \infty} \int_{-\infty}^{+\infty} d\tau \int d^3r \exp \left(-i\mathbf{q} \cdot \mathbf{r} + i\mathbf{q} \cdot \frac{\mathbf{K}}{m}\tau \right) \delta \left(\hat{\mathbf{K}} \cdot \mathbf{r} \right) \\ &\cdot \int \mathcal{D}^3v \mathcal{D}^3w \exp \left\{ i \int_{-T}^{+T} dt \frac{m}{2} [\mathbf{v}^2(t) - \mathbf{w}^2(t)] \right\} \\ &\cdot \left\{ \exp \left[-i \int_{-T}^{+T} dt V \left(\mathbf{r} + \frac{\mathbf{K}}{m}t + \mathbf{x}_v(t) - \mathbf{x}_w(0) \right) \right] - 1 \right\}, \end{aligned} \quad (1.174)$$

where we have replaced the variables with a bar by the original ones in order to simplify our notation. The only dependence on τ which remains in the integrand is now in the factor $\exp(i\tau\mathbf{q} \cdot \mathbf{K}/m)$, so that integration over it exactly generates the energy-conserving δ -function:

$$2\pi \delta \left(\frac{\mathbf{q} \cdot \mathbf{K}}{m} \right) = 2\pi \delta \left(\frac{\mathbf{k}_f^2}{2m} - \frac{\mathbf{k}_i^2}{2m} \right). \quad (1.175)$$

In addition, after the transformation the longitudinal component of \mathbf{r} in the path integral is set to zero. If we keep in mind that $q_{\parallel} = 0$ then we obtain the following expression for the T matrix

²⁴Actually this is a delicate interchange of limits whose justification has to be checked.

$$T_{i \rightarrow f} = i \frac{K}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} \int \mathcal{D}^3v \mathcal{D}^3w \exp \left\{ i \int_{-\infty}^{+\infty} dt \frac{m}{2} [\mathbf{v}^2(t) - \mathbf{w}^2(t)] \right\} \left\{ e^{i\chi(\mathbf{b}, K; \mathbf{v}, \mathbf{w})} - 1 \right\}. \quad (1.176)$$

Here a phase

$$\chi(\mathbf{b}, K; \mathbf{v}, \mathbf{w}) = - \int_{-\infty}^{+\infty} dt V \left(\mathbf{b} + \frac{\mathbf{K}}{m} t + \mathbf{x}_v(t) - \mathbf{x}_w(0) \right) \quad (1.177)$$

has been defined which depends on the velocities $\mathbf{v}(t), \mathbf{w}(t)$ and the transverse component \mathbf{b} of the vector \mathbf{r} . $E = E_i = E_f = k^2/(2m)$ is the scattering energy. In addition, the magnitudes of momentum transfer and average momentum are given by

$$q \equiv |\mathbf{q}| = 2k \sin \frac{\theta}{2}, \quad K \equiv |\mathbf{K}| = k \cos \frac{\theta}{2}. \quad (1.178)$$

One can check that Eq. (1.176) reproduces the exact Born series in all orders, i.e. all manipulations have been correct. More interesting than a derivation of perturbation theory, however, is that this result can serve as a starting point for high-energy approximations. In this case, we expect that the particle moves preferentially along a **straight line path** with the (constant) velocity K/m and that the functional integral over \mathbf{v} and \mathbf{w} only describes the fluctuations around this path. That this is indeed the case can be seen when

$$t = \frac{m}{K} z, \quad \mathbf{v}(t) = \frac{\sqrt{K}}{m} \bar{\mathbf{v}}(z), \quad \mathbf{w}(t) = \frac{\sqrt{K}}{m} \bar{\mathbf{w}}(z) \quad (1.179)$$

is substituted in the path integral (1.176): It basically keeps its form in the new variables²⁵ but the phase becomes

$$\chi(\mathbf{b}, K; \bar{\mathbf{v}}, \bar{\mathbf{w}}) = - \frac{m}{K} \int_{-\infty}^{+\infty} dz V \left(\mathbf{b} + \hat{\mathbf{K}} z + \frac{1}{\sqrt{K}} [\mathbf{x}_{\bar{v}}(z) - \mathbf{x}_{\bar{w}}(0)] \right). \quad (1.180)$$

This shows that for a fixed momentum transfer a **systematic** expansion in inverse powers of $K = k \cos(\theta/2)$ is obtained by expanding the phase χ simultaneously in powers of $\mathbf{v}(t)$ and $\mathbf{w}(t)$ and integrating functionally term by term. One can expect that this will be valid for large values of the energy, small scattering angles θ and weakly varying potentials.

This can be seen as follows: Obviously the correction from the next term of the Taylor expansion of the potential should be small compared to the leading term, i.e. $|\nabla V \cdot \mathbf{x}_{\bar{v}}/\sqrt{K}| \ll V$. Assuming now that the velocity fluctuations are only relevant within the range R of the potential, then we find that $\bar{v} = \mathcal{O}(1/\sqrt{R})$ and $x_{\bar{v}} = \mathcal{O}(\sqrt{R})$ and thus

$$KR \gg \left(R \frac{\nabla V}{V} \right)^2 \simeq \left(\frac{R}{a} \right)^2, \quad (1.181)$$

where a is the distance over which the potential changes appreciably. So for the application of the eikonal approximation it is not necessary that the velocity k/m of the scattered particle should be very large; in atomic physics, for example, this is almost never the case as the masses involved are large and the energies small. On the other hand, for large scattering angles $K = k \cos(\theta/2)$ gets smaller and smaller and one sees that the criterion (1.181) cannot be fulfilled anymore.

²⁵Except that the kinetic energies of velocity and anti-velocity now read $(\bar{\mathbf{v}}^2(t) - \bar{\mathbf{w}}^2(t))/2$, i.e. do not contain anymore the mass of the particle.

The leading approximation is simply obtained by setting $\mathbf{v} = \mathbf{w} = 0$ in the argument of the potential:

$$T_{i \rightarrow f} \simeq i \frac{K}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} \left\{ \exp \left[-i \frac{m}{K} \int_{-\infty}^{+\infty} dz V(\mathbf{b} + \hat{\mathbf{K}}z) \right] - 1 \right\}, \quad (1.182)$$

as the functional integrals are trivially one by normalization. In forward direction the difference between $K = k \cos(\theta/2)$ and k is irrelevant so that one obtains the usual **eikonal approximation**²⁶

$$T_{i \rightarrow f}^{\text{eik}} = i \frac{k}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} \left(e^{i\chi_0(\mathbf{b})} - 1 \right). \quad (1.183)$$

Here

$$\chi_0(\mathbf{b}) = - \int_{-\infty}^{+\infty} dt V \left(\mathbf{b} + \hat{\mathbf{K}} \frac{k}{m} t \right) = - \frac{m}{k} \int_{-\infty}^{+\infty} dz V(\mathbf{b}, z) \quad (1.184)$$

is the phase which the particle has "accumulated" along its straight line path²⁷. Note that the first Born approximation for the T matrix follows from Eq. (1.183) if – for weak potentials – $\exp(i\chi_0)$ is expanded till first order:

$$T_{i \rightarrow f}^{\text{eik}} \longrightarrow i \frac{k}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} \left[-i \frac{m}{k} \int_{-\infty}^{+\infty} dz V(\mathbf{b}, z) \right] = \int d^3r e^{-i\mathbf{q} \cdot \mathbf{r}} V(\mathbf{r}) = \tilde{V}(\mathbf{q}) \equiv T_{i \rightarrow f}^{1^{\text{st}} \text{Born}}. \quad (1.185)$$

However, unlike the first Born approximation the eikonal approximation yields a **complex** scattering amplitude as required by **unitarity** (the "**optical theorem**").

Detail 8: Unitarity

Unitarity is one of the 'sacred' principles of quantum physics; roughly speaking, it requires that in every process no more gets out than what entered in the beginning. More formally (but more accurately) it means that the S matrix should fulfill

$$\hat{S}^\dagger \hat{S} = \hat{S} \hat{S}^\dagger = 1. \quad (1.186a)$$

If the relation (1.150) is written representation free as

$$\hat{S} = 1 - 2\pi i \delta(E_i - \hat{H}_0) \hat{T} \quad (1.186b)$$

then the unitarity (1.186a) of the S matrix requires the T matrix to obey

$$\hat{T} - \hat{T}^\dagger = \frac{2\pi}{i} \hat{T}^\dagger \delta(E_i - \hat{H}_0) \hat{T}. \quad (1.186c)$$

Taking matrix elements for the special case $i = f$, i.e. for forward scattering one obtains

$$\text{Im } T_{i \rightarrow i} = - \frac{mk}{8\pi^2} \int d\Omega_p |T_{i \rightarrow p}|_{p=k}^2, \quad (1.186d)$$

because the δ -function in Eq. (1.186c) fixes the magnitude of the internal momentum \mathbf{p} to be the magnitude of the exterior momentum $k = |\mathbf{k}_i| = |\mathbf{k}_f|$. Usually one discusses the unitarity relation (the optical theorem) for the scattering amplitude (1.151)

$$\text{Im } f(\theta = 0) = \frac{k}{4\pi} \int d\Omega |f(\theta)|^2 = \frac{k}{4\pi} \sigma_{\text{tot}}. \quad (1.186e)$$

Since the first Born approximation (1.185) gives a real scattering amplitude it is clear that the optical theorem is violated in this frequently employed approximation. However, the scattering amplitude of the eikonal approximation has an imaginary part in forward direction

$$\text{Im } f^{\text{eik}}(\theta = 0) = \frac{k}{2\pi} \int d^2b [1 - \cos \chi_0(\mathbf{b})], \quad (1.186f)$$

so that the l.h.s. of the optical theorem is non-zero for this approximation. The total cross section on the r.h.s. is

$$\sigma_{\text{tot}}^{\text{eik}} = \frac{k^2}{4\pi^2} \int d\Omega \int d^2b' e^{i\mathbf{q} \cdot (\mathbf{b} - \mathbf{b}')} \left(e^{i\chi_0(\mathbf{b})} - 1 \right) \cdot \left(e^{i\chi_0(\mathbf{b}')} - 1 \right). \quad (1.186g)$$

²⁶The variant (1.182) is due to Ref. [15].

²⁷The index indicates the inverse power of K while m/K may have an arbitrary value.

Replacing the angle integration by an integration over the momentum transfer $q = 2k \sin(\theta/2)$

$$d\Omega = 2\pi \sin \theta d\theta = \frac{2\pi}{k^2} q dq = \frac{1}{k^2} d^2 q \quad (1.186h)$$

one obtains

$$\sigma_{\text{tot}}^{\text{eik}} = \frac{1}{4\pi^2} \int d^2 b d^2 b' \int_{q < 2k} d^2 q e^{i\mathbf{q} \cdot (\mathbf{b} - \mathbf{b}')} \left(e^{i\chi_0(\mathbf{b})} - 1 \right) \left(e^{i\chi_0(\mathbf{b}')} - 1 \right) . \quad (1.186i)$$

If we split up the 2-dimensional q -integral into one part in which the momentum transfer is unrestricted and a "defect" which corrects this assumption, the first part gives a δ -function

$$\int_{q < 2k} d^2 q e^{i\mathbf{q} \cdot (\mathbf{b} - \mathbf{b}')} = (2\pi)^2 \delta(\mathbf{b} - \mathbf{b}') - \int_{q > 2k} d^2 q e^{i\mathbf{q} \cdot (\mathbf{b} - \mathbf{b}')} , \quad (1.186j)$$

which exactly leads to the fulfillment of the optical theorem:

$$\sigma_{\text{tot}}^{\text{eik}} = \int d^2 b \underbrace{\left| e^{i\chi_0(\mathbf{b})} - 1 \right|^2}_{=2(1-\cos \chi_0)} + \Delta^{\text{eik}} . \quad (1.186k)$$

The defect of the total eikonal cross section obviously is negative

$$\Delta^{\text{eik}} = -\frac{1}{4\pi^2} \int_{q > 2k} d^2 q \left| \int d^2 b e^{-i\mathbf{q} \cdot \mathbf{b}} \left(e^{i\chi_0(\mathbf{b})} - 1 \right) \right|^2 \quad (1.186l)$$

and small if the cross section has its maximum in forward direction and falls off rapidly at larger scattering angles (momentum transfers) which usually is the case at high energy. Let us estimate roughly the defect by using the first Born approximation, i.e. we assume that the phase $\chi_0(\mathbf{b})$ is small. Then we obtain

$$\Delta^{\text{eik}} \simeq \frac{1}{4\pi^2} \frac{m^2}{k^2} \int_{q > 2k} d^2 q \left[\tilde{V}(\mathbf{q}) \right]^2 \quad (1.186m)$$

and we have to evaluate the Fourier transform of a (for simplicity assumed spherically symmetric) potential

$$\tilde{V}(q) = \frac{4\pi}{q} \int_0^\infty dr r \sin(qr) V(r) \quad (1.186n)$$

for large values of $q = |\mathbf{q}|$. This is done most easily by subsequent integrations by parts ($\sin(qr) = -[\cos(qr)]'/q$; $\cos(qr) = [\sin(qr)]'/q$) and gives

$$\tilde{V}(q) = \frac{4\pi}{q} \left\{ \frac{[rV(r)](0)}{q} - \frac{[rV(r)]''(0)}{q^3} + \dots \right\} . \quad (1.186o)$$

Depending on the behaviour of the potential at the origin, the power of the fall-off is different; for example, the Fourier transform of a Yukawa potential $V(r) = V_0 \exp(-\mu r)/r$ falls off asymptotically like $1/q^2$. More general, the behaviour of the potential at the origin determines the asymptotic fall-off:

$$V(r) \xrightarrow{r \rightarrow 0} V_0 r^\alpha \quad \Rightarrow \quad \tilde{V}(q) \xrightarrow{q \rightarrow \infty} \frac{\text{const.}}{q^{\alpha+3}} . \quad (1.186p)$$

From Eq. (1.186m) we then conclude that for these classes of potentials the defect

$$\Delta^{\text{eik}} \sim \frac{1}{k^{2\alpha+6}} . \quad (1.186q)$$

vanishes rapidly at high energies: The eikonal approximation is then (nearly) unitary!

If one considers scattering in a spherically symmetric potential, one can perform the angular integration in Eq. (1.183) ²⁸ and one obtains for the scattering amplitude

$$f^{\text{eik}}(\theta) = \frac{k}{i} \int_0^\infty db b J_0(qb) \left(e^{i\chi_0(b)} - 1 \right) . \quad (1.187)$$

Here $J_0(x)$ is a Bessel function of order zero and the eikonal phase explicitly reads

$$\chi_0(b) = -\frac{m}{k} \int_{-\infty}^{+\infty} dz V \left(\sqrt{b^2 + z^2} \right) . \quad (1.188)$$

Comparing with the well-known partial wave expansion of the scattering amplitude

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \left(e^{2i\delta_l(k)} - 1 \right) , \quad (1.189)$$

²⁸See, e.g., {Handbook}, eq. 9.1.21 .

reveals a close connection: For large scattering energies so many partial waves contribute that summation over l can be replaced by an integral over the **impact parameter** $b = (l + 1/2)/k$. If, in addition an asymptotic expansion²⁹ of the Legendre polynomials $P_l(\cos\theta)$ is used for large values of l , then one finds complete agreement with the form of the eikonal result (1.187) and the simple relation $2\delta_l(k) \simeq \chi_0(b)$ between scattering phase and eikonal phase.

It is (relatively) easy to calculate the first correction to the eikonal result: We expand the phase (1.177) up to first order

$$\begin{aligned} \chi(\mathbf{b}, \mathbf{K}; \mathbf{v}, \mathbf{w}) &= - \int_{-\infty}^{+\infty} dt V \left(\mathbf{b} + \frac{\mathbf{K}}{m} t \right) \\ &\quad - \int_{-\infty}^{+\infty} dt \nabla V \left(\mathbf{b} + \frac{\mathbf{K}}{m} t \right) \frac{1}{2} \int_{-\infty}^{+\infty} ds \left[\mathbf{v}(s) \operatorname{sgn}(t-s) - \mathbf{w}(s) \operatorname{sgn}(-s) \right] \end{aligned} \quad (1.190)$$

and perform the Gaussian integrals over \mathbf{v} and \mathbf{w} . The corrected result

$$T_{i \rightarrow f} \simeq i \frac{K}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} \left\{ e^{i\chi_0(\mathbf{b}) + i\chi_1(\mathbf{b})} - 1 \right\} \quad (1.191)$$

now contains an additional phase

$$\chi_1(\mathbf{b}) = -\frac{1}{8m} \lim_{T \rightarrow \infty} \int_{-T}^{+T} ds \int_{-T}^{+T} dt_1 dt_2 \nabla V_1 \cdot \nabla V_2 \left[\operatorname{sgn}(t_1 - s) \operatorname{sgn}(t_2 - s) - \operatorname{sgn}^2(-s) \right]. \quad (1.192)$$

Here the second term in the square bracket is due to the integration over the anti-velocity and $V_{1/2}$ is a shortform for $V(\mathbf{b} + \mathbf{K}t_{1/2}/m)$. The s -integration can be performed with the help of

$$\int_{-T}^{+T} ds \operatorname{sgn}(t-s) \operatorname{sgn}(s-t') = 2 \left[|t-t'| - T \right] \quad (1.193)$$

and one obtains

$$\chi_1(\mathbf{b}) = \frac{1}{4m} \lim_{T \rightarrow \infty} \int_{-T}^{+T} dt_1 dt_2 \nabla V_1 \cdot \nabla V_2 |t_1 - t_2|. \quad (1.194)$$

As expected the T -dependent terms have been canceled completely by the contribution from the anti-velocity. For a spherically symmetric potential Eq. (1.194) can be simplified by using the relations $\partial V(r)/\partial z = zV'(r)/r$, $\partial V(r)/\partial b = bV'(r)/r$ and by integrations by parts. One obtains

$$\chi_1(b) = -\frac{1}{2K} \left(\frac{m}{K} \right)^2 \left[1 + b \frac{\partial}{\partial b} \right] \int_{-\infty}^{+\infty} dz V^2(r), \quad r \equiv \sqrt{b^2 + z^2}, \quad (1.195)$$

which shows explicitly that this phase is $\mathcal{O}(1/K)$, if one allows arbitrary values for the velocity K/m . The result is identical (except for the appearance of $K = k \cos(\theta/2)$ instead of k which, however, is irrelevant in this order) with the next term in a systematic eikonal expansion where also higher orders have been calculated by quantum mechanical methods [16], [17].

Example: Scattering in a Coulomb Potential

The Coulomb potential

$$V_C(r) = \frac{Z\alpha}{r} \quad (1.196)$$

²⁹{Handbook}, eq. 22.15.1 .

causes well-known difficulties in scattering theory due to its slow decrease at infinity. From the solution of Schrödinger's equation, for example, it is known that the scattered wave in the asymptotic region not only exhibits the characteristic spherical wave but an additional logarithmic r -dependency ³⁰:

$$\psi_{\text{scattered}} \xrightarrow{r \rightarrow \infty} \frac{1}{r} \exp [i (kr - \gamma \ln 2kr)] \cdot f_C(\theta), \quad (1.197)$$

where $\gamma = Z\alpha m/k$ is the Sommerfeld parameter and

$$f_C(\theta) = -\frac{\gamma}{2k \sin^2(\theta/2)} \exp \left[-i\gamma \ln \left(\sin^2 \frac{\theta}{2} \right) + 2i\sigma_0 \right], \quad \sigma_0 = \arg \Gamma(1 + i\gamma) \quad (1.198)$$

the Coulomb scattering amplitude. In eikonal approximation the long range of the potential leads to a divergent eikonal phase χ_0 (see Eq. (1.188)). In order to be able to treat this potential anyway we introduce a cut-off at large radius R

$$V_C(r) \longrightarrow V_C^{(R)}(r) = \frac{Z\alpha}{r} \Theta(R - r). \quad (1.199)$$

Indeed, in nature this screening is always realized, e.g. in an atom where the bare charge of the nucleus is neutralized by the electrons which predominantly are far away at atomic distances. Having modified (regularized) the pure Coulomb potential we can now calculate the eikonal phase (1.188) and find

$$\chi_C^{(R)}(b) = -2\gamma\Theta(R - b) \int_b^R \frac{dr}{\sqrt{r^2 - b^2}} = -2\gamma\Theta(R - b) \ln \frac{R + \sqrt{R^2 - b^2}}{b} \xrightarrow{R \gg b} -2\gamma \ln \frac{2R}{b}. \quad (1.200)$$

An alternative regularization is to consider the pure Coulomb potential as limit $\mu \rightarrow 0$ of a Yukawa potential $V_Y(r) = Z\alpha \exp(-\mu r)/r$. With **{Handbook}**, eq. 9.6.23 its eikonal phase is $\chi_Y(b) = 2\gamma K_0(\mu b)$, where K_0 denotes the modified Bessel function of second type. For small μb one may use the expansion **{Handbook}**, eq. 9.6.13 to find the same logarithmic impact-parameter dependence as in Eq. (1.200) but with a cut-off radius $R_Y = \exp(\gamma_E)/\mu$ where $\gamma_E = 0.57721566\dots$ is Euler's constant.

Since

$$e^{i\chi_C^{(R)}(b)} \simeq \left(\frac{kb}{2kR} \right)^{2i\gamma}, \quad b \ll R \quad (1.201)$$

is then a power in b , the impact-parameter integral in Eq. (1.187) can be performed analytically ³¹ and one finds

$$f_C^{(R)\text{eik}}(\theta) = \frac{1}{2ik} \frac{(2kR)^{-2i\gamma}}{(\sin \theta/2)^{2+2i\gamma}} \frac{\Gamma(1 + i\gamma)}{\Gamma(-i\gamma)} = e^{-2i\gamma \ln 2kR} f_C(\theta). \quad (1.202)$$

Except for the additional phase from the shielding the eikonal approximation thus reproduces the **exact result for the Coulomb scattering amplitude**. An additional phase $-\gamma \ln 2kR$ is also obtained from Eq. (1.197) when the potential is truncated at $r = R$ and the spherical wave is then allowed to spread out freely into the asymptotic region ³².

Detail 9: Correct Treatment of the Coulomb Potential

In the derivation of Eq. (1.202) there was some "cheating" to obtain the correct result: First, we have assumed $b \ll R$, then used the formula

$$\int_0^\infty dx x^\mu J_0(ax) = 2^\mu a^{-\mu-1} \frac{\Gamma((1+\mu)/2)}{\Gamma((1-\mu)/2)} \quad (1.203a)$$

with $\mu = 1 + 2i\gamma$ which only holds for $-1 < \text{Re } \mu < 1/2$ and finally have heedlessly omitted the "1" in the integrand following the exponential function ... A correct derivation would keep the cut-off radius R finite during integration and let it tend to infinity only **after** performing the (now convergent) integral. That is more complicated but can be done as the indefinite integral

$$\int_0^1 dx x^\mu J_0(ax) = a^{-\mu-1} \left[(\mu - 1) a J_0(a) S_{\mu-1,-1}(a) + a J_1(a) S_{\mu,0}(a) + 2^\mu \frac{\Gamma((1+\mu)/2)}{\Gamma((1-\mu)/2)} \right] \quad (1.203b)$$

³⁰See, e.g., **{Messiah 1}**, p. 430.

³¹See, e.g., **{Gradshteyn-Ryzhik}**, eq. 6.561.14 .

³²A closer examination of the truncated Coulomb potential can be found in Ref. [18].

can be expressed analytically³³ by Lommel functions $S_{\mu,\nu}(z)$ and converges for $\text{Re } \mu > -1$.

If we set $x = b/R$ the scattering amplitude for the screened Coulomb potential in eikonal approximation therefore is given by

$$f_C^{(R)\text{eik}} = -ikR^2 \int_0^1 dx x \left(\frac{x}{1 + \sqrt{1-x^2}} \right)^{2i\gamma} J_0(qRx) - (\gamma = 0) \quad (1.203c)$$

where the previously missing "1" is generated by subtracting the same expression with $\gamma = 0$. The expansion

$$\left(\frac{x}{1 + \sqrt{1-x^2}} \right)^{2i\gamma} = \left(\frac{x}{2} \right)^{2i\gamma} \sum_{n=0}^{\infty} a_n x^{2n} \quad (1.203d)$$

now allows term-by-term integration over x using formula (1.203b) and we obtain

$$f_C^{(R)\text{eik}} = -ikR^2 2^{-2i\gamma} \sum_{n=0}^{\infty} \frac{a_n}{(qR)^{1+2n+2i\gamma}} \left[(2n + 2i\gamma) J_0(qR) S_{2n+2i\gamma,-1}(qR) \right. \\ \left. + J_1(qR) S_{1+2n+2i\gamma,0}(qR) + 2^{1+2n+2i\gamma} \frac{1}{qR} \frac{\Gamma(n+1+i\gamma)}{\Gamma(-n-i\gamma)} \right] - (\gamma = 0). \quad (1.203e)$$

Now we may use the asymptotic behaviour of the Lommel and Bessel functions³⁴

$$S_{\mu,\nu}(z) \xrightarrow{z \rightarrow \infty} z^{\mu-1} \left[1 + \mathcal{O}\left(\frac{1}{z}\right) \right], \quad J_\nu(z) \xrightarrow{z \rightarrow \infty} \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{\pi}{2}\nu - \frac{\pi}{4}\right) \quad (1.203f)$$

to let the cut-off radius R (more precisely: qR , therefore not for $\theta = 0$) go to infinity. In the last term of Eq. (1.203e) only the term with $n = 0$ contributes while the second term is dominant and the first subdominant. This gives

$$f_C^{(R)\text{eik}} \rightarrow -ikR^2 2^{-2i\gamma} \sum_{n=0}^{\infty} a_n \left[\frac{J_1(qR)}{qR} + \frac{\delta_{n,0}}{2} \left(\frac{qR}{2} \right)^{-2-2i\gamma} \frac{\Gamma(1+i\gamma)}{\Gamma(-i\gamma)} + \mathcal{O}\left(\frac{\cos(qR - \pi/4)}{(qR)^{5/2}}\right) \right] - (\gamma = 0). \quad (1.203g)$$

From the expansion (1.203d) we read off for $x \rightarrow 0$: $a_0 = 1$ and for $x = 1$: $\sum_n a_n = 2^{2i\gamma}$. With this we obtain

$$f_C^{(R)\text{eik}} \rightarrow -ikR^2 \left[\frac{J_1(qR)}{qR} + \frac{2}{(qR)^{2+2i\gamma}} \frac{\Gamma(1+i\gamma)}{\Gamma(-i\gamma)} \right] - (\gamma = 0), \quad (1.203h)$$

and we see that subtracting the term with $\gamma = 0$, i.e. the "1" in the impact-parameter integral precisely cancels the (unwanted) term $J_1(qR)/(qR)$. Thus we indeed find the expression (1.202) for the Coulomb scattering amplitude.

By an analytic continuation of the scattering amplitude in the wavenumber k we also can obtain the energies of bound states: It is clear that as a function of k , Eq. (1.202) has simple poles exactly where the Gamma function in the numerator diverges. This happens at

$$1 + i\gamma_n = 1 + i \frac{Z\alpha m}{k_n} = -(n-1), \quad n = 1, 2, \dots \quad k_n = -i \frac{Z\alpha m}{n} \quad (1.204)$$

and, indeed, gives the well-known binding energies of hydrogenlike atoms³⁵

$$E_n = \frac{k_n^2}{2m} = -\frac{(Z\alpha)^2}{2n^2} m. \quad (1.205)$$

Of course, it is a coincidence that the (lowest-order) eikonal approximation gives the exact result for the Coulomb potential – the general estimates for the region of validity of this approximation remain unchanged. Note that the first correction (1.195) indeed vanishes for this potential.

As a quantitative test of the various eikonal approximations Fig. 6 shows the relative deviation of the corresponding scattering amplitude

$$\left| \frac{\Delta f}{f} \right| := \left| \frac{f_{\text{approx}} - f_{\text{exact}}}{f_{\text{exact}}} \right| \quad (1.206)$$

³³{Gradshteyn-Ryzhik}, eq. 6.56.13; caution misprint!

³⁴{Gradshteyn-Ryzhik}, eq. 8.576, and eq. 8.451, respectively.

³⁵Note that bound states only exist for $Z < 0$ as $\text{Im } k_n$ has to be positive for a wavefunction $\sim \exp(ik_n r)$ vanishing at infinity.

from the exact result. In this case the potential is an attractive Gaussian potential

$$V(r) = V_0 e^{-r^2/R^2}, \quad \text{with } 2m V_0 R^2 = -4. \quad (1.207)$$

at a ("high") energy so that $kR = 4$. The relative difference (1.206) is sensitive for the correct phase of the scattering amplitude whereas the deviation of the cross sections may be misleading. The comparison with the numerically calculated exact partial-wave amplitude³⁶ shows that the eikonal approximation is excellent in forward direction but that the deviations increase systematically with increasing scattering angle. Although it is known that large-angle scattering for a Gaussian potential is particularly difficult to describe, it can be seen that the eikonal approximation is far superior when compared with the 1st and 2nd Born approximation.

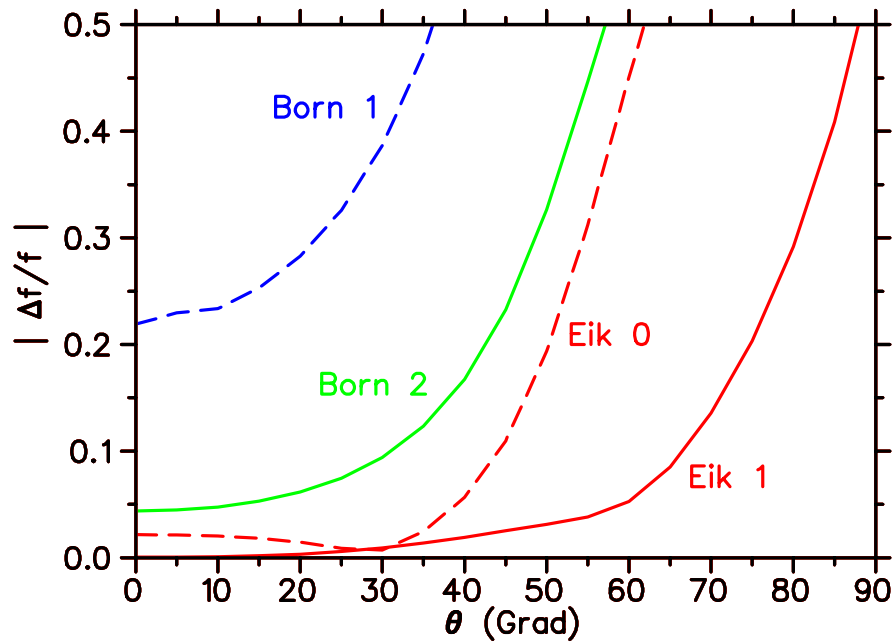


Fig. 6 : Relative deviation (1.206) of several approximations for the scattering amplitude from the exact partial-wave amplitude for scattering from the Gaussian potential (1.207). The 0th-order eikonal approximation (1.183) is denoted by "Eik 0", the 1st-order eikonal approximation (1.191) by "Eik 1". Also depicted are the 1st Born ("Born 1") and the 2nd Born approximation ("Born 2").

The good description of potential scattering by the eikonal approximation is used in the so-called **Glauber theory** to describe high-energy scattering of strongly interacting particles from composite targets (say, nuclei) in terms of the elementary scattering of the projectile from the constituents (in the example: proton and neutron). This turns out to be quite successful although there is actually no good reason to expect that these processes may be adequately described in terms of potential scattering.

³⁶The phase-shift method for central potentials is well explained in {Messiah 1}, ch. 10.

Detail 10: Basics of Glauber Theory

The elimination of the potential is possible because the relation (1.183) is a 2-dimensional Fourier transform which can be inverted

$$\Gamma(\mathbf{b}) := e^{i\chi_0(\mathbf{b})} - 1 = \frac{m}{ik} \int \frac{d^2q}{(2\pi)^2} e^{i\mathbf{q}\cdot\mathbf{b}} T(\mathbf{q}) = \frac{i}{2\pi k} \int d^2q e^{i\mathbf{q}\cdot\mathbf{b}} f(\mathbf{q}). \quad (1.208a)$$

Therefore the "profile function" $\Gamma(\mathbf{b})$ may be obtained directly from (a parametrization of) the scattering amplitude. In the case of nucleon-nucleon scattering at a fixed, high energy this is usually done by writing

$$f(q) = \frac{ik}{4\pi} \sigma_{\text{tot}} (1 - i\rho) e^{-\beta^2 q^2/2}, \quad (1.208b)$$

which has the following parameters: The measured total cross section σ_{tot} (obviously the optical theorem (1.186e) is built in), the ratio ρ of real to imaginary part of the scattering amplitude in forward direction (determinable from interference with the Coulomb scattering amplitude) and the parameter β which describes the fall-off of the differential cross section with momentum transfer. All these parameters are empirical and measurable quantities – and the potential description of the interaction has disappeared! This assumption only comes back into play if we assume that for scattering from a composite object (say, an atomic nucleus) the interaction of the projectile with the A constituents is given by

$$V(\mathbf{r}) = \sum_{i=1}^A V(\mathbf{r} - \mathbf{x}_i), \quad (1.208c)$$

as is customary in non-relativistic many-body physics (see Eq. (2.97)). As the eikonal phase $\chi_0(\mathbf{b})$ in Eq. (1.184) is **linear** in the potential, the profile function for the composite target reads

$$\Gamma(\mathbf{x}_1 \dots \mathbf{x}_A; \mathbf{b}) = \exp \left[i \sum_{i=1}^A \chi_0(\mathbf{b} - \mathbf{x}_i) \right] - 1 = \prod_{i=1}^A [1 + \Gamma(\mathbf{b} - \mathbf{x}_i)] - 1 \quad (1.208d)$$

and the total scattering amplitude at fixed scattering centers \mathbf{x}_i becomes

$$f_{i \rightarrow f}(\mathbf{x}_1 \dots \mathbf{x}_A) = \frac{k}{2\pi i} \int d^2b e^{-i\mathbf{q}\cdot\mathbf{b}} \left\{ \prod_{i=1}^A [1 + \Gamma(\mathbf{b} - \mathbf{x}_i)] - 1 \right\} \quad (1.208e)$$

$$= \frac{k}{2\pi i} \int d^2b e^{-i\mathbf{q}\cdot\mathbf{b}} \left\{ \sum_{i=1}^A \Gamma(\mathbf{b} - \mathbf{x}_i) + \sum_{i>j}^A \Gamma(\mathbf{b} - \mathbf{x}_i) \Gamma(\mathbf{b} - \mathbf{x}_j) + \dots \right\}. \quad (1.208f)$$

In the second line the product has been expanded in powers of the individual profile functions – this gives a (finite) series of **multiple scatterings** from the individual constituents. If, in addition, one assumes that at high energies the target does not change during the ultra-short scattering process ("frozen nucleus approximation"), then the total scattering amplitude simply is the matrix element of Eq. (1.208f) taken between the wave function Ψ_I of the initial target state and the one Ψ_F of the final target state

$$f_{i,I \rightarrow f,F} = \langle \Psi_F | f_{i \rightarrow f}(\mathbf{x}_1 \dots \mathbf{x}_A) | \Psi_I \rangle. \quad (1.208g)$$

For mehr details see, e.g., **{Eisenberg-Koltun}** or **{Scheck}**.

1.7 Green Functions as Path Integrals

Up to now we have discussed the path-integral representation of the time-evolution operators \hat{U} in different formulations. Now we want to consider **Green functions**

$$G_{AB}(t_1, t_2) := \left\langle 0 \left| \mathcal{T} \left[\hat{A}_H(t_1) \hat{B}_H(t_2) \right] \right| 0 \right\rangle \quad (1.209)$$

where $|0\rangle$ is the exact ground state of the system,

$$\hat{A}_H(t) = e^{i\hat{H}t/\hbar} \hat{A}_H(0) e^{-i\hat{H}t/\hbar} \quad (1.210)$$

a quantum mechanical operator in the Heisenberg picture (as is $\hat{B}_H(t)$) and

$$\mathcal{T} \left[\hat{A}_H(t_1) \hat{B}_H(t_2) \right] = \Theta(t_1 - t_2) \hat{A}_H(t_1) \hat{B}_H(t_2) + \Theta(t_2 - t_1) \hat{B}_H(t_2) \hat{A}_H(t_1) \quad (1.211)$$

the time-ordered product of these two operators. Such objects play a central role in many-body physics and in field theory, as it is straight-forward to evaluate them in perturbation theory and all important quantities (ground-state energy, expectation values of operators, S matrix elements) can be calculated from them.

If we insert into the definition (1.209) a complete set of position eigenstates

$$1 = \int dq |q\rangle\langle q| = \int dq e^{i\hat{H}t/\hbar} |q\rangle\langle q| e^{-i\hat{H}t/\hbar}, \quad (1.212)$$

then we obtain

$$G_{AB}(t_1, t_2) = \int dq dq' \langle 0 | e^{i\hat{H}t'/\hbar} |q'\rangle \langle q' | e^{-i\hat{H}t'/\hbar} \mathcal{T} [\hat{A}_H(t_1) \hat{B}_H(t_2)] e^{i\hat{H}t/\hbar} |q\rangle \cdot \langle q | e^{-i\hat{H}t/\hbar} |0\rangle. \quad (1.213)$$

The individual factors in this expression may be rewritten in the following way: The first one

$$\langle 0 | e^{i\hat{H}t'/\hbar} |q'\rangle = e^{iE_0 t'/\hbar} \langle 0 | q'\rangle = e^{iE_0 t'/\hbar} \psi_0^*(q') \quad (1.214)$$

can be expressed by the wave function of the ground state and the ground-state energy – similarly, also the last one.

Therefore we now concentrate on a path-integral representation for the middle factor and first assume that $\hat{A} = \hat{B} = \hat{x}$ and that $t_1 > t_2$. After inserting two complete sets of position eigenstates we then obtain

$$\begin{aligned} \langle q' | e^{-i\hat{H}t'/\hbar} \hat{x}_H(t_1) \hat{x}_H(t_2) e^{i\hat{H}t/\hbar} |q\rangle &= \langle q' | e^{-i\hat{H}(t'-t_1)/\hbar} \hat{x} e^{-i\hat{H}(t_1-t_2)/\hbar} \hat{x} e^{-i\hat{H}(t_2-t)/\hbar} |q\rangle \\ &= \int dq_1 dq_2 q_1 q_2 \langle q' | e^{-i\hat{H}(t'-t_1)/\hbar} |q_1\rangle \langle q_1 | e^{-i\hat{H}(t_1-t_2)/\hbar} |q_2\rangle \langle q_2 | e^{-i\hat{H}(t_2-t)/\hbar} |q\rangle. \end{aligned} \quad (1.215)$$

Now we may use the path-integral representation of the individual time-evolution operators and obtain in the Hamilton formulation

$$\begin{aligned} \langle q' | e^{-i\hat{H}t'/\hbar} \hat{x}_H(t_1) \hat{x}_H(t_2) e^{i\hat{H}t/\hbar} |q\rangle &= \int dq_1 dq_2 q_1 q_2 \int_{x(t_1)=q_1}^{x(t')=q'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_1}^{t'} d\tau [p\dot{x} - H(x, p)] \right\} \\ &\quad \cdot \int_{x(t_2)=q_2}^{x(t_1)=q_1} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_2}^{t_1} d\tau [p\dot{x} - H(x, p)] \right\} \\ &\quad \cdot \int_{x(t)=q}^{x(t_2)=q_2} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_t^{t_2} d\tau [p\dot{x} - H(x, p)] \right\}. \end{aligned} \quad (1.216)$$

Similar as in the proof of the composition law (1.42) we can concentrate the exponents into one exponent and all integrations can be combined into one functional integral if one integrates additionally over the endpoints q_1, q_2 . For $t_1 > t_2$ the result therefore is

$$\begin{aligned} \langle q' | e^{-i\hat{H}t'/\hbar} \mathcal{T} [\hat{x}_H(t_1) \hat{x}_H(t_2)] e^{i\hat{H}t/\hbar} |q\rangle &= \int_{x(t)=q}^{x(t')=q'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} x(t_1)x(t_2) \exp \left\{ \frac{i}{\hbar} \int_t^{t'} d\tau [p\dot{x} - H(x, p)] \right\}. \end{aligned} \quad (1.217)$$

For $t_2 > t_1$, a similar calculation gives the same expression, i.e. the time-ordering operator is **automatically** built into the path-integral representation! This is not quite so surprising as it first seems, since the time ordering is necessary because the Heisenberg operator do not commute at different times – the path integral, however, deals with ordinary numbers. Eq. (1.217) is easily generalized to any operator $\hat{A} = A(\hat{x}, \hat{p})$, $\hat{B} = B(\hat{x}, \hat{p})$ and then reads

$$\begin{aligned} \langle q' | e^{-i\hat{H}t'/\hbar} \mathcal{T} [\hat{A}_H(t_1) \hat{B}_H(t_2)] e^{i\hat{H}t/\hbar} |q\rangle &= \int_{x(t)=q}^{x(t')=q'} \frac{\mathcal{D}'x \mathcal{D}p}{2\pi\hbar} A(p(t_1), x(t_1)) B(p(t_2), x(t_2)) \exp \left\{ \frac{i}{\hbar} S[x(t), p(t)] \right\}. \end{aligned} \quad (1.218)$$

Let us return to the formula (1.213) for the Green function in which we now can insert the result (1.218). However, the appearance of the ground-state wave function $\psi_0(q)$ is unsatisfactory since the exact ground state is unknown in general. We would like to have an expression available in which the ground state is generated at the same time. This is possible by “filtering” out the lowest lying state of the system. Indeed, in an expression of the form

$$\langle q' | e^{-i\hat{H}t'/\hbar} \hat{O} e^{i\hat{H}t/\hbar} | q \rangle = \sum_{n,m} \psi_m(q') e^{-iE_m t'/\hbar} \langle m | \hat{O} | n \rangle e^{iE_n t/\hbar} \psi_n^*(q) \quad (1.219)$$

only the ground state contribution survives if one formally lets approach

$$t \rightarrow i\infty, \quad t' \rightarrow -i\infty \quad (1.220)$$

as is easily seen:

$$\begin{aligned} \langle q' | e^{-i\hat{H}t'/\hbar} \hat{O} e^{i\hat{H}t/\hbar} | q \rangle &\xrightarrow[t' \rightarrow -i\infty]{t \rightarrow i\infty} \psi_0(q') \psi_0^*(q) e^{-E_0(|t|+|t'|)/\hbar} \langle 0 | \hat{O} | 0 \rangle \\ &= \lim_{\substack{t \rightarrow i\infty \\ t' \rightarrow -i\infty}} \langle q' | e^{-i\hat{H}(t'-t)/\hbar} | q \rangle \langle 0 | \hat{O} | 0 \rangle. \end{aligned} \quad (1.221)$$

This is due to the fact that for $n > 0$, $E_n > E_0$, so that the contributions of the excited states decay more rapidly than those from the ground state. If we use Eq. (1.221) for the Green function of the operators \hat{A}, \hat{B} we obtain

$$G_{AB}(t_1, t_2) = \lim_{\substack{t \rightarrow i\infty \\ t' \rightarrow -i\infty}} \frac{\langle q' | e^{-i\hat{H}t'/\hbar} \mathcal{T} [\hat{A}_H(t_1) \hat{B}_H(t_2)] e^{i\hat{H}t/\hbar} | q \rangle}{\langle q' | e^{-i\hat{H}(t'-t)/\hbar} | q \rangle} \quad (1.222)$$

or as path integral

$$G_{AB}(t_1, t_2) = \lim_{\substack{t \rightarrow i\infty \\ t' \rightarrow -i\infty}} \frac{\int \mathcal{D}'x \mathcal{D}p A(x(t_1), p(t_1)) B(x(t_2), p(t_2)) e^{iS[x,p]/\hbar}}{\int \mathcal{D}'x \mathcal{D}p e^{iS[x,p]/\hbar}}. \quad (1.223)$$

Note that in the expression (1.223) all normalization factors cancel! The unphysical limits (1.220) are quite natural for **Euclidean** Green functions where the time t is replaced by $-\tau$ everywhere. Instead of oscillations one has damping everywhere and the path integral is well-defined mathematically. Therefore one frequently investigates Euclidean Green functions and transforms back – if possible – to real time by an analytic continuation. It is clear that in order to project out the ground state by the boundary conditions (1.220) one doesn't necessarily have to go to infinity along the imaginary axis but that it is sufficient to do that along a suitable ray in the complex time plane (see, e.g. ch. 7 in Ref. [19]).

The operators \hat{A}, \hat{B} can be expressed in terms of the fundamental operators \hat{x}, \hat{p} , say by a Taylor expansion. However, it is not necessary that in the matrix element the products of operators \hat{x}, \hat{p} all are taken at the same time: One can define **n-point functions**

$$G(t_1 \dots t_j, t_{j+1} \dots t_n) := \langle 0 | \mathcal{T} [\hat{x}_H(t_1) \dots \hat{x}_H(t_j) \hat{p}_H(t_{j+1}) \dots \hat{p}_H(t_n)] | 0 \rangle \quad (1.224)$$

and write as path integral (in the following we do not indicate the limits anymore explicitly):

$$G(t_1 \dots t_j, t_{j+1} \dots t_n) = \frac{\int \mathcal{D}'x \mathcal{D}p x(t_1) \dots x(t_j) p(t_{j+1}) \dots p(t_n) e^{iS[x,p]/\hbar}}{\int \mathcal{D}'x \mathcal{D}p e^{iS[x,p]/\hbar}}. \quad (1.225)$$

The full set of n -point functions can be obtained from a **generating functional**

$$Z[J, K] = \int \mathcal{D}'x \mathcal{D}p \exp \left\{ \frac{i}{\hbar} S[x, p] + \frac{i}{\hbar} \int dt [J(t)x(t) + K(t)p(t)] \right\} \quad (1.226)$$

by functional differentiation with respect to artificially introduced sources which are set to zero thereafter ³⁷

$$G(t_1 \dots t_j, t_{j+1} \dots t_n) = (-i\hbar)^n \frac{\delta^j}{\delta J(t_1) \dots \delta J(t_j)} \frac{\delta^{n-j}}{\delta K(t_{j+1}) \dots \delta K(t_n)} \frac{Z[J, K]}{Z[0, 0]} \Bigg|_{J=K=0} . \quad (1.227)$$

Detail 11: Generating Functions

The generating functional is a generalization of the notion of a generating function which exists for a multitude of orthogonal polynomials (**{Handbook}**, Table 22.9). For example,

$$g(x, t) = \exp(2xt - t^2) = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \quad (1.228a)$$

is the generating function for the Hermite polynomials $H_n(x)$. Obviously we have

$$H_n(x) = \frac{\partial^n}{\partial t^n} g(x, t) \Big|_{t=0} \quad (1.228b)$$

and it easily is found that $H_0 = 1, H_1 = 2x, H_2 = 4x^2 - 2, H_3 = 8x^3 - 12x, \dots$. Also quite known is the generating function for the Legendre polynomials

$$\frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n, \quad |t|, |x| < 1, \quad (1.228c)$$

which is important for the multipole expansion of the Coulomb potential or the phase-shift method in scattering.

In general the generating functional cannot be evaluated exactly. However, if one can split up the Hamiltonian

$$\hat{H} = \hat{H}_0 + V(\hat{x}, \hat{p}) \quad (1.229)$$

in such a way that the generating functional $Z_0[J, K]$ is known then one can give a closed expression for the full generating functional: First one also splits up the exponent in the path integral as

$$\int dt [p\dot{x} - H_0(x, p) + J(t)x(t) + K(t)p(t)] - \int dt V(x(t), p(t)) \quad (1.230)$$

and then one uses the fact that $x(t)$ can be generated by functional differentiation w.r.t. the source $J(t)$, $p(t)$ by differentiation w.r.t. $K(t)$. With this procedure the exponent of the ‘‘perturbation’’ V can be taken out from the path integral and we obtain the representation

$$\begin{aligned} Z[J, K] &= \int \mathcal{D}'x \mathcal{D}p \exp \left[-\frac{i}{\hbar} \int dt V(x(t), p(t)) \right] \exp \left\{ \frac{i}{\hbar} S_0 + \frac{i}{\hbar} \int dt [J(t)x(t) + K(t)p(t)] \right\} \\ &= \exp \left[-\frac{i}{\hbar} \int dt V \left(\frac{\hbar}{i} \frac{\delta}{\delta J(t)}, \frac{\hbar}{i} \frac{\delta}{\delta K(t)} \right) \right] Z_0[J, K]. \end{aligned} \quad (1.231)$$

Of course, this is only a formal solution and in most cases one has to expand the exponential function in powers of the perturbation in order to perform the functional differentiations. This produces the perturbation series for the generating functional and therefore for alle n -point functions.

³⁷ ‘‘Der Mohr hat seine Arbeit [Schuldigkeit] getan, der Mohr kann gehn’’ – ‘‘The moor has done his obligation, the moor can go’’, in **{Schiller}**, 3. Aufzug, 4. Auftritt .

Examples:

The Hamiltonian for the anharmonic oscillator in one dimension ($m = \hbar = 1$)

$$\hat{H} = \underbrace{\frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{x}^2}_{=H_0} + \lambda\hat{x}^4 \quad (1.232)$$

is a prototype for many similar problems. Indeed Eq. (1.232) can be seen as a ϕ^4 field theory in (0+1) (space + time)-dimensions. Also the Hamiltonian of a non-relativistic many-body system (in “2nd quantization”) has a similar structure.

The free generating functional can be determined easily by completing the square: First, one writes

$$p\dot{x} - \frac{1}{2}p^2 + Kp = -\frac{1}{2}[p - (\dot{x} + K)]^2 + \frac{1}{2}(\dot{x} + K)^2 \quad (1.233)$$

and performs the functional momentum integration which simply gives a constant. The remaining integral is a Gaussian one again:

$$Z_0[J, K] = \text{const.} \int \mathcal{D}x e^{iS_0[x, J, K]} \quad (1.234)$$

with

$$\begin{aligned} S_0[x, J, K] &= \int dt \left[\frac{1}{2}(\dot{x} + K)^2 - \frac{\omega^2}{2}x^2 + Jx \right] \\ &= \int dt \left[\frac{1}{2}x \underbrace{\left(-\frac{\partial^2}{\partial t^2} - \omega^2 \right)}_{:=\mathcal{O}} x + (J - \dot{K})x + \frac{1}{2}K^2 \right] \\ &\equiv \frac{1}{2}(x, \mathcal{O}x) + (J - \dot{K}, x) + \frac{1}{2}(K, K) . \end{aligned} \quad (1.235)$$

Here an integration by parts has been performed in the second line and we have assumed that no boundary terms appear at $t_a = i\infty, t_b = -i\infty$; The third line is a shorthand, e.g. for

$$(x, \mathcal{O}x) := \int dt dt' x(t) \mathcal{O}(t, t') x(t') \quad \text{with} \quad \mathcal{O}(t, t') = \left(-\frac{\partial^2}{\partial t^2} - \omega^2 \right) \delta(t - t') . \quad (1.236)$$

Completing the square another time allows to perform the Gaussian x -integral and gives the result

$$Z_0[J, K] = \text{const.} \exp \left\{ \frac{i}{2}(K, K) - \frac{i}{2}(J - \dot{K}, \mathcal{O}^{-1}, J - \dot{K}) \right\} . \quad (1.237)$$

We now have to evaluate the inverse operator $\mathcal{O}^{-1}(t, t')$. This can be done by Fourier transformation

$$\mathcal{O}^{-1}(t, t') = \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \tilde{\mathcal{O}}^{-1}(E) e^{-iE(t-t')} \quad (1.238)$$

and one obtains an algebraic equation with the solution $\mathcal{O}^{-1}(E) = 1/(E^2 - \omega^2)$.

How to treat the pole at $E = \omega$? The easiest way is to require a damping of the functional integral in the factor

$$e^{iS_0} = \exp \left[-\frac{i}{2} \left(x, \frac{\partial^2}{\partial t^2} + \omega^2, x \right) + \dots \right] \quad (1.239)$$

which leads to Feynman’s prescription

$$\boxed{\omega^2 \longrightarrow \omega^2 - i0^+} \quad (1.240)$$

($i0^+$ is a shorthand for a small, positive imaginary part which is set to zero at the end of the calculation).

Detail 12: Derivation of Feynman's Rule

In some sense, this comes out of the blue and we would better look more carefully into the previous result for the forced harmonic oscillator. First, we notice that the prefactor (1.74) does not matter, because the Green functions are ratios of path integrals. Then we consider the result (1.98) for the classical action with a linear perturbation $e(t) = -J(t)$ and the boundary conditions $x_a = x_b = 0$. These conditions we have already used to perform an integration by parts without troublesome boundary terms (for the current discussion this is just pure convenience – as we shall see below, one could use arbitrary boundary conditions). We now have

$$S_{\text{cl}} = \frac{m}{2 \sin \omega(t_b - t_a)} \left(-\frac{2}{m^2 \omega^2} \right) \int_{t_a}^{t_b} dt J(t) \sin \omega(t_b - t) \int_{t_a}^t dt' J(t') \sin \omega(t' - t_a). \quad (1.241a)$$

Assuming that the perturbation $J(t)$ only acts during the time interval $|t| < \tau$ ($\tau \rightarrow +\infty$) we now make an analytic continuation of initial and final times into the complex time plane

$$t_a = -\tau + i\kappa\tau, \quad t_b = \tau - i\kappa\tau \quad \Longrightarrow \quad e^{-i\hat{H}(t_b - t_a)} = e^{-2\hat{H}\kappa\tau} e^{-2i\hat{H}\tau} \quad (1.241b)$$

with $\kappa > 0$. The integration path in the complex t -plane thus looks as shown in Fig. 7.

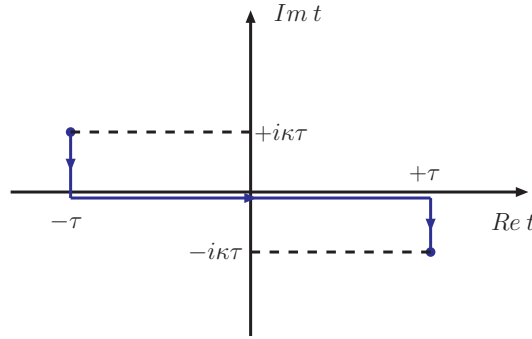


Fig. 7: Deformation of the integration path in the complex t -plane for projecting out the ground state.

However, the trigonometric functions will now increase exponentially

$$\sin \omega(t_b - t_a) \xrightarrow{\tau \rightarrow \infty} \frac{1}{2i} e^{2\omega\kappa\tau} e^{2i\omega\tau}, \quad \sin \omega(t_b - t) \xrightarrow{\tau \rightarrow \infty} \frac{1}{2i} e^{\omega\kappa\tau} e^{i\omega(\tau-t)}, \quad \sin \omega(t' - t_a) \xrightarrow{\tau \rightarrow \infty} \frac{1}{2i} e^{\omega\kappa\tau} e^{i\omega(t'+\tau)}, \quad (1.241c)$$

and the classical action takes the form

$$S_{\text{cl}} \xrightarrow{\tau \rightarrow \infty} \frac{i}{2m\omega} \int_{-\infty}^{+\infty} dt J(t) e^{-i\omega t} \int_{-\infty}^t dt' J(t') e^{i\omega t'} = \frac{i}{4m\omega} \int_{-\infty}^{+\infty} dt dt' J(t) J(t') e^{-i\omega|t-t'|}. \quad (1.241d)$$

The generating functional for the Green function of the harmonic oscillator therefore is (for $m = 1$)

$$Z_0[J] = \text{const.} e^{iS_{\text{cl}}} = \text{const.} \exp \left[-\frac{1}{4\omega} \int_{-\infty}^{+\infty} dt dt' J(t) J(t') e^{-i\omega|t-t'|} \right]. \quad (1.241e)$$

But this is exactly the same result as if we perform the Gaussian integral for the generating functional (disregarding all boundary conditions) and apply Feynman's rule for treating the pole while doing the complex integration:

$$Z_0[J] = \text{const.} \exp \left[-\frac{i}{2} (J, O^{-1} J) \right] = \text{const.} \exp \left\{ -\frac{i}{2} \int_{-\infty}^{+\infty} dt dt' J(t) J(t') \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \exp[-i\omega(t-t')] \frac{1}{E^2 - \omega^2 + i0^+} \right\}. \quad (1.241f)$$

The derivation given above also shows that the boundary terms x_a, x_b are irrelevant: The terms linear in $J(t)$ appearing in Eq. (1.98) do not contribute anything in the limit $\tau \rightarrow \infty$ since they contain only *one* complex time t_a/b and the first, $J(t)$ -independent term indeed makes a (constant) contribution (because it is multiplied by a factor $\cos \omega(t_b - t_a)$) but not for the Green functions after dividing by $Z_0[0]$.

a) Ground-state Energy for the Anharmonic Oscillator

We now concentrate our interest on the special 2-point function

$$\begin{aligned} G_{xx}(E) &:= \int_{-\infty}^{+\infty} dt e^{iEt} \langle 0 | \mathcal{T} [\hat{x}_H(t) \hat{x}_H(0)] | 0 \rangle \\ &= \int_{-\infty}^{+\infty} dt e^{iEt} (-) \frac{\delta^2}{\delta J(t) \delta J(0)} \frac{Z[J, 0]}{Z[0, 0]} \Bigg|_{J=0}, \end{aligned} \quad (1.242)$$

which is also called “single-particle Green function”. This quantity is particularly important because the ground-state energy of the system can be derived from it in the most simple way (see, e.g. **{Fetter-Walecka}**, p. 66 - 68 .):

$$E_0 = \frac{1}{4} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} e^{-i\epsilon E} (\omega^2 + 3E^2) G_{xx}(E), \quad (1.243)$$

Detail 13: Ground-State Energy from the Single-Particle Green Function

This relation is based on the equations of motion $p_H(t) = \dot{x}_H(t)$ and $\dot{p}_H(t) = \ddot{x}_H(t) = -\omega^2 x_H(t) - 4\lambda x_H^3(t)$. From the first one, one obtains

$$\frac{1}{2} \langle 0 | p^2 + \omega^2 x^2 | 0 \rangle = \frac{1}{2} \lim_{t_1, t_2 \rightarrow 0} \left(\frac{\partial^2}{\partial t_1 \partial t_2} + \omega^2 \right) \langle 0 | x_H(t_1) x_H(t_2) | 0 \rangle = \frac{1}{2} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} e^{-iE\epsilon} (E^2 + \omega^2) G_{xx}(E), \quad (1.244a)$$

from the second one after multiplication with $x \equiv x_H(0)$

$$\langle 0 | \lambda x^4 | 0 \rangle = -\frac{1}{4} \lim_{t \rightarrow 0} \left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) \langle 0 | x_H(t) x_H(0) | 0 \rangle = \frac{1}{4} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} e^{-iE\epsilon} (E^2 - \omega^2) G_{xx}(E). \quad (1.244b)$$

Adding both leads to Eq. (1.243).

A simple calculation gives

$$G_{xx}^{(0)}(E) = i \int_{-\infty}^{+\infty} dt e^{iEt} \mathcal{O}^{-1}(t, 0) = i\tilde{\mathcal{O}}^{-1}(E) = \frac{i}{E^2 - \omega^2 + i0^+} \quad (1.245)$$

and therefore the expected result is obtained from Eq. (1.243)

$$E_0^{(0)} = \frac{i}{8\pi} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} dE e^{-i\epsilon E} \frac{3E^2 + \omega^2}{E^2 - \omega^2 + i0^+} = \frac{1}{2}\omega. \quad (1.246)$$

Here the theorem of residues has been used after closing the integration contour in the lower complex E -plane. In first-order perturbation theory we have to expand the exponential function $\exp\left(-i\lambda \int_{-\infty}^{+\infty} dt \delta^4 / \delta J(t)^4\right)$ (see Eq. (1.231)) in the numerator and the denominator of Eq. (1.227), differentiate functionally and perform the Fourier transformation. The result of this – admittingly a bit lengthy – calculation is

$$\begin{aligned} G_{xx}^{(1)}(E) &= G_{xx}^{(0)}(E) - 12i\lambda \left[G_{xx}^{(0)}(E) \right]^2 \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} G_{xx}^{(0)}(E') \\ &= \frac{i}{E^2 - \omega^2 - i0^+} + \frac{6i\lambda}{\omega} \frac{1}{(E^2 - \omega^2 - i0^+)^2}. \end{aligned} \quad (1.247)$$

With that we find for the ground state energy

$$E_0 = \frac{1}{2}\omega + \frac{3i\lambda}{2\omega} \underbrace{\int_{-\infty}^{+\infty} \frac{dE}{2\pi} e^{-i\epsilon E} \frac{\omega^2 + 3E^2}{(E^2 - \omega^2 - i0^+)^2}}_{=-\frac{i}{2\omega}} = \frac{1}{2}\omega + \frac{3\lambda}{4\omega^2}. \quad (1.248)$$

Of course, this is exactly the result which we would obtain in ordinary perturbation theory:

$$\Delta E_0 = \langle 0 | \lambda \hat{x}^4 | 0 \rangle = \lambda \left\langle 0 \left| \left[\frac{1}{\sqrt{2\omega}} (\hat{a} + \hat{a}^\dagger) \right]^4 \right| 0 \right\rangle = \frac{3\lambda}{4\omega^2}. \quad (1.249)$$

b) Structure Function of the Harmonic Oscillator

An important, experimentally measurable quantity is the so-called **structure function** of a bound system (e.g. a proton, a nucleus or a quantum liquid) which can be determined by inelastic scattering of electrons or

neutrons and gives us – as the name implies – information on the structure of the object under investigation. In this (inclusive) process the projectile transfers momentum q and energy ν to the target which gets excited but whose final states are not observed: Only the final energy E_f and the scattering angle Ω_f of the projectile are measured. Therefore, one has to sum **incoherently** over all (energetically accessible) final states $|n\rangle$:

$$\frac{d^2\sigma}{d\Omega_f dE_f} = \left(\frac{d\sigma}{d\Omega_f} \right)_0 \cdot S(q, \nu) \quad (1.250)$$

$$S(q, \nu) = \sum_n \delta(\nu - (E_n - E_0)) \left| \langle 0 | \hat{\mathcal{O}} | n \rangle \right|^2. \quad (1.251)$$

Here the excitation operator essentially is the Fourier transform of the density operator

$$\hat{\mathcal{O}} = e^{-iq \cdot \hat{x}} \quad (1.252)$$

since the elementary interaction is already taken care of by the factor $(d\sigma/d\Omega_f)_0$ (which, e.g., is the Rutherford or Mott cross section in the case of electromagnetic interactions) ³⁸.

The **inelastic** structure function (for which the elastic contribution $n = 0$ is excluded) may be determined by the Green function ³⁹

$$G_{\mathcal{O}\mathcal{O}^\dagger}(T) := \langle 0 | \hat{\mathcal{O}}_H(T) \hat{\mathcal{O}}_H^\dagger(0) | 0 \rangle \quad (1.253)$$

where

$$\hat{\mathcal{O}}_H(T) = e^{i\hat{H}T} e^{-iq \cdot x} e^{-i\hat{H}T} \quad (1.254)$$

is the excitation operator in the Heisenberg picture. Due to the well-known relation

$$\frac{1}{x - x_0 \pm i0^+} = \mathcal{P} \frac{1}{x - x_0} \mp i\pi \delta(x - x_0) \quad (1.255)$$

(\mathcal{P} denotes the principal value) we indeed have for $\nu > 0$

$$S^{\text{inelast.}}(q, \nu) = \frac{1}{\pi} \text{Re} \int_{-\infty}^{+\infty} dT e^{i\nu T} G_{\mathcal{O}\mathcal{O}^\dagger}(T). \quad (1.256)$$

Proof:

Completeness of the final states ($\sum_n |n\rangle \langle n| = 1$) allows to write the Fourier transform of the Green function in Eq. (1.253) as

$$\begin{aligned} \int_{-\infty}^{+\infty} dT e^{i\nu T} G_{\mathcal{O}\mathcal{O}^\dagger}(T) &= \sum_{n=0} \left\{ \int_0^\infty dT e^{iT(\nu - (E_n - E_0) + i0^+)} |\langle 0 | \mathcal{O} | n \rangle|^2 + \int_{-\infty}^0 dT e^{iT(\nu + (E_n - E_0) - i0^+)} |\langle n | \mathcal{O} | 0 \rangle|^2 \right\} \\ &= i \sum_{n=0} \left\{ \frac{|\langle 0 | \hat{\mathcal{O}} | n \rangle|^2}{\nu - (E_n - E_0) + i0^+} + \frac{|\langle n | \hat{\mathcal{O}} | 0 \rangle|^2}{\nu + (E_n - E_0) - i0^+} \right\}. \end{aligned} \quad (1.257a)$$

Applying the relation (1.255) then gives

$$\text{Re} \int_{-\infty}^{+\infty} dT e^{i\nu T} G_{\mathcal{O}\mathcal{O}^\dagger}(T) = \pi \sum_{n=0} \left\{ \left| \langle 0 | \hat{\mathcal{O}} | n \rangle \right|^2 \delta(\nu - (E_n - E_0)) + \left| \langle n | \hat{\mathcal{O}} | 0 \rangle \right|^2 \delta(\nu + (E_n - E_0)) \right\}, \quad (1.257b)$$

which leads to Eq. (1.256) for positive excitation energies. For $\nu > 0^-$ the elastic line is also included

$$\frac{1}{\pi} \text{Re} \int_{-\infty}^{+\infty} dT e^{i\nu T} G_{\mathcal{O}\mathcal{O}^\dagger}(T) = S^{\text{inelast.}}(q, \nu) + 2 F_{00}^2(q) \delta(\nu), \quad (1.257c)$$

³⁸Eq. (1.251) only holds under some simplifying assumptions: The interaction must be weak and scalar or transferred by a single impulse. Velocity-dependent (magnetic) parts and the recoil of the target are neglected, see, e.g. Ref. [20].

³⁹See, e.g., **{Fetter-Walecka}**, eq. 17.13. Note that in this work the so-called **polarisations propagator** $\Pi = -iG$ is used which requires a corresponding modification of Eq. (1.256).

where

$$F_{00}(q) = \langle 0 | \hat{\mathcal{O}} | 0 \rangle \quad (1.257d)$$

is the elastic **form factor**.

This Green function is easily evaluated for the harmonic oscillator:

$$\begin{aligned} G_{\mathcal{O}\mathcal{O}^\dagger}^{\text{h.O.}}(T) &= \int \mathcal{D}x \exp \left\{ i \int_{-\infty}^{+\infty} dt \left[\frac{m}{2} \dot{x}^2(t) - \frac{m}{2} \omega^2 x^2(t) \right] - iq \cdot x(T) + iq \cdot x(0) \right\} \\ &= \int \mathcal{D}x \exp \left\{ i \int_{-\infty}^{+\infty} dt \left[\frac{m}{2} x(t) (-\partial_t^2 - \omega^2 + i0^+) x(t) - b(t) \cdot x(t) \right] \right\}, \end{aligned} \quad (1.258)$$

where we have defined

$$b(t) := q [\delta(t-T) - \delta(t)]. \quad (1.259)$$

Inevitably for problems involving the harmonic oscillator, the functional integral is a Gaussian one giving the result (the normalization is such that $G = 1$ for $q = 0$)

$$\begin{aligned} G_{\mathcal{O}\mathcal{O}^\dagger}^{\text{h.O.}}(T) &= \exp \left[-\frac{i}{2m} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' b(t) \left(t \left| \frac{1}{-\partial_t^2 - \omega^2 + i0^+} \right| t' \right) b(t') \right] \\ &= \exp \left[-i \frac{q^2}{2m} \int_{-\infty}^{+\infty} \frac{dE}{\pi} \frac{1}{E^2 - \omega^2 + i0^+} (1 - \cos(ET)) \right]. \end{aligned} \quad (1.260)$$

The E -integral can be easily calculated by the theorem of residues and one obtains

$$G_{\mathcal{O}\mathcal{O}^\dagger}^{\text{h.O.}}(T) = \exp \left[-\frac{q^2}{2m\omega} \left(1 - e^{-i\omega|T|} \right) \right]. \quad (1.261)$$

Inserted into Eq. (1.256) this gives

$$S^{\text{inelast.h.O.}}(q, \nu) = \exp \left(-\frac{q^2}{2m\omega} \right) \sum_{n=1}^{\infty} \left(\frac{q^2}{2m\omega} \right)^n \frac{1}{n!} \delta(\nu - n\omega). \quad (1.262)$$

The square of the elastic form factor is given by the T -independent part in Eq. (1.260) and reads

$$\left(F_{00}^{\text{h.O.}}(q) \right)^2 = \exp \left[-i \frac{q^2}{2m} \int_{-\infty}^{+\infty} \frac{dE}{\pi} \frac{1}{E^2 - \omega^2 + i0^+} \right] = \exp \left(-\frac{q^2}{2m\omega} \right). \quad (1.263)$$

This supplies exactly the missing ($n = 0$)-contribution in the sum of Eq. (1.262) and agrees with the result which one obtains if one calculates the matrix element $\langle 0 | \mathcal{O} | n \rangle$ in Eq. (1.251) with the explicit wave functions (1.78b) and then incoherently sums over all excited states. It goes without saying that such a calculation is much more involved than the derivation presented here. However, the biggest advantage of Green function methods is that they can easily be extended to many-body and field-theoretical problems.

From Eq. (1.262) one sees that the structure function of a harmonically bound particle consists – as expected – of a collection of δ - functions because the entire spectrum is discrete. In general, however, the interactions in the target are such that also a continuous spectrum exists; then the structure function contains – besides the excitation of individual discrete levels – at large momentum transfer a broad, continuous ”quasi-elastic peak” that corresponds to the knock-out of the bound particle into the continuum. Although the model of the harmonic oscillator is unrealistic (even for confined quarks) Eq. (1.262) also contains this information in terms of the weight which a single δ -functions carries: If $q^2 \gg 2m\omega$, we can estimate the excitation number of maximal strength by using Stirling’s formula (1.130e) and we obtain $n_{max} \simeq q^2/(2m\omega)$, i.e. the strongest excitation occurs at $\nu_{max} \simeq q^2/(2m)$, which exactly is the energy of a particle initially at rest after it has absorbed a momentum q .

1.8 Symmetries and Conservation Laws

From the usual operator formulation of quantum mechanics we know that the time-dependence of an Heisenberg operator is given by

$$\frac{d\hat{A}_H(t)}{dt} = \frac{d}{dt} \left(e^{i\hat{H}t/\hbar} \hat{A} e^{-i\hat{H}t/\hbar} \right) = \frac{i}{\hbar} \left[\hat{H}, \hat{A}_H(t) \right] = \frac{i}{\hbar} e^{i\hat{H}t/\hbar} \left[\hat{H}, \hat{A} \right] e^{-i\hat{H}t/\hbar} \quad (1.264)$$

if the operator \hat{A} does not depend explicitly on time. By that it follows in particular that operators which commute with the Hamiltonian of the system are **conserved**

$$\frac{d\hat{A}_H(t)}{dt} = 0 \quad , \quad \text{if} \quad \left[\hat{H}, \hat{A} \right] = 0 \quad , \quad (1.265)$$

i.e. they don't change during the evolution of the system in time. Since in most cases of interest an exact solution of the equation of motion (1.264) is not possible such constants of motion are of highest importance in quantum physics.

This is also the case in classical physics where **Noether's theorem** links the existence of a conserved quantity to the invariance of the action under a (continuous) symmetry transformation. In the usual proof ⁴⁰ one uses the Euler-Lagrange equations for the system: Let

$$x(t) \longrightarrow x'(t) = x(t) + \alpha \Delta x(t) \quad (1.266)$$

be an infinitesimal transformation of the classical path with a constant parameter α , which leaves the action invariant (up to boundary terms which do not change the equation of motion). This means that the Lagrange function changes at most by a total time derivative:

$$L \longrightarrow L + \alpha \frac{d}{dt} \Lambda(t) \quad (1.267)$$

Here $\Lambda(t)$ is a quantity which can be calculated from the symmetry transformation and the Lagrange function under discussion. However, the change of $L(x, \dot{x})$ can be also calculated from the change of the path

$$\begin{aligned} \alpha \Delta L &= \frac{\partial L}{\partial x} \alpha \Delta x + \frac{\partial L}{\partial \dot{x}} \frac{d}{dt} (\alpha \Delta x) \\ &= \alpha \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \Delta x \right) + \alpha \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right] \Delta x \end{aligned} \quad (1.268)$$

Due to the equation of motion the term in the square bracket vanishes. If we equate the two changes of the Lagrange function then we obtain

$$\frac{d}{dt} j(t) = 0 \quad \text{with} \quad j(t) := \frac{\partial L}{\partial \dot{x}} \Delta x - \Lambda(t) \quad , \quad (1.269)$$

i.e. $j(t)$ is a conserved "current" (the normalization is arbitrary).

Example : Time-Translation Invariance

Consider a particle in a time-independent potential with the Lagrange function $L = m\dot{x}^2/2 - V(x)$. It is obvious that its motion does not depend on the moment when we start counting the time, i.e. we can shift $t \rightarrow t + \alpha$. Infinitesimally this induces the transformation

$$x(t) \longrightarrow x(t) + \alpha \dot{x}(t) \quad , \quad (1.270)$$

under which the Lagrange function changes as

$$\alpha \Delta L = m\dot{x} \alpha \ddot{x} - V'(x) \alpha \dot{x} = \alpha \frac{d}{dt} \left(\frac{m}{2} \dot{x}^2 - V(x) \right) \quad . \quad (1.271)$$

⁴⁰See, e.g. **{Landau-Lifschitz 1}**, ch. 2. This chapter mainly follows **Peskin & Schroeder**, ch. 2.2 and 9.6 .

From Eq. (1.269) we therefore find that

$$j = m\dot{x}\dot{x} - \left(\frac{m}{2}\dot{x}^2 - V(x) \right) = \frac{m}{2}\dot{x}^2 + V(x) = \text{const}_t, \quad (1.272)$$

i.e. the **energy** of the system is conserved due to the homogeneity in time.

How does that come out in the path integral formalism which doesn't know anything about operators or classical equations of motion? To answer this question we will investigate the behavior of the path integral (in the Lagrange form) under the general **time-dependent** transformation

$$x(t) \longrightarrow x'(t) = x(t) + \alpha(t) \Delta x(t). \quad (1.273)$$

We will assume again that the transformation with a constant α is a symmetry transformation, i.e. as in Eq. (1.267) it changes the Lagrangian only by a total derivative. With a time-dependent parameter, however, we now obtain

$$\begin{aligned} L(x, \dot{x}) \longrightarrow L(x + \alpha\Delta x, \dot{x} + \alpha\Delta\dot{x}) + \dot{\alpha}\Delta x &= L(x + \alpha\Delta x, \dot{x} + \alpha\Delta\dot{x}) + \dot{\alpha}\frac{\partial L}{\partial \dot{x}}\Delta x \\ &= \alpha\frac{d}{dt}\Lambda(t) + \dot{\alpha}\frac{\partial L}{\partial \dot{x}}\Delta x, \end{aligned} \quad (1.274)$$

because we have to consider the change in velocity induced by $\alpha(t)$. Of course, the transformation (1.273) is not allowed to change the fixed boundary conditions $x(t_a) = x_a$, $x(t_b) = x_b$ (we recall that there is **no** integration over the boundary points in the path integral) so that we have to require that

$$\alpha(t_a) = \alpha(t_b) = 0. \quad (1.275)$$

As in the classical case we will restrict ourselves to infinitesimal transformations, i.e. in the following we will only consider terms up to order α . Since the path integral does not change we have

$$\int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x e^{iS[x]/\hbar} = \int_{x'(t_a)=x_a}^{x'(t_b)=x_b} \mathcal{D}x' |\mathcal{J}| e^{iS[x'+\alpha\Delta\xi]/\hbar}, \quad (1.276)$$

where

$$\mathcal{J} = \mathcal{D}\text{et}_{t,t'} \left(\frac{\delta x(t)}{\delta x'(t')} \right) \quad (1.277)$$

is the Jacobi determinant of the transformation. Here we will assume that $\mathcal{J} = 1$, i.e. that the "measure" $\mathcal{D}x$ of the path integral is also invariant under the symmetry transformation. If we expand the r.h.s. of Eq. (1.276) up to order α , we therefore obtain

$$\int_{x'(t_a)=x_a}^{x'(t_b)=x_b} \mathcal{D}x' \frac{i}{\hbar} \Delta S[x'] e^{iS[x']/\hbar} = \int_{x'(t_a)=x_a}^{x'(t_b)=x_b} \mathcal{D}x' \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left\{ \alpha(t) \frac{d}{dt} \Lambda(t) + \dot{\alpha}(t) \frac{\partial L}{\partial \dot{x}'} \Delta x' \right\} e^{iS[x']/\hbar} = 0. \quad (1.278)$$

Now we perform an integration by parts in the second term: Due to Eq. (1.275) the boundary terms at $t = t_a$ and $t = t_b$ vanish and we get

$$\int_{t_a}^{t_b} dt \alpha(t) \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \frac{i}{\hbar} \frac{d}{dt} \left\{ \Lambda(t) - \frac{\partial L}{\partial \dot{x}} \Delta x \right\} e^{iS[x]/\hbar} = 0, \quad (1.279)$$

where we again have written $x(t)$ as integration variable in the functional integral. As $\alpha(t)$ is arbitrary the integrand in the curly bracket has to vanish at any time t , i.e.

$$\boxed{\frac{d}{dt} \langle j(t) \rangle := \mathcal{N} \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \frac{d}{dt} \left\{ \frac{\partial L}{\partial \dot{x}} \Delta x - \Lambda(t) \right\} e^{iS[x]/\hbar} = 0} \quad \text{for all } t \quad (1.280)$$

must hold. Here $\mathcal{N}^{-1} = \int \mathcal{D}x \exp(iS[x]/\hbar)$ is the normalization which ensures that $\langle 1 \rangle = 1$.

Example: Space-Translation Invariance

As simplest example we will consider a free particle when its coordinate is shifted by a constant: $x(t) \rightarrow x(t) + \alpha$. Obviously, the Jacobi determinant here is $\mathcal{J} = 1$ and the Lagrange function $m\dot{x}^2/2$ remains unchanged under this transformation. Therefore we have $\Lambda(t) = 0$ and the path-integral version of Noether's theorem (1.280) says, that the momentum

$$P := \langle m\dot{x}(t) \rangle = \text{const}_t \quad (1.281)$$

is conserved.

This we may check by calculating the path integral exactly. The easiest way is to introduce an external force $e(t)$, to differentiate functionally w.r.t. this source and then to switch it off. For that purpose we can use the explicit results obtained in **chapter 1.3**: Since the prefactor in Eq. (1.84) does not depend on $e(t)$, we have to calculate

$$P^{\text{free}} = m e^{-iS_{\text{cl}}/\hbar} \frac{\partial}{\partial t} \left(-\frac{\hbar}{i} \right) \frac{\delta}{\delta e(t)} e^{iS_{\text{cl}}/\hbar} \Big|_{e=0} = -m \frac{\partial}{\partial t} \frac{\delta S_{\text{cl}}}{\delta e(t)} \Big|_{e=0}. \quad (1.282)$$

The classical action of a particle under the influence of a time-dependent force $e(t)$ is obtained from Eq. (1.98) in the limit $\omega \rightarrow 0$:

$$S_{\text{cl}} = \frac{m}{2T} \left[(x_b - x_a)^2 - \frac{2x_b}{m} \int_{t_a}^{t_b} ds e(s) (s - t_a) - \frac{2x_a}{m} \int_{t_a}^{t_b} ds e(s) (t_b - s) + \mathcal{O}(e^2) \right]. \quad (1.283)$$

Differentiation in Eq. (1.282) then gives

$$P^{\text{free}} = m \frac{x_b - x_a}{T}, \quad T \equiv t_b - t_a, \quad (1.284)$$

which, indeed, is independent of the arbitrary time $t \in [t_a, t_b]$ and illustrates the classical result "momentum = mass \times (constant) velocity between a and b ".

A less trivial example is given by a system of two particles (although this rather belongs into **section 2**) interacting via a potential which only depends on their mutual distance:

$$L = \frac{m_1}{2} \dot{x}_1^2 + \frac{m_2}{2} \dot{x}_2^2 - V(x_1 - x_2). \quad (1.285)$$

This system is again translation invariant as the previously considered free particle and therefore Noether's theorem (1.280) (with obvious modifications for several particles) tells us that the total momentum

$$P^{\text{total}} := \langle m_1 \dot{x}_1 + m_2 \dot{x}_2 \rangle = \text{const}_t \quad (1.286)$$

is conserved. However, the quantum dynamics of the system described by Eq. (1.285) is far from being so simple as in the previous example. Fortunately, the path-integral average needed in Eq. (1.286) can be evaluated easily by introducing center-of-mass and relative coordinates

$$R := \frac{m_1 x_1 + m_2 x_2}{M}, \quad r := x_1 - x_2, \quad M \equiv m_1 + m_2. \quad (1.287)$$

It is well-known that the Lagrange function (1.285) then separates into a center-of-mass part $M\dot{R}^2/2$ and a relative part $m_1 m_2 \dot{r}^2 / (2M) - V(r)$, which leads to a factorization of the corresponding path integrals. Because of $m_1 \dot{x}_1 + m_2 \dot{x}_2 = M\dot{R}$ the path integral over the relative coordinate – which, in general, cannot be performed – cancels in the averaging procedure. Therefore we can employ the result for the free particle and obtain

$$P^{\text{total}} = M \frac{R_b - R_a}{T}. \quad (1.288)$$

If the Jacobian contributes, i.e. if the "measure" is not invariant, additional terms appear which are called an **anomaly**: The quantum theory does not have the symmetry of the classical theory. This plays an important role in field theory (see **chapter 3.5**).

1.9 Numerical Treatment of Path Integrals

If neither an exact analytic evaluation of the path integral is possible nor perturbation theory or semi-classical expansions are applicable one has to try to calculate the functional integral numerically. In practice, this is only possible in **Euclidean time** since in real time the oscillations in the integrand are not under control numerically ⁴¹: One changes to **imaginary times**

$$T = -i\beta, \quad t = -i\tau \quad (1.289)$$

and investigates the **partition function**

$$Z(\beta) = \text{tr} \left(e^{-\beta \hat{H}/\hbar} \right). \quad (1.290)$$

We can write down immediately a path-integral representation for the partition function of a particle utilizing the one derived for time-evolution operators. If in

$$\text{tr} \left(\hat{U}(T, 0) \right) = \text{tr} \left(e^{-iT\hat{H}/\hbar} \right) = \int dx \int_{x(0)=x}^{x(T)=x} \mathcal{D}x \exp \left[\frac{i}{\hbar} \int_0^T dt \left(\frac{m}{2} \dot{x}^2 - V(x) \right) \right] \quad (1.291)$$

we perform the transformation (1.289), then we obtain the required result

$$Z(\beta) = \int dx \int_{x(0)=x}^{x(\beta)=x} \mathcal{D}x \exp \left[-\frac{1}{\hbar} \int_0^\beta d\tau \left(\frac{m}{2} \dot{x}^2 + V(x) \right) \right] \equiv \oint_{x(0)=x(\beta)} \mathcal{D}x e^{-S_E[x]/\hbar}. \quad (1.292)$$

Here

$$S_E[x] = \int_0^\beta d\tau \left[\frac{m}{2} \dot{x}^2 + V(x) \right] \quad (1.293)$$

is the **Euclidean action** ⁴². Notice the change of sign in Eq. (1.293) between kinetic and potential energy compared to the normal action!

Similar as the ground state is projected out in the expression for the Green function the **ground-state energy** of the system $E_0 = \langle 0 | \hat{H} | 0 \rangle$ can be filtered out from the partition function by considering large Euclidean times:

$$\begin{aligned} E_0 &= \lim_{\beta \rightarrow \infty} \frac{\text{tr} \left(\hat{H} e^{-\beta \hat{H}/\hbar} \right)}{\text{tr} \left(e^{-\beta \hat{H}/\hbar} \right)} = \lim_{\beta \rightarrow \infty} \frac{E_0 e^{-\beta E_0/\hbar} + E_1 e^{-\beta E_1/\hbar} + \dots}{e^{-\beta E_0/\hbar} + e^{-\beta E_1/\hbar} + \dots} \\ &= \lim_{\beta \rightarrow \infty} \left[-\hbar \frac{\partial}{\partial \beta} \ln Z \right]. \end{aligned} \quad (1.294)$$

If we consider the discretized form of the path integral (1.292)

$$Z = \lim_{N \rightarrow \infty} A_\epsilon^N \int dx_0 \dots dx_{N-1} \exp \left[-S_E(x_0 \dots x_N)/\hbar \right] \quad (1.295)$$

⁴¹There are some attempts to treat path integrals numerically in real time, e.g. in Ref. [21].

⁴²The name derives from the fact that this transformation changes the relativistic indefinite metric into a four-dimensional Euclidean one: $x_\mu x^\mu = c^2 t^2 - \mathbf{x}^2 = -(\mathbf{x}^2 + c^2 \tau^2)$.

with $x_0 = x_N$, $A_\epsilon = [m/(2\pi\epsilon\hbar)]^{1/2}$ and

$$S_E(x_0 \dots x_N) = \epsilon \sum_{j=1}^N \left[\frac{m}{2} \left(\frac{x_j - x_{j-1}}{\epsilon} \right)^2 + V(x_j) \right] \quad (1.296)$$

then we obtain

$$E_0 = \lim_{\substack{N \rightarrow \infty \\ \epsilon \rightarrow 0}} \frac{\int dx_0 \dots dx_{N-1} \frac{1}{N} \sum_{j=1}^N \left[\frac{m}{2} \left(\frac{x_j - x_{j-1}}{\epsilon} \right)^2 + V(x_j) - \frac{\hbar}{2\epsilon} \right] \exp(-S_E/\hbar)}{\int dx_0 \dots dx_{N-1} \exp(-S_E/\hbar)}. \quad (1.297)$$

This is not well suited for numerical purposes because terms inverse in ϵ have to cancel to produce a finite result in the limit $\epsilon \rightarrow 0$. As can be seen the culprit is the operator of the kinetic energy which is non-local and causes these difficulties when taking expectation values.

One can circumvent this difficulty by using the **virial theorem** ⁴³

$$\left\langle 0 \left| \frac{\hat{p}^2}{2m} \right| 0 \right\rangle = \frac{1}{2} \langle 0 | \hat{x} V'(\hat{x}) | 0 \rangle. \quad (1.298)$$

By this we obtain

$$\begin{aligned} E_0 &= \lim_{\substack{N \rightarrow \infty \\ \epsilon \rightarrow 0}} \frac{\int dx_0 \dots dx_{N-1} \frac{1}{N} \sum_{j=1}^N \left[\frac{1}{2} x_j V'(x_j) + V(x_j) \right] \exp(-S_E/\hbar)}{\int dx_0 \dots dx_{N-1} \exp(-S_E/\hbar)} \\ &\equiv \left\langle \frac{1}{N} \sum_{j=1}^N \left[\frac{1}{2} x_j V'(x_j) + V(x_j) \right] \right\rangle. \end{aligned} \quad (1.299)$$

Excitation energies can be obtained from the euclidean Green functions (also called correlation functions) if the expectation value of the corresponding operator vanishes in the ground state

$$\begin{aligned} G_{AA}(t = -i\beta) &= \sum_n \left| \langle 0 | \hat{A} | n \rangle \right|^2 e^{-(E_n - E_0)\beta/\hbar} \\ &\xrightarrow{\beta \rightarrow \infty} \underbrace{\left| \langle 0 | \hat{A} | 0 \rangle \right|^2}_{=0} + \left| \langle 0 | \hat{A} | 1 \rangle \right|^2 e^{-(E_1 - E_0)\beta/\hbar} \dots \end{aligned} \quad (1.300)$$

In other words, the correlation functions fall off exponentially in Euclidean time and their decay constant is determined by the excitation energy of the first state which has an overlap with the ground state by means of the operator \hat{A} . For the numerical calculation it is crucial that the expectation value of the operator in the ground state vanishes *exactly* because any contribution of the first term in Eq. (1.300), no matter how small, would overwhelm the exponentially vanishing signal of the excited state.

The simplest operator whose expectation value vanishes in the ground state due to the parity selection rule, is $\hat{A} = \hat{x}$. Thus we have, for example

$$E_1 - E_0 = \lim_{\beta \rightarrow \infty} \left\{ -\frac{\hbar}{\beta} \ln \frac{\int \mathcal{D}x x(\beta)x(0) \exp[-S_E/\hbar]}{\int \mathcal{D}x \exp[-S_E/\hbar]} \right\} \quad (1.301)$$

and the corresponding discrete form can be used for a numerical analysis. In the 3-dimensional case, for instance, the lowest-lying state for a given angular momentum ℓ can be projected out by the operator $\hat{A} = Y_{\ell 0}(\hat{r})$.

Similarly one proceeds in field theory in which the particles are considered as excitations above a "vacuum" whose energy is set to $E_0 = 0$. For example, in Quantum Chromo Dynamics (to be discussed in greater detail

⁴³Proof: Evaluate the commutator $[\hat{x}\hat{p}, \hat{p}^2/(2m) + V(\hat{x})]$ and take the ground-state expectation value on both sides.

in **section 3**) the operator $\hat{A} = \bar{\psi}\gamma_5\psi$, where ψ are suitable quark field operators connects the vacuum with the pion, the lowest pseudoscalar state. In this way, one can (in principle) determine the masses of the lowest-lying hadrons numerically from the fundamental field theory (more on this in **chapter 3.6**).

Up to now we only have discussed the formal tools to extract energies or masses from the Euclidean path integral. How does one calculate in reality those functional integrals numerically? Let's take again as a concrete example the case of a particle moving in one dimension under the influence of a given potential. In order to get the ground-state energy we see from Eq. (1.299) that we have to evaluate a N -dimensional integral numerically and that N has to be very large. Direct integration by means of methods for one- or low-dimensional integrals (for example Simpson's rule or Gaussian integration) is clearly not feasible as the required computing time would increase like (integration points) ^{N} , a feature sometimes called "the curse of dimensions". Fortunately, one can use statistical (stochastic) methods which depend much less on the dimensions of the integrals. However, such **Monte-Carlo methods** have the disadvantage that the accuracy of the result only increases like the square root of the number of "thrown dices". Nevertheless, at present they are the only methods to treat high-dimensional integrals (like the discretized path integral).

If, for example, one wants to evaluate the one-dimensional integral

$$I = \int_0^1 dx f(x) \quad (1.302)$$

over an arbitrary function $f(x)$ by "rolling the dices", one simply generates M uniformly distributed random numbers $x_i \in [0, 1]$ and takes the average

$$I \simeq \frac{1}{M} \sum_{i=1}^M f(x_i) \equiv \bar{f}. \quad (1.303)$$

The error made by this procedure can be estimated by

$$(\Delta I)^2 = \frac{1}{M} \left[\frac{1}{M} \sum_{i=1}^M f^2(x_i) - \left(\frac{1}{M} \sum_{i=1}^M f(x_i) \right)^2 \right] \equiv \frac{1}{M} [\overline{f^2} - (\bar{f})^2]. \quad (1.304)$$

This is not very effective and a simple improvement is obtained by rolling the dice more specifically, i.e by using "**importance sampling**": Let $w(x) > 0$ be a weight function which essentially mimicks the behaviour of the function $f(x)$. Then we write

$$I = \int_0^1 dx \frac{f(x)}{w(x)} w(x) \quad (1.305)$$

and the transformation

$$y(x) = \int_0^x dz w(z) \quad \Rightarrow \quad dy = w(x)dx \quad (1.306)$$

has the effect that in the integral

$$I = \int_0^{y(1)} dy \frac{f(x(y))}{w(x(y))} \quad (1.307)$$

the integrand varies much less. If

$$y(1) = \int_0^1 dz w(z) = 1 \quad (1.308)$$

then we can calculate immediately

$$I \simeq \frac{1}{M} \sum_{i=1}^M \frac{f(x(y_i))}{w(x(y_i))} \quad (1.309)$$

where $y_i \in [0, 1]$ are uniformly distributed random numbers. $x_i = x(y_i)$ are now the integration points weighted by the function $w(x)$, i.e. they are more concentrated at those points where $w(x) \simeq f(x)$ is large. The disadvantage of this method is that an inversion $x(y)$ is needed.

There exist methods to generate weighted integration points x_i *without* inversion. As the most prominent (and oldest) we now discuss the **Metropolis method** although it is - as may be expected - not the most efficient method anymore. In general, one starts with an arbitrary point x_0 in the region of integration and generates a new one x_1 by a specific algorithm, from that a new one etc.

$$x_0 \rightarrow x_1 \rightarrow x_2 \rightarrow \dots \quad (1.310)$$

This is called a "random walk" through the integration region. The Metropolis algorithm chooses a new point, for example by the scheme

$$x_t = x_n + \delta \cdot (z_1 - 0.5) , \quad (1.311)$$

where δ is a given interval and z_1 a uniformly distributed random number between 0 and 1. Then one forms the ratio

$$r = \frac{w(x_t)}{w(x_n)} \quad (1.312)$$

and accepts the new point x_t according to the following criteria

- a) if $r > 1$ then one sets $x_{n+1} = x_t$,
- b) if $r < 1$ then x_t is accepted with probability r , otherwise $x_{n+1} = x_n$ remains. In practice, this is done by generating a second, uniformly distributed random number $z_2 \in [0, 1]$ and by setting $x_{n+1} = x_t$, if $z_2 < r$, but $x_{n+1} = x_n$ if $z_2 > r$.

Assertion : If n becomes large, then the distribution of points generated in such a way approaches more and more accurately the one weighted by $w(x)$.

Proofs : Consider a large collection of "random walks" with density $N_n(x)$ in the n^{th} step. At the $(n + 1)^{\text{th}}$ step the net effect is

$$\Delta N_n(x, y) = N_n(x) P(x \rightarrow y) - N_n(y) P(y \rightarrow x) , \quad (1.313)$$

where $P(x \rightarrow y)$ is the transition probability from x to y . If

$$\frac{N_n(x)}{N_n(y)} = \frac{P(x \rightarrow y)}{P(y \rightarrow x)} = \frac{N(x)}{N(y)} \quad (1.314)$$

then there will be an equilibrium. In the Metropolis algorithm the probability that a move is made from x to y is given by

$$P(x \rightarrow y) = T(x \rightarrow y) A(x \rightarrow y) \quad (1.315)$$

where $A(x \rightarrow y)$ is the probability of acceptance and $T(x \rightarrow y)$ the probability that a move leads from x to y . It is crucial that in the prescription of Eq. (1.311) to generate the point x_t the probability to move from y to x is equally large ("**detailed balance**"):

$$T(x \rightarrow y) = T(y \rightarrow x) \quad \Rightarrow \quad \frac{N_n(x)}{N_n(y)} = \frac{A(y \rightarrow x)}{A(x \rightarrow y)} . \quad (1.316)$$

We now distinguish two cases:

a) $w(x) > w(y)$; then $A(y \rightarrow x) = 1$ since $r > 1$ and $A(x \rightarrow y) = r = w(y)/w(x)$. From this it follows that

$$\frac{N(x)}{N(y)} = \frac{1}{w(y)/w(x)} = \frac{w(x)}{w(y)}. \quad (1.317)$$

b) $w(x) < w(y)$; then $A(y \rightarrow x) = w(x)/w(y)$ and $A(x \rightarrow y) = 1$ since $r > 1$. Again Eq. (1.317) follows.

In both cases we therefore have the desired result that the equilibrium distribution of the "random walks" generated by the Metropolis-Algorithmus is proportional to the weight function $w(x)$.

Detail 14: Ground-State Energy of the Anharmonic Oscillator by Monte-Carlo Methods and FORTRAN Program

From Eq. (1.299) we obtain for the potential $V(x) = m\omega^2 x^2/2 + \lambda x^4$

$$E_0 = \lim_{\substack{N \rightarrow \infty \\ \epsilon \rightarrow 0}} \left\langle \frac{1}{N} \sum_{i=1}^N [x_i^2 + 3\lambda x_i^4] \right\rangle, \quad (1.318a)$$

with the weight function

$$w(\mathbf{x}) = \frac{e^{-S_E(\mathbf{x})}}{\int dx_0 \dots dx_{N-1} e^{-S_E(\mathbf{x})}}, \quad \mathbf{x} = (x_0 \dots x_{N-1}) \quad (1.318b)$$

$$S_E(\mathbf{x}) = \sum_{i=1}^N \left[\frac{(x_i - x_{i-1})^2}{2\epsilon} + \frac{\epsilon}{2} x_i^2 + \epsilon \lambda x_i^4 \right]. \quad (1.318c)$$

It fulfills all requirements: $w > 0$, $\int dx_0 \dots dx_{N-1} w(\mathbf{x}) = 1$. According to the Metropolis algorithm one has to calculate

$$r = \frac{w(\mathbf{x}_t)}{w(\mathbf{x})} = \exp[-(S_E(\mathbf{x}_t) - S_E(\mathbf{x}))] = e^{-\Delta S_E}. \quad (1.318d)$$

This change of action is only made at a single point of the "time lattice"; then one doesn't have to evaluate the full action but only

$$\begin{aligned} \Delta S_E &= S_E[\dots x_i^{\text{neu}} \dots] - S_E[\dots x_i^{\text{alt}} \dots] = (x_i^{\text{neu}} - x_i^{\text{alt}}) \\ &\cdot \left\{ \left[\frac{1}{\epsilon} + \frac{\epsilon}{2} + \epsilon \lambda (x_i^{\text{neu}2} + x_i^{\text{alt}2}) \right] (x_i^{\text{neu}} + x_i^{\text{alt}}) - \frac{1}{\epsilon} (x_{i+1}^{\text{alt}} + x_{i-1}^{\text{alt}}) \right\}, \end{aligned} \quad (1.318e)$$

where one has to take $i = 0, \dots, N-1$, $x_{-1} \equiv x_{N-1}$, $x_N = x_0$.

A simple FORTRAN program which performs this algorithm is given in the following. It only serves for illustration and is not really up to professional rules – both for the statistical analysis as well for the random number generator⁴⁴ – even for this simple quantum mechanical example.

```

C
C Calculates the ground-state energy of the anharmonic oscillator
C by the Metropolis method for the Euclidean path integral
C
C Units : h bar = m = omega = 1
C
C Parameter : ALA      = lambda (anharmonicity)
C              EPS      = time step
C              N         = number of (time) lattice points
C              NTH       = number of thermalisation sweeps
C              NHIT      = number of additional Monte-Carlo trials
C                      at each lattice point
C              NSWEEP    = total number of sweeps
C              NMESS     = number of sweeps after which a measurement is made
C              DELTA     = max. increase of x at each lattice point
C
      DOUBLE PRECISION DSEED
      DIMENSION X(-1:200)
      WRITE(*,*) 'Eingabe: ala,eps,n,nth,nhit,nsweep,nmess,delta'
      READ(5,*) ALA, EPS, N, NTH, NHIT, NSWEEP, NMESS, DELTA
      WRITE(6,1) ALA, EPS, N, NTH, NHIT, NSWEEP, NMESS, DELTA
1  FORMAT(/'   lambda = ',F6.2,2X,' EPS = ',F6.2,2X,' N = ',I3,2X,
&         ' NTH = ',I4,2X,' NHIT = ',I2// ' NSWEEP = ',I7,2X,' NMESS = ',
&         I4,2X,' DELTA = ',F6.3/)

```

⁴⁴Linear congruent generator: $X_{j+1} = aX_j + b \pmod{c}$, $z_j = X_j/c$ with $a = 7^5$, $b = 0$, $c = 2^{31} - 1$. For a more detailed discussion see, e.g. {Num. Recipes}, ch. 7.

```

C
  DSEED = 3.72D2
  WRITE(6,2) DSEED
2  FORMAT(/' SEED =',D15.8//)
C
C auxiliary calculations
C
  HILF = 1./EPS
  HELF= HILF + 0.5*EPS
  HALF = ALA*EPS
  N1 = N - 1
C
C setting of initial values
C
  NACC = 0
  SUM1 = 0.
  SUM2 = 0.
  DO 10 I = -1,N
10  X(I) = 0.5
C
C Sweep
C
  WRITE(6,5)
5  FORMAT(/' sweep',5x,'energy',4x,'mean energy',5x,'error',
& 5x,'acceptance'//)
  DO 20 I =1,NSWEEP
    DO 30 K = 0,N1
      DO 35 M = 1,NHIT
        Z = ZUFALL(DSEED)
        XT = X(K) + DELTA*(Z-0.5)
C
C change of action
C
        DS = HALF*(XT*XT + X(K)*X(K))
        DS = (HELF + DS)*(XT+X(K))
        DS = DS - HILF*(X(K-1) + X(K+1))
        DS = (XT - X(K))*DS
C
C Metropolis test
C
        IF(DS .GE. 0.) THEN
          R = EXP(-DS)
          Z = ZUFALL(DSEED)
          IF(Z .GT. R) GO TO 35
        ENDIF
        X(K) = XT
        NACC = NACC + 1
35  CONTINUE
        IF(K .EQ. 0) X(N) = X(0)
        IF(K .EQ. N1) X(-1) = X(N1)
30  CONTINUE
        IF(I .LE. NTH) GO TO 20
C
C measurement
C
        II = I - NTH
        IC = II/NMESS
        IF(NMESS*IC .NE. II) GO TO 20
        E = 0.
        DO 25 K = 0,N1
25  E = E + X(K)*X(K) + 3.*ALA*X(K)**4
        E = E/N
        SUM1 = SUM1 + E
        SUM2 = SUM2 + E*E
        EM = SUM1/IC
        EMM = SUM2/IC
        DE = SQRT((EMM-EM*EM)/IC)
        ACC = FLOAT(NACC)/(I*N*NHIT)
C
C print out
C
        WRITE(6,3) II,E,EM,DE,ACC
3  FORMAT(I8,4(3X,F10.4))
20  CONTINUE
    STOP
    END

C+++++ subprogram ZUFALL +++++
      FUNCTION ZUFALL(DSEED)
C
C generates uniformly distributed random numbers in the interval [0,1]
C
      DOUBLE PRECISION DSEED,A,C
      DATA A,C /16807.DO,2147483647.DO/
      DSEED = DMOD(A*DSEED,C)
      ZUFALL = DSEED/C
      RETURN
      END

```

With this program we produce a new x_i -value at any point of the "time lattice" and then calculate the change in the action. According to the Metropolis method the new value is then accepted or not. It is crucial for the correct description of quantum fluctuations that also configurations with a larger action as the foregoing ones have to be accepted with a certain probability, otherwise one would end up inevitably in the state of deepest Euclidean action (= energy), i.e. in the classical ground state. Once one has gone through the lattice one has performed a "sweep". Since the random walk is not completely random (the new points generated are more or less in the neighborhood of the old ones) one rolls the dice several times at each point of the lattice (NHIT = 3 in our example), before moving on and calculates the ground-state energy after each "sweep". The δ -parameter is adjusted so that approximately 50% of all trials are accepted; with too small δ more is accepted but one remains too close to the old configuration; at large δ one indeed has more independent configurations, but most have such a large action that they are not accepted. The time step ϵ should be small compared to the period of oscillation ($2\pi/\omega = 2\pi$ for the pure harmonic oscillator) and N should be so large that the first excited state is sufficiently suppressed, that is, $\exp(-\hbar(E_1 - E_0)N\epsilon) = \exp(-N\epsilon) \ll 1$ for the pure harmonic oscillator.

Initially all x_i -values are set arbitrarily to the fixed value $x_i = 0.5$ – this is called a "cold start" (as the system in Euclidean time is equivalent to a statistical system at a given temperature, a thermodynamic nomenclature is frequently used: At low temperatures all spins in a spin system point in the same direction). A "hot start" would have the x_i -values randomly distributed at the beginning. Of course, the result of the calculation must be independent from the initial preparations. Therefore one disregards the first NTH (= 1000 in our example) "sweeps" until "thermalisation" has been achieved and after NMESS (= 500 in the example) "sweeps" one then "measures" the ground state energy. For example, for $\lambda = 0$ (i.e. the harmonic oscillator) one obtains the following printout

```
lambda = 0.00  EPS = 0.10  N = 100  NTH = 1000  NHIT = 3
NSWEEP = 110000  NMESS = 500  DELTA = 1.300
SEED = 0.37200000D+03
```

sweep	energy	mean energy	error	acceptance
500	0.5407	0.5407	0.0000	0.5045
1000	0.3529	0.4468	0.0664	0.5039
1500	0.2990	0.3976	0.0598	0.5037
2000	0.2488	0.3604	0.0552	0.5037
2500	0.4176	0.3718	0.0454	0.5037
3000	0.4441	0.3839	0.0394	0.5033
3500	0.5483	0.4073	0.0401	0.5035
4000	0.4838	0.4169	0.0362	0.5033
4500	0.4182	0.4171	0.0322	0.5033
5000	0.5140	0.4267	0.0304	0.5032
5500	0.4527	0.4291	0.0277	0.5033
6000	0.1740	0.4078	0.0326	0.5031
6500	1.0234	0.4552	0.0545	0.5030
7000	0.3397	0.4469	0.0513	0.5031
7500	0.8015	0.4706	0.0530	0.5031
8000	0.4014	0.4663	0.0499	0.5030
8500	0.6237	0.4755	0.0478	0.5031
9000	0.3360	0.4678	0.0458	0.5030
9500	0.4740	0.4681	0.0434	0.5031
10000	0.5682	0.4731	0.0415	0.5031

i.e. after 10000 sweeps one obtains

$$E_0^{\text{h.o.}} = 0.473 \pm 0.042, \quad (1.318\text{f})$$

in good agreement with the exact value $E_0 = 0.5$. As already mentioned the error estimate is much too naive and should take into account the correlations which obviously still exist between the different configurations (see the printout).

For the anharmonic case we obtain with the same stochastic parameters the values collected in Table 1:

λ	perturbation theory	Monte-Carlo	exact
0.	0.50	0.473 ± 0.042	0.500000
1.	1.25	0.809 ± 0.067	0.803771
10.	8.00	1.386 ± 0.122	1.504972

Tab. 1 : Ground-state energy of the anharmonic oscillator for several values of the anharmonicity parameter λ . The column titled "perturbation theory" gives the values obtained in 1st order perturbation theory (see Eq. (1.248)), the column "Monte-Carlo" the results of the stochastic calculation and the last column the exact values (see, e.g. Ref. [22]).

As one can see the stochastic calculation of the ground-state energy even works well for large anharmonicities while 1st-order perturbation theory fails completely as expected. There is no much help when including higher terms of the perturbative series since this is an asymptotic (i.e. in the mathematical sense divergent) series.

1.10 Tunneling and Instanton Solutions

Again we are considering the anharmonic oscillator with the potential

$$V(x) = V_0 + \frac{m}{2}\Omega^2 x^2 + \lambda x^4, \quad (1.319)$$

but this time for $\Omega^2 < 0$. In this "double-well potential" (see Fig. 8) new effects arise by the fact that there are two degenerate minima of the potential lying at

$$x_{\pm} = \pm \sqrt{-\frac{m\Omega^2}{4\lambda}} =: \pm a \quad (1.320)$$

For convenience we choose V_0 such that $V(x_{\pm}) = V_0 - m^2\Omega^4/(16\lambda) = 0$ – this we can do as a constant term in the potential does not have any influence on the dynamics of the system but only fixes the scale of the energy. By this choice the potential becomes

$$V(x) = -\frac{m\Omega^2}{4a^2} (x^2 - a^2)^2 =: \frac{m\omega^2}{8a^2} (x - a)^2 (x + a)^2, \quad \omega^2 = -2\Omega^2. \quad (1.321)$$

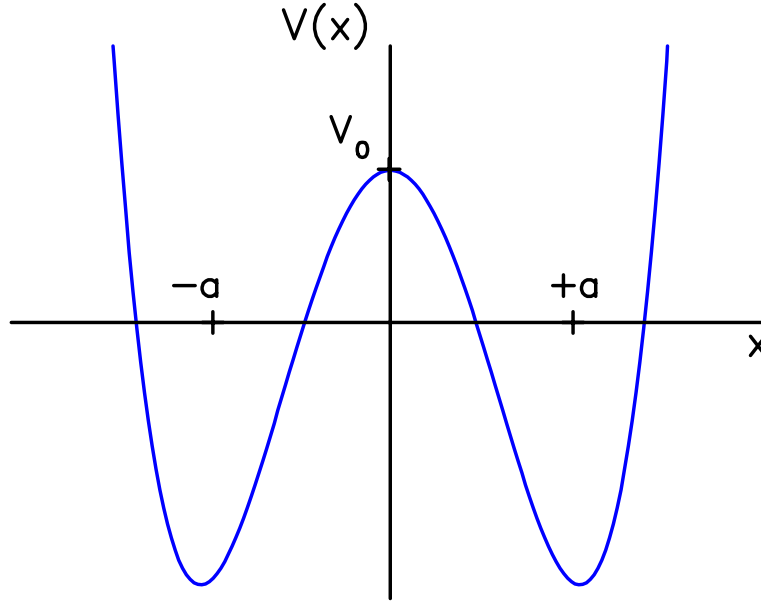


Fig. 8 : Double-well potential.

In the vicinity of $x = \pm a$ we have approximately an oscillator potential

$$V(x) \xrightarrow{x \rightarrow \pm a} \frac{m\omega^2}{2} (x \mp a)^2 \quad (1.322)$$

and therefore we obtain for the case of far-away minima separated by high barriers approximately as ground-state energy

$$E_0 \simeq \frac{1}{2} \hbar\omega. \quad (1.323)$$

The corresponding ground-state wave functions are superpositions of the ground-state wave functions of the oscillators localized at $x = \pm a$

$$\psi_0(x) \simeq \frac{1}{\sqrt{2}} \left[\phi_0(x - a) \pm \phi_0(x + a) \right]. \quad (1.324)$$

This is because in quantum mechanics the wave functions must exhibit the symmetry of the Hamiltonian (there is no "spontaneous symmetry breaking"). Here this means that one can classify the wave functions according to their behaviour under parity transformations (the Hamiltonian is invariant under $x \rightarrow -x$); obviously Eq. (1.324) describes wave functions of positive and negative parity which are degenerate in energy.

Since for $\lambda \neq 0$ the barrier at $x = 0$

$$V(0) = \frac{m\omega^2}{8}a^2 = \frac{m^2\Omega^4}{16\lambda} \quad (1.325)$$

is not infinitely high (and thick) the particle can "tunnel" through the wall and lift the degeneracy: We expect an energy splitting between the state with positive parity (which is the lowest-lying state) and the state of negative parity. This energy splitting can be calculated for small anharmonicities by semi-classical methods – best in the path-integral formalism (and not in the usual WKB approximation for Schrödinger's equation) because this can be extended with not too much effort to systems with many, even infinite many degrees of freedom.

Therefore we consider the matrix element of the **Euclidean** time-evolution operator which brings the particle from the minimum at $x = -a$ to the minimum at $x = +a$

$$\begin{aligned} U\left(a, \frac{\beta}{2}; -a, -\frac{\beta}{2}\right) &\equiv \langle +a | e^{-\beta\hat{H}/\hbar} | -a \rangle = \sum_n \psi_n(a)\psi_n(-a) e^{-\beta E_n/\hbar} \\ &= \int_{x(-\beta/2)=-a}^{x(\beta/2)=+a} \mathcal{D}x e^{-S_E[x]/\hbar} \end{aligned} \quad (1.326)$$

$$\xrightarrow{\beta \rightarrow \infty} \psi_0(a)\psi_0(-a)e^{-\beta E_0/\hbar} + \psi_1(a)\psi_1(-a)e^{-\beta E_1/\hbar} + \dots \quad (1.327)$$

Thus we can determine both the ground-state energy as well as the energy of the first excited state from the behaviour of the time-evolution operators at large Euclidean times. Moreover, the sign of $\psi_0(a)\psi_0(-a) = \pm|\psi_0(a)|^2$ tells us which parity state is the lowest.

We will proceed in several steps:

(i) Determine the classical path

In the semi-classical approximation we first determine the path which makes the action stationary. Since we are working in Euclidean time this is a path in the **inverted** potential (see Fig. 9):

$$\frac{\delta S_E[x]}{\delta x(\tau)} = 0 \implies m \frac{d^2 x_{cl}}{d\tau^2} - V'(x_{cl}) = 0, \quad \text{with } x_{cl}(-\beta/2) = -a, x_{cl}(\beta/2) = +a. \quad (1.328)$$

From the path-integral representation (1.326) of the Euclidean time-evolution operator it follows that those paths determine the ground-state energy in the limit $\beta \rightarrow \infty$ which have an Euclidean action as low as possible. Since $V(x) \geq 0$ we have

$$S_E[x] = \int_{-\beta/2}^{+\beta/2} d\tau \left[\frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right] \geq \int_{-\beta/2}^{+\beta/2} d\tau \frac{m}{2} \left(\frac{dx}{d\tau} \right)^2, \quad (1.329)$$

and therefore all paths whose speed is finite at $\tau = \pm\beta/2$ will give an infinite Euclidean action for $\beta \rightarrow \infty$. Only that path which reaches the points $\pm a$ with zero velocity at $\tau \rightarrow \infty$ is excluded from this, i.e. a trajectory with Euclidean "energy" = 0 where the particle "crawls" up and down the hills in the inverted

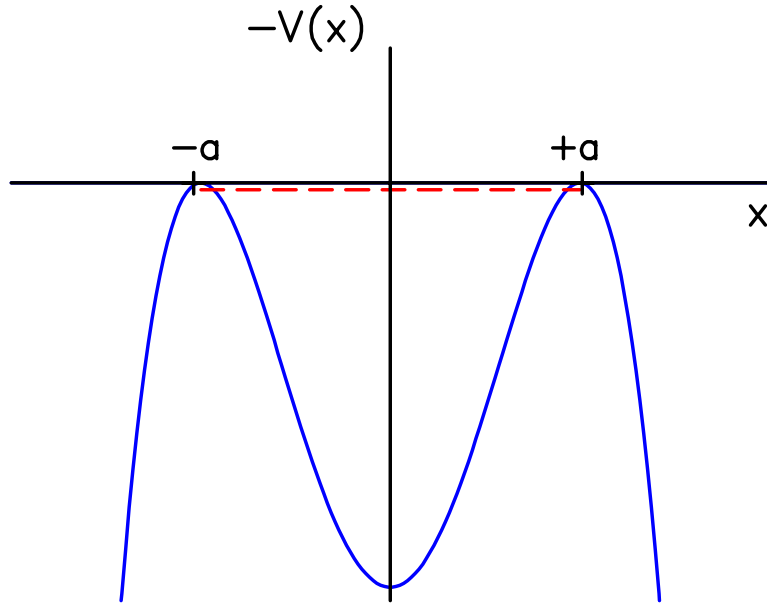


Fig. 9 : Motion in the inverted potential for Euclidean "energy" = 0.

potential. This path can be determined easily by integrating the classical equation of motion (1.328): The Euclidean "energy" is

$$\frac{m}{2} \left(\frac{dx_1}{d\tau} \right)^2 - V(x_1) \stackrel{!}{=} 0 \quad (1.330)$$

and another integration by separating the variables gives

$$\tau = \tau_0 + \int_{x_1(\tau_0)}^{x_1(\tau)} dx \sqrt{\frac{m}{2V(x)}}. \quad (1.331)$$

For the double-well potential (1.321) it is possible to do the integral analytically and also to solve the implicit equation for this special path. One obtains (**Problem 10 a**)

$$x_1(\tau) \equiv x_{cl}(\tau - \tau_0) = a \tanh \left[\frac{\omega}{2} (\tau - \tau_0) \right], \quad (1.332)$$

where the time τ_0 has been fixed (arbitrarily) by demanding that the origin of the potential is traversed at this time.

This solution is called an **instanton** (or also a **kink**) because the particle spends most of its time to crawl up and down the potential hills but then relatively fast – localized in time around $\tau = \tau_0$ – crosses over from the negative x -axis to the positive x -axis. The solution $-x_1(\tau)$ which connects the ($x = +a$)-minimum of the potential with the one at $x = -a$ is called an **anti-instanton**.

The action of this instanton solution is most easily calculated by using the "energy" conservation (1.330)

$$\begin{aligned} S_1 &= \int_{-\beta/2}^{\beta/2} d\tau m \left(\frac{dx_1(\tau)}{d\tau} \right)^2 \stackrel{\beta \rightarrow \infty}{\rightarrow} m \int_{-a}^{+a} dx_1 \frac{dx_1(\tau)}{d\tau} \\ &= \int_{-a}^{+a} dx_1 \sqrt{2mV(x_1)} = \int_{-a}^{+a} dx_1 \frac{m\omega}{2a} (a^2 - x_1^2) = \frac{2}{3} m\omega a^2 \end{aligned} \quad (1.333)$$

and, indeed, a finite action is found.

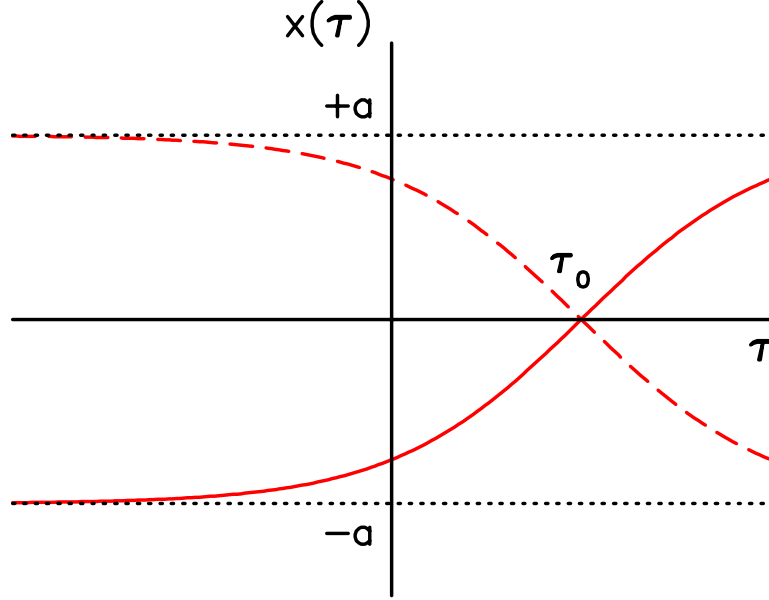


Fig. 10 : The instanton solution and the anti-instanton solution (dashed line).

(ii) Evaluate the quadratic fluctuations and treat the zero mode

Although this (one-)instanton solution is not sufficient to obtain the energy splitting in the double-well potential, we first concentrate on calculating the quadratic fluctuations around this solution in the euclidean path integral. If we set

$$x(\tau) = x_{\text{cl}}(\tau - \tau_0) + \eta(\tau, \tau_0) \quad (1.334)$$

the functional Taylor expansion of the action gives

$$S_E[x_1 + \eta] = S_n + \frac{1}{2} \int_{-\beta/2}^{+\beta/2} d\tau d\tau' \left. \frac{\delta^2 S}{\delta x(\tau) \delta x(\tau')} \right|_{x=x_{\text{cl}}} \eta(\tau) \eta(\tau') + \dots \quad (1.335)$$

since the first functional derivative vanishes. Here we have

$$\left. \frac{\delta^2 S}{\delta x(\tau) \delta x(\tau')} \right|_{x=x_{\text{cl}}} = \left[-m \frac{d^2}{d\tau^2} + V''(x_{\text{cl}}(\tau)) \right] \delta(\tau - \tau') =: \mathcal{O}_{V''} \delta(\tau - \tau'). \quad (1.336)$$

As usual quadratic actions can be integrated out exactly in the path integral: Expand the fluctuations in a complete, orthonormal system (preferently in eigenfunctions of the operator $\mathcal{O}_{V''}$)

$$\eta(\tau) = \sum_{n=0} c_n y_n(\tau), \quad \mathcal{O}_{V''} y_n(\tau) = e_n y_n(\tau), \quad \langle y_m | y_n \rangle := \int_{-\beta/2}^{+\beta/2} d\tau y_m(\tau) y_n(\tau) = \delta_{mn} \quad (1.337)$$

which turns the functional integral into a product of Gaussian integrals over the expansion coefficients c_n . If the eigenvalues are positive $e_n > 0$, then the result of the integrations simply is

$$U\left(a, \frac{\beta}{2}; -a, -\frac{\beta}{2}\right) \simeq \mathcal{N} e^{-S_1/\hbar} \prod_{n=0} \left[\int_{-\infty}^{+\infty} dc_n \exp\left(-\frac{1}{2\hbar} e_n c_n^2\right) \right] =: F_1^{\text{d.w.}}(\beta) e^{-S_1/\hbar} \quad (1.338)$$

where

$$F_1^{\text{d.w.}}(\beta) = \mathcal{N} \prod_{n=0} \left(\frac{2\pi\hbar}{e_n} \right)^{1/2} = \sqrt{\frac{m}{2\pi\hbar \prod_n e_n}} = \sqrt{\frac{m}{2\pi\hbar [\text{Det } \mathcal{O}_{V''}]}} \quad (1.339)$$

is the one-instanton prefactor of the semi-classical path integral for the double well (d.w.) potential due to the fluctuations around the classical path. Note that from our previous derivation of the semi-classical approximation (see Eqs. (1.66) and (1.90) transformed to Euclidean times) we know the correct normalization factor to be

$$\mathcal{N} = \sqrt{\frac{m}{2\pi\hbar}} \prod_{n=0} (2\pi\hbar)^{-1/2}. \quad (1.340)$$

However, as should be investigated in more detail in **Problem 10 b**), there is an eigenfunction of $\mathcal{O}_{V''}$ with eigenvalue 0

$$\left[-m \frac{d^2}{d\tau^2} + V''(x_1(\tau)) \right] \frac{\partial x_1(\tau - \tau_0)}{\partial \tau_0} = \left[-m \frac{d^2}{d\tau^2} + m\omega^2 - \frac{3}{2} \frac{m\omega^2}{\cosh^2(\omega(\tau - \tau_0)/2)} \right] \frac{\partial x_1(\tau - \tau_0)}{\partial \tau_0} = 0, \quad (1.341)$$

a **zero mode** or **Goldstone mode**! This zero mode is a consequence of the translational invariance of the solution in the limit $\beta \rightarrow \infty$: The position of the center of the instanton is then irrelevant and it doesn't "cost" to shift the center by an infinitesimal amount. Therefore, the zero-mode wavefunction must be proportional to the derivative of the classical (instanton) solution

$$y_0(\tau - \tau_0) = A_0 \lim_{\epsilon \rightarrow 0} \frac{x_{\text{cl}}(\tau - (\tau_0 + \epsilon)) - x_{\text{cl}}(\tau - \tau_0)}{\epsilon} = A_0 \frac{\partial x_{\text{cl}}(\tau - \tau_0)}{\partial \tau_0} \equiv -A_0 \dot{x}_{\text{cl}}(\tau - \tau_0) \quad (1.342)$$

(see **Problem 10 b**). Hence, the integration over c_0 is undamped and the euclidean path integral diverges. This problem can be remedied by the **method of collective co-ordinates**: The integration over c_0 is replaced by an integration over "the collective co-ordinate" τ_0 . This is achieved by applying the Faddeev-Popov trick (as in **chapter 1.6**), i.e. by multiplying the path integral by the following "one"

$$1 = \int_{-\beta/2}^{+\beta/2} d\tau_0 \delta[f(\tau_0)] \left| \frac{\partial f}{\partial \tau_0} \right|. \quad (1.343)$$

This means that one first fixes τ_0 by requiring that an arbitrary function of it should vanish (due to the δ -function) and then integrates over all possible τ_0 . Choosing

$$f(\tau_0) = \langle \eta | y_0 \rangle = A_0 \int_{-\beta/2}^{+\beta/2} d\tau \left[x(\tau) - x_{\text{cl}}(\tau, \tau_0) \right] \frac{\partial x_{\text{cl}}(\tau, \tau_0)}{\partial \tau_0} \quad (1.344)$$

demands the fluctuations to be orthogonal to the zero mode. If this is inserted one finds that the expansion coefficient c_0 for the zero mode is set to zero and replaced by the integration over the "center" τ_0 of the instanton. More precisely, one obtains for the one-instanton prefactor of the semi-classical approximation to the path integral for the double-well potential

$$F_1^{\text{d.w.}}(\beta) = \mathcal{N} \int_{-\beta/2}^{+\beta/2} d\tau_0 \frac{1}{A_0} \prod_{n=1} \left(\frac{2\pi\hbar}{e_n} \right)^{1/2} \equiv \beta \sqrt{\frac{m}{2\pi\hbar}} \sqrt{\frac{1}{2\pi\hbar A_0^2 \text{Det}' \mathcal{O}_{V''}}}. \quad (1.345)$$

where Det' indicates the functional determinant with the zero mode removed. Thus the usual factor for the quadratic fluctuations is replaced by

$$\frac{1}{\sqrt{\text{Det}' \mathcal{O}_{V''}}} \longrightarrow \sqrt{\frac{1}{2\pi\hbar A_0^2 \text{Det}' \mathcal{O}_{V''}}} \int_{-\beta/2}^{+\beta/2} d\tau_0, \quad (1.346)$$

where

$$\frac{1}{A_0^2} = \left\langle \frac{\partial x_{\text{cl}}}{\partial \tau_0} \left| \frac{\partial x_{\text{cl}}}{\partial \tau_0} \right. \right\rangle = \frac{S_1}{m} \quad (1.347)$$

is from the normalization of the zero mode (see **Problem 10 b**). The factor $(2\pi\hbar)^{-1/2}$ is a left-over from the $(n=0)$ -term in the product of Eq. (1.340) for the normalization factor \mathcal{N} . Note that we are only interested in the limit $\beta \rightarrow \infty$.

Detail 15: Path integral with Zero Mode

As the original path-integral variable $x(\tau) = x_{cl}(\tau, \tau_0) + \eta(\tau, \tau_0)$ does not depend on the collective variable τ_0 we find from Eqs. (1.343), (1.344)

$$\frac{\partial f(\tau_0)}{\partial \tau_0} = -\frac{1}{A_0} \langle y_0 | y_0 \rangle + \left\langle \eta \left| \frac{\partial y_0}{\partial \tau_0} \right. \right\rangle. \quad (1.348a)$$

Thus with $\langle y_0 | y_0 \rangle = 1$ and the usual integral representation of the δ -function the one-instanton prefactor of the semi-classical path integral for the double well potential becomes (suppressing the subscript of the fluctuation operator \mathcal{O})

$$F_1^{d.w.}(\beta) = \int_{-\beta/2}^{+\beta/2} d\tau_0 \int \frac{d\alpha}{2\pi\hbar} \int_{\eta(-\beta/2)=0}^{\eta(+\beta/2)=0} \mathcal{D}\eta \exp \left[-\frac{1}{2\hbar} \langle \eta | \mathcal{O} | \eta \rangle + \frac{i}{\hbar} \alpha \langle \eta | y_0 \rangle \right] \left| -\frac{1}{A_0} + \left\langle \eta \left| \frac{\partial y_0}{\partial \tau_0} \right. \right\rangle \right|. \quad (1.348b)$$

The exchange $\eta \rightarrow -\eta$ and $\alpha \rightarrow -\alpha$ leaves the exponent invariant but changes the sign of the last term (linear in η) which therefore vanishes. As \mathcal{O} has a zero mode one cannot perform the Gaussian functional integral over η immediately. Following **Negele & Orland** p. 214 - 217 we regularize the operator, i.e. we replace

$$\mathcal{O} \rightarrow \mathcal{O}_\epsilon := \epsilon | y_0 \rangle \langle y_0 | + \mathcal{O}_\perp \quad (1.348c)$$

where $\epsilon > 0$ at the end is set to zero. \mathcal{O}_\perp is the projection of \mathcal{O} on the subspace orthogonal to the zero mode y_0 . Thus

$$\mathcal{O}_\epsilon = \begin{pmatrix} \epsilon & 0 \\ 0 & \mathcal{O}_\perp \end{pmatrix}, \quad \text{Det } \mathcal{O}_\epsilon = \epsilon \text{Det } \mathcal{O}_\perp. \quad (1.348d)$$

With the proper normalization of the fluctuation path integral we then obtain

$$F_1^{d.w.}(\beta) = \int_{-\beta/2}^{+\beta/2} d\tau_0 \int \frac{d\alpha}{2\pi\hbar} \left(\frac{m}{2\pi\hbar A_0^2 \text{Det } \mathcal{O}_\epsilon} \right)^{1/2} \exp \left[-\frac{\alpha^2}{2\hbar} \langle y_0 | \mathcal{O}_\epsilon^{-1} | y_0 \rangle \right]. \quad (1.348e)$$

Since y_0 is the zero mode, one has $\mathcal{O}_\epsilon^{-1} y_0 = \frac{1}{\epsilon} y_0$ and after performing the Gaussian α -integration and performing the limit $\epsilon \rightarrow 0$ one arrives at

$$F_1^{d.w.}(\beta) = \lim_{\epsilon \rightarrow 0} \int_{-\beta/2}^{+\beta/2} d\tau_0 \sqrt{\frac{m}{2\pi\hbar}} \left(2\pi\hbar A_0^2 \epsilon \text{Det } \mathcal{O}_\perp \right)^{-1/2} \sqrt{\epsilon} \equiv \beta \sqrt{\frac{m}{2\pi\hbar} \frac{1}{2\pi\hbar A_0^2 \text{Det}' \mathcal{O}}}. \quad (1.348f)$$

More generally: If there is a continuous symmetry for which the classical equations of motion ($\delta S / \delta x(t)|_{cl} = 0$) have degenerate solutions $x_{cl}(t, \tau_i)$, $i = 1 \dots n$, then there exist n Goldstone modes $\partial x_{cl}(t, \vec{\tau}) / \partial \tau_i$ which are annihilated by $\delta^2 S / \delta x(t) \delta x(t')|_{cl}$ and Eq. (1.348f) generalizes to

$$F_n(\beta) = \sqrt{\frac{m}{2\pi\hbar \text{Det}' \mathcal{O}_\perp}} \prod_{i=1}^n \left(\int \frac{d\tau_i}{\sqrt{2\pi\hbar}} \right) \left[\det_{i,j} \left(\left\langle \frac{\partial x_{cl}}{\partial \tau_i} \left| \frac{\partial x_{cl}}{\partial \tau_j} \right. \right\rangle \right) \right]^{1/2} \quad (1.348g)$$

(Problem 4.6 in **Negele & Orland**, p. 228 - 230).

(iii) Calculate the functional determinant without the zero mode

How do we calculate the reduced determinant $\text{Det}' \mathcal{O}_{V''}$? The straight-forward way would be to determine the other eigenvalues of the operator $\mathcal{O}_{V''}$, i.e. solving the Schrödinger-like equation (after evaluating $V''(x_1(\tau))$)

$$\left\{ -m \frac{d^2}{d\tau^2} + m\omega^2 - \frac{3m\omega^2}{2} \frac{1}{\cosh^2[\omega(\tau - \tau_0)/2]} \right\} y_n(\tau - \tau_0) = e_n y_n(\tau - \tau_0) \quad (1.349)$$

with **boundary conditions** $y_n(-\beta/2) = y_n(+\beta/2) = 0$ as the fluctuations vanish at the boundaries. Then

$$\text{Det}' \mathcal{O}_{V''} = \prod_{n=1} e_n \equiv \frac{\text{Det}' \mathcal{O}_{V''}}{e_0} \quad (1.350)$$

This is possible since these are potentials of the Rosen-Morse type for which analytic solutions are available (see **Kleinert**, ch. 17.3). However, this is very cumbersome, in part because one also has to consider the continuous spectrum. Fortunately, there is a simpler method⁴⁵ based on the **Gel'fand-Yaglom formula** :

⁴⁵This derivation follows **Kleinert**, ch. 17.5.

We have to find the solution $f_{\text{GY}}(\tau)$ of the differential equation (1.349) with the r.h.s. vanishing (i.e. for eigenvalue zero) subject to the **initial condition** $f_{\text{GY}}(-\beta/2) = 0, \dot{f}_{\text{GY}}(-\beta/2) = 1$ and the determinant is then given by

$$\text{Det } \mathcal{O}_{V''} = f_{\text{GY}}(\beta/2). \quad (1.351)$$

We already know one solution for the full Gel'fand-Yaglom equation: It is (proportional to) the zero-mode solution

$$f^{(1)}(\tau) \equiv y_0(\tau) = -A_0 \dot{x}_{\text{cl}}(\tau) = -A_0 a \frac{\omega/2}{\cosh^2[\omega(\tau - \tau_0)/2]} \xrightarrow{\tau \rightarrow \pm\infty} -2\omega a A_0 e^{-\omega|\tau|}, \quad (1.352)$$

which, however, does not fulfill the initial conditions. To achieve that we need a second independent solution $f^{(2)}(\tau)$ which behaves at infinity like

$$f^{(2)}(\tau) \xrightarrow{\tau \rightarrow \pm\infty} \mp 2\omega a A_0 e^{\omega|\tau|} \quad (1.353)$$

(it should have asymptotic behaviour and parity opposite to the first solution). Then we may form the linear combination

$$f_{\text{GY}}(\tau) = C \left[f^{(1)}(-\beta/2) f^{(2)}(\tau) - f^{(2)}(-\beta/2) f^{(1)}(\tau) \right] \quad (1.354)$$

which obviously vanishes at $\tau = -\beta/2$. From the requirement that $\dot{f}_{\text{GY}}(-\beta/2) \stackrel{!}{=} 1$ one determines the constant as

$$C = \frac{1}{W(f^{(1)}, f^{(2)})} = \frac{1}{8\omega^3 a^2 A_0^2} \quad (1.355)$$

where $W(f^{(1)}, f^{(2)}) \equiv f^{(1)} \dot{f}^{(2)} - \dot{f}^{(1)} f^{(2)}$ is the Wronskian of the two solutions evaluated at $\tau = -\beta/2$. As is well known the Wronskian of a linear second-order differential equation is a constant (**Problem 10 c**). Thus

$$f_{\text{GY}}(+\beta/2) = C \left[f^{(1)}(-\beta/2) f^{(2)}(+\beta/2) - f^{(2)}(-\beta/2) f^{(1)}(+\beta/2) \right] = C \cdot 8\omega^2 a^2 A_0^2 = \frac{1}{\omega}. \quad (1.356)$$

It remains to evaluate the would-be zero eigenvalue e_0 at finite β to obtain

$$\text{Det}' \mathcal{O}_{V''} = \frac{f_{\text{GY}}(+\beta/2)}{e_0}. \quad (1.357)$$

At finite β there is no exactly vanishing eigenvalue – instead we expect that $e_0 \sim \exp(-\omega\beta)$. Indeed (as to be shown in **Problem 10 d**) the leading behaviour of the eigenvalue e_0 at large β can be found in perturbation theory as

$$e_0 = 24 m \omega^2 e^{-\omega\beta}. \quad (1.358)$$

Thus

$$F_1^{\text{d.w.}}(\beta) \xrightarrow{\beta \rightarrow \infty} \beta \sqrt{\frac{m}{2\pi\hbar}} e^{-\omega\beta/2} \sqrt{\frac{24\omega^3 S_1}{2\pi\hbar}} =: \beta \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\omega\beta/2} \cdot \sqrt{K_1} \quad (1.359)$$

where

$$K_1 = \frac{4ma^2\omega^3}{\pi\hbar} \quad (1.360)$$

is the single-instanton correction factor to the result which would be obtained for individual harmonic oscillators, i.e. if the inverse \cosh^2 - term would be neglected in the Gel'fand-Yaglom equation.

(iv) Consider n instantons

However, this 1-instanton solution is not sufficient to calculate the energy splitting in the double-well potential; one has to take into account additional solutions with finite action. These solutions (called

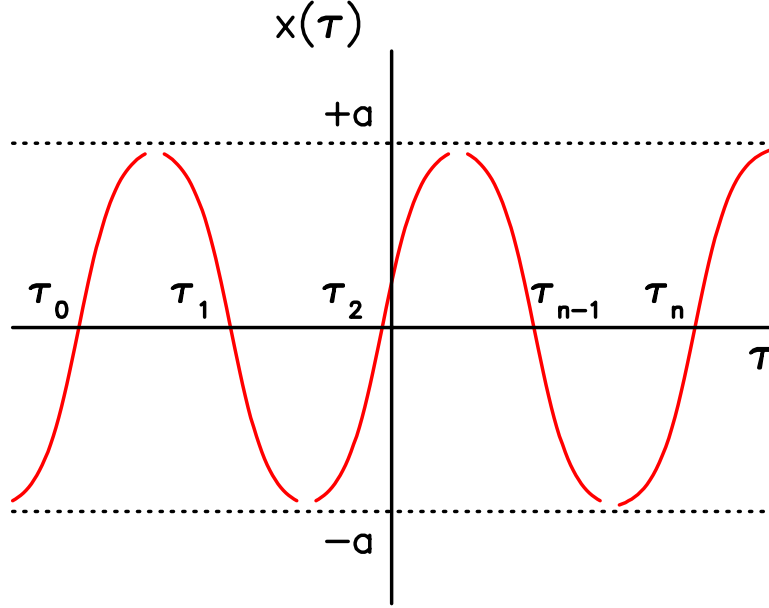


Fig. 11 : Multi-instanton-anti-instanton solution.

$x_n(\tau)$ consist of 3, 5... instantons/anti-instantons which connect the classical minimum at $x = -a$ with the one at $x = +a$ (see Fig. 11).

Strictly speaking these are not exact solutions anymore since, of course, the superposition principle doesn't hold in the non-linear equation of motion (1.328). However, $\delta S_E / \delta x|_{x=x_n}$ is very small if the mutual distance (in Euclidean time) fulfills $\tau_k - \tau_{k-1} \gg 1/\omega$. This approximation is called the "dilute instanton gas". Under these conditions it is also allowed to set

$$S_n \simeq n S_1, \quad n = 3, 5 \dots \quad (1.361)$$

for the corresponding actions. When we calculate the quadratic fluctuations we encounter n zero modes which are treated in a completely analogous way as in the case of a single instanton: Again the method of collective co-ordinates replaces the integration over the undamped modes by an integration over the centers τ_k , $k = 1 \dots n$ of the multi-instantons, under the condition

$$-\frac{\beta}{2} \leq \tau_1 \leq \tau_2 \dots \leq \tau_{n-1} \leq \tau_n \leq \frac{\beta}{2}. \quad (1.362)$$

With Eqs. (1.348g), (1.347) this gives

$$\int dc_0^{(1)} dc_0^{(2)} \dots dc_0^{(n)} \longrightarrow \int_{-\beta/2}^{+\beta/2} d\tau_n \int_{-\beta/2}^{\tau_n} d\tau_{n-1} \dots \int_{-\beta/2}^{\tau_2} d\tau_1 \left(\frac{1}{\sqrt{2\pi\hbar}A_0} \right)^n = \left(\frac{\beta}{\sqrt{2\pi\hbar}A_0} \right)^n \frac{1}{n!} \quad (1.363)$$

and therefore an n -instanton correction factor of $K_n \simeq K_1^n$.

The Euclidean time-evolution operator then is

$$\begin{aligned} U\left(a, \frac{\beta}{2}; -a, -\frac{\beta}{2}\right) &\simeq \sum_{n=1,3,\dots} \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\omega\beta/2} \frac{1}{n!} \left(\sqrt{K_1}\beta e^{-S_1/\hbar}\right)^n = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\omega\beta/2} \sinh\left(\sqrt{K_1}\beta e^{-S_1/\hbar}\right) \\ &= \frac{1}{2} \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\omega\beta/2} \left\{ \exp\left[\beta\sqrt{K_1}e^{-S_1/\hbar}\right] - \exp\left[-\beta\sqrt{K_1}e^{-S_1/\hbar}\right] \right\}. \end{aligned} \quad (1.364)$$

Comparing with the spectral representation (1.327) we thus conclude that

$$E_0 = \frac{1}{2}\hbar\omega - \hbar\sqrt{K_1}e^{-S_1/\hbar}, \quad \psi_0(a)\psi_0(-a) = \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \quad (1.365)$$

$$E_1 = \frac{1}{2}\hbar\omega + \hbar\sqrt{K_1}e^{-S_1/\hbar}, \quad \psi_1(a)\psi_1(-a) = -\frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}, \quad (1.366)$$

i.e. the ground state has positive parity and is lowered while the first excited state has negative parity and has been raised in energy by tunneling. The wave function at $x = \pm a$ agrees with Eq. (1.324) if one neglects the (exponentially suppressed) tail of wave function from the other well and recalls that the wave function of the harmonic oscillator has $\phi_0(0) = (m\omega/\pi\hbar)^{1/4}$ (see Eq. (1.76a)). Taking the value (1.360) for the constant K_1 we obtain the (leading term for the) splitting of the energy levels

$$\Delta E = E_1 - E_0 = 2\hbar\sqrt{K_1}e^{-S_1/\hbar} = 4\hbar\omega\sqrt{\frac{m\omega a^2}{\pi\hbar}} \exp\left[-\frac{2}{3}m\omega a^2/\hbar\right]. \quad (1.367)$$

Remarks

1. The factor $e^{-S_1/\hbar}$ is the expected suppression factor for the tunneling probability. From Eq. (1.333) it can be seen that this is exactly the usual WKB result.
2. In terms of the usual oscillator length $b = \sqrt{\hbar/(m\omega)}$ the result (1.367) reads

$$\Delta E = \frac{4}{\sqrt{\pi}}\hbar\omega\frac{a}{b} \exp\left(-\frac{2}{3}\frac{a^2}{b^2}\right). \quad (1.368)$$

3. Since $1/a^2 \sim \lambda$ essentially is the anharmonicity parameter (cf. Eq. (1.320)) one sees that the result (1.367) for the splitting

$$\Delta E \sim \frac{\text{const}}{\sqrt{\lambda}} e^{-\text{const}_2/\lambda} \quad (1.369)$$

depends non-analytically on λ and hence cannot be obtained in perturbation theory.

4. Higher-order terms for the splitting have been calculated (see, e.g. Ref. [23] and references therein).

2. Path Integrals in Statistical Mechanics and Many-Body Physics

2.1 Partition Function

The partition function

$$Z(\beta) = \text{tr} \left(e^{-\beta \hat{H}} \right), \quad \beta = \frac{1}{k_B T} \quad (2.1)$$

(k_B : Boltzmann's constant, T : temperature) is a central quantity in statistical mechanics as the following thermodynamical quantities can be derived from it

- free energy $F = -\frac{1}{\beta} \ln Z$, i.e.

$$Z = \exp(-\beta F) \quad (2.2)$$

- pressure $P = -\partial F / \partial V$ (V : volume)

- entropy $S = -\partial F / \partial T$ etc.

To calculate expectation values of arbitrary observables \hat{A} in the thermodynamical equilibrium one needs the (equilibrium) density matrix

$$\hat{\rho}_\beta = \frac{1}{Z} e^{-\beta \hat{H}}, \quad \langle \hat{A} \rangle = \text{tr} \left(\hat{A} \hat{\rho}_\beta \right). \quad (2.3)$$

We already have derived a path-integral representation for the partition function of a particle in a potential in **chapter 1.9** and only have to replace there $\beta \rightarrow \beta \hbar$:

$$\begin{aligned} Z(\beta) &= \int dx \int_{x(0)=x}^{x(\beta\hbar)=x} \mathcal{D}x \exp \left[-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left(\frac{m}{2} \dot{x}^2 + V(x) \right) \right] \equiv \oint_{x(0)=x(\beta\hbar)} \mathcal{D}x e^{-S_E[x]/\hbar}, \\ S_E[x] &= \int_0^{\beta\hbar} d\tau \left(\frac{m}{2} \dot{x}^2 + V(x) \right). \end{aligned} \quad (2.4)$$

For example, when we consider a particle in a harmonic potential we obtain from Eqs. (1.66, 1.64, 1.74) after transformation to Euclidean times ⁴⁶ the following expression for the density matrix

$$\begin{aligned} \rho_\beta^{\text{h.o.}}(x, x') &:= \frac{1}{Z} \langle x | \exp(-\beta \hat{H}^{\text{h.o.}}) | x' \rangle \\ &= \frac{1}{Z} \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)}} \exp \left[-\frac{m\omega}{2\hbar} \frac{(x^2 + x'^2) \cosh(\beta\hbar\omega) - 2xx'}{\sinh(\beta\hbar\omega)} \right]. \end{aligned} \quad (2.5)$$

After performing the trace the corresponding partition function reads

$$Z^{\text{h.o.}}(\beta) = \int_{-\infty}^{+\infty} dx \langle x | \exp(-\beta \hat{H}^{\text{h.o.}}) | x \rangle = \frac{1}{2 \sinh(\beta\hbar\omega/2)}, \quad (2.6)$$

where we have used $\cosh z - 1 = 2 \sinh^2(z/2)$. Of course, this agrees with the sum over all energy levels of the harmonic oscillator:

$$Z^{\text{h.o.}}(\beta) = \sum_n \exp(-\beta E_n) \stackrel{\text{h.o.}}{=} \sum_{n=0}^{\infty} \exp \left[-\beta\hbar\omega \left(n + \frac{1}{2} \right) \right]. \quad (2.7)$$

⁴⁶Set $t_a = 0$, $t_b = T = -i\beta\hbar$ and $\sin(iz) = i \sinh(z)$, $\cos(iz) = \cosh(z)$.

For many applications one needs the **partition function of the forced harmonic oscillator**:

$$Z^{\text{forced h.o.}}(\beta) = Z^{\text{h.o.}}(\beta) \exp \left\{ \frac{1}{2m\omega\hbar} \int_0^{\beta\hbar} d\tau \int_0^\tau d\tau' e(\tau) K(\omega(\tau - \tau'), \omega\beta\hbar) e(\tau') \right\} \quad (2.8)$$

with the integral kernel

$$K(x, y) = \frac{\cosh(y/2 - x)}{\sinh(y/2)}. \quad (2.9)$$

Detail 16: Partition Function of the Forced Harmonic Oscillator

The derivation of this result can be made by direct calculation but is a little bit cumbersome. One starts from the result (1.98) in real time and performs, in addition to the transformation $t_a = 0, t_b = T = -i\beta\hbar$, the substitution $t = -i\tau, t' = -i\tau'$ in the integrals over the external force. This gives

$$Z^{\text{forced h.o.}}(\beta) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\omega\beta\hbar)}} \int_{-\infty}^{+\infty} dx \exp(-ax^2 - bx + c) \quad (2.10a)$$

with

$$\begin{aligned} a &= \frac{m\omega}{\hbar \sinh(\omega\beta\hbar)}, & b &= \frac{1}{\hbar \sinh(\omega\beta\hbar)} \\ c &= \frac{1}{m\omega\hbar \sinh(\omega\beta\hbar)} \int_0^{\beta\hbar} d\tau \int_0^\tau d\tau' e(\tau) e(\tau') \sinh \omega(\beta\hbar - \tau) \sinh(\omega\tau'). \end{aligned} \quad (2.10b)$$

The Gaussian integral can be done immediately and gives

$$Z^{\text{forced h.o.}}(\beta) = Z^{\text{h.o.}}(\beta) \exp\left(\frac{b^2}{4a} + c\right). \quad (2.10c)$$

If one evaluates the exponent, uses the relation (1.118) with $j = 2$ for combining the double integrals of b^2 and c and employs the addition theorems for the hyperbolic functions, one obtains Eq. (2.8) with the kernel (2.9).

We may take over the result (2.4) immediately to the case where we have a system of N **distinguishable** quantum mechanical particles moving in an exterior (or mean) potential:

$$\hat{H} = \sum_{i=1}^N \left[\frac{\hat{p}_i^2}{2m} + V(\hat{x}_i) \right] = \sum_{i=1}^N \hat{H}_i. \quad (2.11)$$

Then

$$Z = \text{tr} \left(e^{-\beta \sum_{i=1}^N \hat{H}_i} \right) = \left[\text{tr} \left(e^{-\beta \hat{H}} \right) \right]^N, \quad (2.12)$$

since the particles are moving independently. For each of the sub-partition functions the path-integral representation (2.4) is valid.

As another application we will derive the **high-temperature expansion** of the partition function from the path integral. This is also known as **Wigner-Kirkwood expansion**. For this purpose we write the path which leads from the point x at "time" $\tau = 0$ to x at "time" $\tau = \beta\hbar$ as

$$x(\tau) = x + \xi(\tau) \quad (2.13)$$

and assume that in the high-temperature case ξ is small compared to x . Then we can expand

$$\begin{aligned} V(x + \xi) &= V(x) + \xi V'(x) + \frac{1}{2} \xi^2 V''(x) + \dots \\ &= V - \frac{V'^2}{2V''} + \frac{1}{2} V'' \left(\xi + \frac{V'}{V''} \right)^2 + \mathcal{O}(\xi^3) \end{aligned} \quad (2.14)$$

and obtain similar as in the semi-classical expansion of the propagator in **chapter 1.5**

$$Z^{1/N} \simeq \int dx \exp[-\beta(V - V'^2/(2V''))] \int \mathcal{D}\eta \exp \left[-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left(\frac{m}{2} \dot{\eta}^2 + \frac{1}{2} V'' \eta^2 \right) \right]. \quad (2.15)$$

The boundary conditions for the shifted integration variable $\eta(\tau) = \xi(\tau) + V'/V''$ are $\eta(0) = \eta(\beta\hbar) = V'/V''$ and all potential values have to be taken at the fixed point x over which finally one also has to integrate. The path integral (2.15) is that of a harmonic oscillator in Euclidean time with $m\omega^2 = V''(x)$ and therefore we can employ immediately the result given in Eq. (2.5). In addition, one has to expand the hyperbolic functions for small β in order to remain consistent with the assumption that $\xi(\tau) = \mathcal{O}(\tau^2)$ is small. In this way one obtains

$$\begin{aligned} Z^{1/N} &\simeq \int dx \exp[-\beta(V - V'^2/(2V''))] \sqrt{\frac{m}{2\pi\hbar^2\beta(1 + \omega^2\beta^2\hbar^2/6 + \dots)}} \\ &\quad \cdot \exp\left[-\frac{m\omega}{\hbar} \left(\frac{V'}{V''}\right)^2 \frac{\omega}{2}\beta\hbar \left(1 - \frac{1}{12}\omega^2\beta^2\hbar^2 + \dots\right)\right] \\ &\simeq \int dx \exp[-\beta V(x)] \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \left[1 + \frac{\beta^2\hbar^2}{24m} (\beta V'^2 - 2V'') + \dots\right]. \end{aligned} \quad (2.16)$$

Realizing that

$$\frac{d^2}{dx^2} e^{-\beta V(x)} = \beta(\beta V'^2 - 2V'') e^{-\beta V(x)} \quad (2.17)$$

one can perform an integration by parts to obtain the result

$$Z^{1/N} \simeq \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \int dx \exp[-\beta V(x)] \left[1 - \frac{\beta^3\hbar^2}{24m} V'^2(x) + \dots\right]. \quad (2.18)$$

The first term

$$Z_{\text{class.}}^{1/N} = \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \int dx \exp[-\beta V(x)] = \int \frac{dx dp}{2\pi\hbar} \exp\left[-\beta \left(\frac{p^2}{2m} + V(x)\right)\right] \quad (2.19)$$

is the classical result as can be seen most clearly in the phase-space representation (the second expression in Eq. (2.19)): Apart from the division of phase space into cells of size $h = 2\pi\hbar$ this form does not contain any dependence on Planck's elementary quantum but only the classical Boltzmann factor $\exp(-\beta H(p, x))$. The second term in the square bracket of Eq. (2.18) is the quantum correction for high temperatures. It is obvious that higher corrections may be calculated by additional terms in the Taylor expansion of the potential.

2.2 The Polaron

A celebrated application of the path-integral method in statistical mechanics or solid-state physics is the motion of electrons in an ionic crystal, e.g. NaCl. Here Feynman's path-integral method [24] gives results which are clearly superior over those obtained in conventional approaches.

The electron interacts with the ions which are not tightly bound and thus generates a distortion of the crystal which it tugs along during its motion. This "quasiparticle" is called a **polaron**. A simple model Hamiltonian describing this effect has been given by H. Fröhlich⁴⁷: One solves the Poisson equation for the potential acting on the electron under the assumption that the induced charge density is proportional to the divergence of a longitudinal displacement wave which can be expanded in modes

$$\mathbf{P}(\mathbf{x}) \sim \sum_{\mathbf{k}} \left[a_{\mathbf{k}} \frac{\mathbf{k}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + c.c. \right]. \quad (2.20)$$

In the quantized theory one interpretes $\hat{a}_{\mathbf{k}}$ as a creation operator for a **phonon** with momentum \mathbf{k} . For small momenta only the optical branch of the phonons contributes with a frequency ω which is constant, i.e.

⁴⁷This "Fröhlich" polaron is also called "large" polaron as its dimensions are so large compared to the lattice constant of the solid that one can treat the crystal as a continuum. This is not the case for "small" or "Holstein" polarons. See, e.g. <http://en.wikipedia.org/wiki/Polaron>.

independent of \mathbf{k} in the simplest approximation. If one adds a free part for the phonons then the Hamiltonian of the system reads (in units $\hbar = \omega = m = 1$)

$$\hat{H} = \frac{1}{2}\hat{\mathbf{p}}^2 + \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + i \left(2\sqrt{2}\pi\alpha\right)^{1/2} \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{|\mathbf{k}|} \left[\hat{a}_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}} - \text{h.c.} \right] \equiv \hat{H}_0 + \hat{H}_1. \quad (2.21)$$

Here V denotes the volume in which the total system is enclosed⁴⁸ and α is the dimensionless electron-phonon coupling constant. In actual applications it takes values between 1 and 10 – and therefore is not necessarily small.

First, however, we assume that perturbation theory is applicable. In lowest order the energy of the electron is $E^{(0)} = \mathbf{p}^2/2$. The next two orders of perturbation theory give $\Delta E^{(1)} = 0$ and

$$\Delta E^{(2)} = \sum_n \frac{\langle 0|\hat{H}_1|n\rangle \langle n|\hat{H}_1|0\rangle}{E^{(0)} - E^{(n)}} = -\frac{2\sqrt{2}\pi\alpha}{V} \sum_{\mathbf{k}} \frac{1}{\mathbf{k}^2} \left[\frac{1}{2}(\mathbf{p} - \mathbf{k})^2 + 1 - \frac{1}{2}\mathbf{p}^2 \right]^{-1}. \quad (2.22)$$

The first order of perturbation theory vanishes since there is no phonon in initial and final state. As usual, the second order leads to a lowering of the (ground-state) energy and can be visualized as the emission and absorption of a phonon with momentum \mathbf{k} from the (bare) electron:

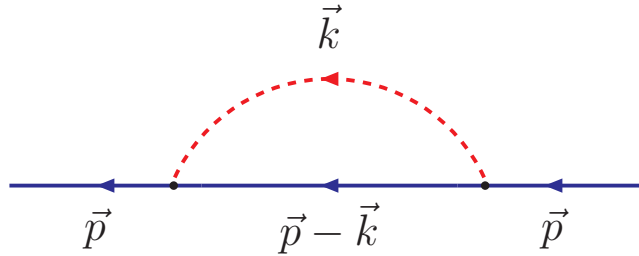


Fig. 12 : Second-order perturbation theory for the self-energy of the polaron.

In the continuum limit we obtain a (loop) integral whose calculation gives

$$\Delta E^{(2)} = -\alpha \frac{\sqrt{2}}{p} \arcsin\left(\frac{p}{\sqrt{2}}\right). \quad (2.23)$$

For small momenta $p = |\mathbf{p}|$ of the electron we therefore have

$$E = \frac{1}{2}\mathbf{p}^2 - \alpha - \frac{\alpha}{12}\mathbf{p}^2 + \mathcal{O}(\alpha^2, \mathbf{p}^4) \simeq -\alpha + \frac{\mathbf{p}^2}{2(1 + \alpha/6)} + \dots. \quad (2.24)$$

In other words: The electron gets an effective mass $m_{\text{eff}}/m = 1 + \alpha/6$ and has a rest energy⁴⁹

$$E_0 = -\alpha + \mathcal{O}(\alpha^2). \quad (2.25)$$

Higher orders of perturbation theory have been calculated (over the years/decades) [25],[26],[27] giving the result

$$E_0(\alpha) = -\alpha - 1.59196 \left(\frac{\alpha}{10}\right)^2 - 0.8061 \left(\frac{\alpha}{10}\right)^3 - 0.533 \left(\frac{\alpha}{10}\right)^4 - 0.38 \left(\frac{\alpha}{10}\right)^5 + \mathcal{O}(\alpha^6). \quad (2.26)$$

⁴⁸This is to make the spectrum discrete and countable: $k_i = n_i\pi/L, V = L^3$. Summation over \mathbf{k} is a shorthand for the summation over $n_i = 1, 2, \dots, i = 1, 2, 3$. For $L \rightarrow \infty$ one can replace this summation by an integral so that $(1/V) \sum_{\mathbf{k}} \rightarrow \int d^3k/(2\pi)^3$.

⁴⁹The numerical factors in front of the interaction term in the Fröhlich Hamiltonian (2.21) look rather arbitrary but have been chosen intentionally such that the term linear in α for the energy has the "nice" coefficient -1 ... This legitimate cosmetics is quite common and leads to a simpler and, in some sense, more "elegant" final result. However, I am far away from supporting Dirac's statement "It is more important to have *beauty* in one's equation than to have them fit experiment", in **{Farmelo}**, p.376. Rather I prefer the attitude of J. W. Tukey "An approximate solution of the exact problem is often more *useful* than the exact solution of an approximate problem", in "Physics Today", July 2001, p. 80.

It is obvious that this series becomes useless for large coupling constants. Here the path-integral method comes to rescue : First, Feynman realized that the phonon coordinates appear at most quadratically and therefore can be **integrated out exactly**.

Detail 17: Integrating out the Phonons

This is done most easily by introducing the (reversed) coordinate and momentum operators instead of the creation and annihilation operators in the Fröhlich Hamiltonian (2.21)

$$\hat{q}_{\mathbf{k}} = \frac{i}{\sqrt{2}} \left(\hat{a}_{-\mathbf{k}}^\dagger - \hat{a}_{\mathbf{k}} \right), \quad \hat{p}_{\mathbf{k}} = -\frac{1}{\sqrt{2}} \left(\hat{a}_{\mathbf{k}}^\dagger + \hat{a}_{-\mathbf{k}} \right). \quad (2.27a)$$

As one can check easily, these operators obey the commutation relations $[\hat{q}_{\mathbf{k}}, \hat{p}_{\mathbf{k}'}] = i\delta_{\mathbf{k}\mathbf{k}'}$, i.e. Eq. (2.27a) is a canonical transformation. Then the Fröhlich Hamiltonian reads

$$\hat{H} = \frac{1}{2} \hat{\mathbf{p}}^2 + \frac{1}{2} \sum_{\mathbf{k}} (\hat{p}_{\mathbf{k}} \hat{p}_{-\mathbf{k}} + \hat{q}_{\mathbf{k}} \hat{q}_{-\mathbf{k}}) - \sum_{\mathbf{k}} \frac{1}{2} + 2 \left(\sqrt{2} \pi \alpha \right)^{1/2} \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{|\mathbf{k}|} \hat{q}_{\mathbf{k}} e^{i\mathbf{k} \cdot \hat{\mathbf{x}}}, \quad (2.27b)$$

where the 3rd term subtracts the (infinite) zero-point energy of all modes \mathbf{k} . The path integral for the partition function now has the following form

$$\begin{aligned} Z(\beta) = & \int_{\mathbf{x}(0)=\mathbf{x}(\beta)} \mathcal{D}^3 x(\tau) \exp \left(- \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2(\tau) \right) \prod_{\mathbf{k}} \left\{ \exp(\beta/2) \int_{q_{\mathbf{k}}(0)=q_{\mathbf{k}}(\beta)} \mathcal{D}q_{\mathbf{k}}(\tau) \right. \\ & \left. \cdot \exp \left[- \int_0^\beta d\tau \sum_{\mathbf{k}} \left(\frac{1}{2} \dot{q}_{\mathbf{k}}(\tau) \dot{q}_{-\mathbf{k}}(\tau) + \frac{1}{2} q_{\mathbf{k}}(\tau) q_{-\mathbf{k}}(\tau) + e_{\mathbf{k}}(\tau) q_{\mathbf{k}}(\tau) \right) \right] \right\} \end{aligned} \quad (2.27c)$$

with

$$e_{\mathbf{k}}(\tau) = 2 \left(\sqrt{2} \pi \alpha \right)^{1/2} \frac{1}{\sqrt{V}} \frac{1}{|\mathbf{k}|} e^{i\mathbf{k} \cdot \mathbf{x}(\tau)}. \quad (2.27d)$$

Due to the canonical transformation (2.27a) we have $q_{\mathbf{k}}^*(\tau) = q_{-\mathbf{k}}(\tau)$ which means $\gamma_{-\mathbf{k}} = \gamma_{\mathbf{k}}$ for the real part and $\eta_{-\mathbf{k}} = -\eta_{\mathbf{k}}$ for the imaginary part. Therefore we only have to integrate over the positive modes with the actions

$$\sum_{\mathbf{k} \geq 0} \int_0^\beta d\tau \left[\dot{\gamma}_{\mathbf{k}}^2 + \gamma_{\mathbf{k}}^2 + (e_{\mathbf{k}} + e_{-\mathbf{k}}) \gamma_{\mathbf{k}} \right], \quad \text{or} \quad \sum_{\mathbf{k} > 0} \int_0^\beta d\tau \left[\dot{\eta}_{\mathbf{k}}^2 + \eta_{\mathbf{k}}^2 + i(e_{\mathbf{k}} - e_{-\mathbf{k}}) \eta_{\mathbf{k}} \right]. \quad (2.27e)$$

In both cases we can use the result (2.8) (by setting there $m = 2, \omega = \hbar = 1$). Then we obtain for each mode the factor

$$Z^{\text{h.o.}}(\beta) \cdot \exp \left\{ \frac{1}{2} \int_0^\beta d\tau \int_0^\tau d\tau' K(\tau - \tau', \beta) \left[e_{\mathbf{k}}(\tau) e_{-\mathbf{k}}(\tau') + e_{-\mathbf{k}}(\tau) e_{\mathbf{k}}(\tau') \right] \right\}. \quad (2.27f)$$

By this the partition function of the electron becomes

$$Z(\beta) = \prod_{\mathbf{k}} \left(\frac{\exp(\beta/2)}{2 \sinh(\beta/2)} \right) \int_{\mathbf{x}(0)=\mathbf{x}(\beta)} \mathcal{D}^3 x(\tau) e^{-S_{\text{eff}}[\mathbf{x}(\tau)]}, \quad (2.27g)$$

with the effective (Euclidean) action

$$S_{\text{eff}}[\mathbf{x}(\tau)] = \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2 - \frac{1}{2} \int_0^\beta d\tau \int_0^\tau d\tau' \frac{\cosh(\beta/2 - (\tau - \tau'))}{\sinh(\beta/2)} \sum_{\mathbf{k}} e_{\mathbf{k}}(\tau) e_{-\mathbf{k}}(\tau').$$

Inserting Eq. (2.27d) and taking the limit of infinite quantization volume gives the result

$$S_{\text{eff}}[\mathbf{x}(\tau)] = \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2 - 2\pi\sqrt{2}\alpha \int_0^\beta d\tau \int_0^\tau d\tau' \frac{\cosh(\beta/2 - (\tau - \tau'))}{\sinh(\beta/2)} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{\mathbf{k}^2} \exp[i\mathbf{k} \cdot (\mathbf{x}(\tau) - \mathbf{x}(\tau'))]. \quad (2.27h)$$

The momentum integral is that for a Coulomb potential

$$\int \frac{d^3 k}{(2\pi)^3} \frac{1}{\mathbf{k}^2} \exp(i\mathbf{k} \cdot \mathbf{y}) = \frac{1}{4\pi} \frac{1}{|\mathbf{y}|}, \quad (2.27i)$$

so that the final result reads

$$S_{\text{eff}}[\mathbf{x}(\tau)] = \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2 - \alpha \sqrt{2} \int_0^\beta d\tau \int_0^\tau d\tau' G_\beta(\tau - \tau') \frac{1}{|\mathbf{x}(\tau) - \mathbf{x}(\tau')|} \quad (2.27j)$$

Here the retardation function is defined by

$$G_\beta(t) := \frac{\cosh(\beta/2 - |t|)}{2 \sinh(\beta/2)} \stackrel{\beta \gg |t|}{\approx} \frac{1}{2} e^{-|t|}. \quad (2.27k)$$

By integrating out the phonons the polaron problem has been reduced to an one-body problem for the electron! If we are only interested in the ground-state energy we can also (partially) perform the limit $\beta \rightarrow \infty$: The zero-point energy of the individual phonon oscillators cancels in the pre-factor of Eq. (2.27g) and the integral kernel can be simplified by assuming $\tau, \tau' \ll \beta$. We then have

$$Z(\beta) = \oint_{\mathbf{x}(0)=\mathbf{x}(\beta)} \mathcal{D}^3 x(\tau) e^{-S_{\text{eff}}[\mathbf{x}(\tau)]} \quad (2.28)$$

with the **effective action**

$$S_{\text{eff}}[\mathbf{x}(\tau)] = \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2 - \frac{\alpha}{\sqrt{2}} \int_0^\beta d\tau \int_0^\tau d\tau' \frac{e^{-(\tau-\tau')}}{|\mathbf{x}(\tau) - \mathbf{x}(\tau')|} . \quad (2.29)$$

However, the remaining path integral cannot be solved exactly anymore. Feynman, in a second step, therefore applied a **variational principle** . It is based on the identity (remember: The path integral works with ordinary, commuting numbers!)

$$\int \mathcal{D}x e^{-S} = \int \mathcal{D}x e^{-S_t} \cdot \frac{\int \mathcal{D}x e^{-(S-S_t)} e^{-S_t}}{\int \mathcal{D}x e^{-S_t}} \equiv \int \mathcal{D}x e^{-S_t} \cdot \langle e^{-(S-S_t)} \rangle \quad (2.30)$$

and **Jensen's inequality** for convex functions

$$\langle e^{-\Delta S} \rangle \geq e^{-\langle \Delta S \rangle} \quad (2.31)$$

which holds for averaging with positive weight functions which is the case for $\exp(-S_t)$. Here S_t is a trial action which should approximate the true action S as well as possible but also allows the path integral to be performed. This technical requirement restricts our choice to the class of **quadratic trial actions**. Since the effective action (2.29) shows a **retardation** which takes into account that phonons emitted at an earlier time are absorbed at a later time, it is crucial to have a retardation also built into the trial action. Therefore one makes the *ansatz*

$$S_t = \int_0^\beta d\tau \frac{1}{2} \dot{\mathbf{x}}^2 + \int_0^\beta d\tau \int_0^\tau d\tau' f(\tau - \tau') [\mathbf{x}(\tau) - \mathbf{x}(\tau')]^2 \quad (2.32)$$

where $f(\sigma)$ is a free, undetermined retardation function. The ground-state energy of the electron in the crystal is obtained from

$$Z(\beta) = e^{-\beta F} \xrightarrow{\beta \rightarrow \infty} e^{-\beta E_0} , \quad (2.33)$$

i.e. with the help of Eqs. (2.30) and (2.31)

$$E_0 \leq E_t + \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle S_{\text{eff}} - S_t \rangle . \quad (2.34)$$

This expression is a generalization of the upper limit of energy from Hamiltonians (i.e. the well-known Rayleigh-Ritz variational principle) to general actions. The calculation of E_t and $\langle S_{\text{eff}} - S_t \rangle$ with the *ansatz* (2.32) is slightly involved but may be done best by Fourier expanding the electron path as in **chapter 1.2**. The result is [28]

$$E_0 \leq \Omega - \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\sigma \frac{e^{-\sigma}}{\mu(\sigma)} , \quad (2.35)$$

with

$$\Omega = \frac{3}{2\pi} \int_0^\infty dE \left[\ln A(E) + \frac{1}{A(E)} - 1 \right] \quad (2.36)$$

$$\mu^2(\sigma) = \frac{4}{\pi} \int_0^\infty dE \frac{\sin^2(\sigma E/2)}{E^2 A(E)} . \quad (2.37)$$

Here, the function $A(E)$ is obtained from the retardation function by

$$A(E) = 1 + \frac{8}{E^2} \int_0^\infty d\sigma f(\sigma) \sin^2\left(\frac{\sigma E}{2}\right). \quad (2.38)$$

Feynman chose

$$f(\sigma) = f_F(\sigma) = C \cdot e^{-w\sigma} \quad (2.39)$$

with two variational parameters C (strength of the retardation) and w (retardation time). Then one obtains

$$\Omega_F = \frac{3}{4v}(v-w)^2, \quad A_F(E) = \frac{v^2 + E^2}{w^2 + E^2}, \quad \mu_F(\sigma) = \left[\frac{w^2}{v^2} \sigma + \frac{v^2 - w^2}{v^3} (1 - e^{-v\sigma}) \right]^{1/2}, \quad (2.40)$$

where one uses – as is customary – the quantity $v = \sqrt{w^2 + 4C/w}$ ($v \geq w$) instead of the strength C . For small coupling constants α one can evaluate the variation w.r.t. the parameters v, w (**Problem 11**) analytically and one obtains

$$E_F = -\alpha - 0.012346 \alpha^2 - 0.6344 \cdot 10^{-3} \alpha^3 - 0.4643 \cdot 10^{-4} \alpha^4 - 0.3957 \cdot 10^{-5} \alpha^5 + \mathcal{O}(\alpha^6). \quad (2.41)$$

This is only slightly worse than the perturbative expansion (2.26). For very large coupling constants one also can work out Feynman's energy analytically and finds

$$E_F = - \underbrace{\frac{1}{3\pi}}_{=0.1061} \alpha^2 - 3 \ln 2 - \frac{3}{4} + \mathcal{O}(\alpha^{-2}) = -0.1061 \alpha^2 - 2.83 + \mathcal{O}(\alpha^{-2}), \quad (2.42)$$

while the exact result in this limit has been derived as

$$E_0(\alpha) = -0.10851 \alpha^2 - 2.84 + \mathcal{O}\left(\frac{1}{\alpha^2}\right), \quad (2.43)$$

(the leading term will be determined in **chapter 2.8**). For arbitrary α one has to calculate the remaining integral in Eq. (2.35) numerically. When doing that it turns out that Feynman's result is the best upper limit⁵⁰ obtained when different approximation schemes are compared for *all* values of α . While perturbation theory is better for $\alpha \ll 1$, it completely fails for large coupling constants where Feynman's result only deviates by at most 2.2%. This success is mainly due to the fact that the infinite phonon degrees of freedom have been integrated out **exactly** so that – irrespective how the electronic part is approximated – the lattice distortion accompanying the electron is treated correctly. Note that although the effective action (2.29) is an one-body action, there is no Hamiltonian description available anymore and therefore also no Schrödinger equation to be solved.

Detail 18: Mean Number of Phonons in the Polaron

It is easy to calculate the mean number of phonons

$$\bar{N} \equiv \langle \hat{N} \rangle = \left\langle \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right\rangle = \lim_{\beta \rightarrow \infty} \frac{\text{tr}(\hat{N} e^{-\beta \hat{H}})}{\text{tr}(e^{-\beta \hat{H}})} \quad (2.44a)$$

which are present in the polaron ground-state – the "dressed electron". This is because one can generate the number operator \hat{N} by differentiating a modified Hamiltonian w.r.t. an artificial parameter λ which then is set to the value "1":

$$\bar{N} = -\frac{\partial}{\partial \lambda} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \text{tr}(e^{-\beta \hat{H} \lambda}) \Big|_{\lambda=1}. \quad (2.44b)$$

Here

$$\hat{H} \lambda = \frac{1}{2} \hat{\mathbf{p}}^2 + \lambda \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + i(2\sqrt{2}\pi\alpha)^{1/2} \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{|\mathbf{k}|} \left[\hat{a}_{\mathbf{k}}^\dagger e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}} - \text{h.c.} \right]. \quad (2.44c)$$

⁵⁰There also exist (in principle exact) Monte-Carlo calculations [29], [30] with which one can compare.

Since for large β the modified partition function fulfills

$$\text{tr} \left(e^{-\beta \hat{H}_\lambda} \right) \xrightarrow{\beta \rightarrow \infty} e^{-\beta E_0(\lambda, \alpha)} \quad (2.44d)$$

one obtains from Eq. (2.44b)

$$\bar{N} = \left. \frac{\partial}{\partial \lambda} E_0(\lambda, \alpha) \right|_{\lambda=1} \quad (2.44e)$$

and one only has to determine the lowest eigenvalue of the Hamiltonian \hat{H}_λ . However, this is easily done by relating it to the original Hamiltonian \hat{H} : First, one divides by λ

$$\frac{1}{\lambda} \hat{H}_\lambda = \frac{1}{2\lambda} \hat{\mathbf{p}}^2 + \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + i \left(2\sqrt{2}\pi\alpha \right)^{1/2} \frac{1}{\lambda\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{|\mathbf{k}|} \left[\hat{a}_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}} - \text{h.c.} \right], \quad (2.44f)$$

and then scales momentum and position operators of the electron (in opposite ways to preserve the commutation relation)

$$\hat{\mathbf{p}} = \sqrt{\lambda} \tilde{\mathbf{p}}, \quad \hat{\mathbf{x}} = \frac{1}{\sqrt{\lambda}} \tilde{\mathbf{x}}. \quad (2.44g)$$

In the interaction term we then set $\mathbf{k} = \sqrt{\lambda} \tilde{\mathbf{k}}$ in the summation and obtain

$$\begin{aligned} \frac{1}{\lambda} \hat{H}_\lambda &= \frac{1}{2} \tilde{\mathbf{p}}^2 + \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + i \left(2\sqrt{2}\pi\alpha \right)^{1/2} \frac{\lambda^{3/4}}{\lambda\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{\lambda}|\mathbf{k}|} \left[\hat{a}_{\mathbf{k}}^\dagger e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{x}}} - \text{h.c.} \right] \\ &= \hat{H}_0 + i \left(2\sqrt{2}\pi \frac{\alpha}{\lambda^{3/2}} \right)^{1/2} \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{|\mathbf{k}|} \left[\hat{a}_{\mathbf{k}}^\dagger e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{x}}} - \text{h.c.} \right]. \end{aligned} \quad (2.44h)$$

Therefore we can read off

$$E_0(\lambda, \alpha) = \lambda E_0 \left(\frac{\alpha}{\lambda^{3/2}} \right) \quad (2.44i)$$

and Eq. (2.44e) gives

$$\bar{N} = E_0(\alpha) - \frac{3}{2} \alpha \frac{\partial}{\partial \alpha} E_0(\alpha). \quad (2.44j)$$

This means that for large α the mean number of phonons grows like $0.217\alpha^2$, i.e. at $\alpha = 10$ a cloud of roughly 22 phonons surrounds a bare electron.

2.3 Dissipative Quantum Systems

Aside from the rather special polaron problem, Feynman's treatment of the phonons has become important for the description of dissipative systems where the heat bath (the rest of the system which is not treated explicitly) is also modelled by a collection of oscillators. This is the topic of the present chapter which essentially follows Ref. [31].

In classical physics dissipation is frequently described in a phenomenological way by adding a velocity-dependent term in the equations of motion. In quantum mechanics this is not possible anymore as a description with a time-independent Hamiltonian implies energy- and probability conservation.

The simple example of a damped pendulum shows how one can get a better, more physical model for a dissipative system: The degree of freedom we are interested in – the elongation of the pendulum – is damped because it interacts with other degrees of freedom (the molecules of the air, the suspension mechanism etc.) We may describe the pendulum, the molecules of the air and the suspension as a large system which conserves the total energy (if isolated well enough from other degrees of freedom). The energy of the pendulum, however, is not conserved in general but will be shared with the environment, i.e. the bath. A popular model due to Caldeira and Leggett [32] therefore assumes a total Hamiltonian of the form

$$H = H_{\text{system}} + H_{\text{bath}} + H_{\text{interaction}} \quad (2.45)$$

where

$$H_{\text{system}} = \frac{p^2}{2m} + V(x) \quad (2.46)$$

describes a particle with mass m moving in a potential V . The model becomes tractable by assuming that the bath degrees of freedom can be described by a collection of N harmonic oscillators

$$H_{\text{bath}} = \sum_{n=1}^N \left(\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 q_n^2 \right) \quad (2.47)$$

and the interaction by a bilinear coupling of particle and bath coordinates

$$H_{\text{interaction}} = -x \sum_{n=1}^N c_n q_n + x^2 \sum_{n=1}^N \frac{c_n^2}{2m_n \omega_n^2} . \quad (2.48)$$

The last term in Eq. (2.48) is really a potential term for the particle, i.e. should be part of V , but it will turn out to be useful if written in this way.

First we want to show that the model describes the expected damping already on the **classical level**. For this purpose we derive the equations of motion for the bath degrees of freedom

$$\dot{p}_n = -m_n \omega_n^2 q_n + c_n x, \quad \dot{q}_n = \frac{p_n}{m_n} \quad (2.49)$$

and for those of the system

$$\dot{p} = -\frac{\partial V}{\partial x} + \sum_{n=1}^N c_n q_n - x \sum_{n=1}^N \frac{c_n^2}{2m_n \omega_n^2}, \quad \dot{x} = \frac{p}{m} . \quad (2.50)$$

Next, we solve Eq. (2.49) for the bath coordinates in such a way that we consider the coordinate $x(t)$ of the particle as a given function of time. Then the inhomogeneous differential equation has the solution

$$q_n(t) = q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n \omega_n} \sin(\omega_n t) + \frac{c_n}{m_n \omega_n} \int_0^t ds \sin[\omega_n(t-s)] x(s), \quad (2.51)$$

and inserting that result into Eq. (2.50) gives

$$\begin{aligned} m \ddot{x}(t) - \int_0^t ds \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n^2} \sin[\omega_n(t-s)] x(s) + \frac{\partial V}{\partial x} + x(t) \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n^2} \\ = \sum_{n=1}^N c_n \left[q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n \omega_n} \sin(\omega_n t) \right] . \end{aligned} \quad (2.52)$$

With the help of an integration by parts in the second term on the l.h.s. the equation of motion of the particle can be brought into the final form

$$m \ddot{x}(t) + m \int_0^t ds \gamma(t-s) \dot{x}(s) + \frac{\partial V}{\partial x} = \xi(t) . \quad (2.53)$$

Note that the damping term needs information about the particle coordinate at earlier times ("memory effect"). On the r.h.s. we have a fluctuating force

$$\xi(t) = \sum_{n=1}^N c_n \left[\left(q_n(0) - \frac{c_n}{m_n \omega_n^2} x(0) \right) \cos(\omega_n t) + \frac{p_n(0)}{m_n \omega_n} \sin(\omega_n t) \right], \quad (2.54)$$

which vanishes if averaged over the bath degrees of freedom. The damping kernel

$$\gamma(t) = \frac{1}{m} \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n^2} \cos(\omega_n t) \quad (2.55)$$

can be expressed by the spectral density of the bath oscillators

$$J(\omega) := \pi \sum_{n=1}^N \frac{c_n^2}{2m_n \omega_n} \delta(\omega - \omega_n) \quad (2.56)$$

as is easily verified:

$$\gamma(t) = \frac{2}{m\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \cos(\omega t). \quad (2.57)$$

Thus, for practical applications there is no need to quantify all parameters m_n, ω_n and c_n which enter Eqs. (2.47, 2.48); it is sufficient to specify the spectral density $J(\omega)$. The form most frequently used is called “**Ohmic damping**”

$$J^{\text{Ohm}}(\omega) = m\gamma\omega, \quad (2.58)$$

which leads to the damping term $\gamma(t) = 2\gamma\delta(t)$ and thus to a classical damping (without ”memory”). However, a realistic spectral density cannot grow without limit and thus Eq. (2.58) has to be modified at high frequencies. One possibility is the suppression of frequencies above a characteristic **Drude frequency** ω_D :

$$J^{\text{Drude}}(\omega) = m\gamma\omega \frac{\omega_D^2}{\omega^2 + \omega_D^2} \implies \gamma(t) = \gamma\omega_D \exp(-\omega_D|t|). \quad (2.59)$$

At first sight, the description of the environment by a ”heat bath” of harmonic oscillators and the bilinear coupling of the particle to it may appear problematic because the system can return to its original state after a sufficient long time and therefore no real, irreversible damping ever happens. However, if the number N of oscillators goes to infinity this so-called **Poincaré recurrence time** also goes to infinity and the system **always** loses energy to the environment. This is also exactly the limiting case, in which the spectral density $J(\omega)$ becomes a continuous function rather than a sum of δ -functions.

Now we want to consider the **quantum mechanical** description of the system by means of Euclidean path integrals. Thus we consider the full partition function of the total system at a temperature $T = 1/(k_B\beta)$ (and we omit the index ”E” for ”Euclidean” in the following)

$$\begin{aligned} Z(\beta) &= \text{tr}_{\text{system+bath+interaction}} \left(\exp(-\beta\hat{H}) \right) \\ &= \oint \mathcal{D}x \left(\prod_{n=1}^N \mathcal{D}q_n \right) \exp \left[-\frac{1}{\hbar} (S_{\text{system}}[x] + S_{\text{bath}}[q_n] + S_{\text{interaction}}[x, q_n]) \right], \end{aligned} \quad (2.60)$$

with

$$S_{\text{system}}[x] = \int_0^{\beta\hbar} d\tau \left[\frac{m}{2} \dot{x}^2 + V(x) \right] \quad (2.61)$$

$$S_{\text{bath}}[q_n] = \int_0^{\beta\hbar} d\tau \sum_{n=1}^N \frac{m_n}{2} (\dot{q}_n^2 + \omega_n^2 q_n^2) \quad (2.62)$$

$$S_{\text{interaction}}[x, q_n] = \int_0^{\beta\hbar} d\tau \sum_{n=1}^N \left(-x c_n q_n + x^2 \frac{c_n^2}{2m_n \omega_n^2} \right). \quad (2.63)$$

The trace in the definition of the partition function again requires periodic boundary conditions for all paths and integration over the endpoints. We can write the partition function in the following form

$$Z(\beta) = \oint \mathcal{D}x \exp\left(-\frac{1}{\hbar} S_{\text{system}}[x]\right) \mathcal{F}[x] \quad (2.64)$$

where the **influence functional** $\mathcal{F}[x]$ is given as a product of path integrals for each environmental oscillator:

$$\mathcal{F}[x] = \prod_{n=1}^N \mathcal{F}_n[x] \quad (2.65)$$

$$\mathcal{F}_n[x] = \oint \mathcal{D}q_n \exp\left\{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \frac{m_n}{2} \left[\dot{q}_n^2(\tau) + \omega_n^2 \left(q_n(\tau) - \frac{c_n}{m_n \omega_n^2} x(\tau) \right)^2 \right]\right\}. \quad (2.66)$$

Similar as in the polaron case we can perform the path integral over the bath oscillators exactly as each mode n is a forced harmonic oscillator. Indeed, the application of Eq. (2.8) immediately gives

$$\mathcal{F}_n[x] = Z_n^{\text{h.o.}} \exp\left[\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \int_0^\tau d\tau' K_n(\tau - \tau') x(\tau) x(\tau') - \frac{c_n^2}{2m_n \omega_n^2 \hbar} \int_0^{\beta\hbar} d\tau x^2(\tau)\right], \quad (2.67)$$

where the kernel reads

$$K_n(s) = \frac{c_n^2}{2m_n \omega_n} \frac{\cosh(\omega_n(\beta\hbar/2 - s))}{\sinh(\omega_n \beta\hbar/2)}, \quad s > 0 \quad (2.68)$$

(see Eq. (2.9)). Different from the polaron problem where we only were interested in the ground-state energy (i.e. $\beta \rightarrow \infty$), it is not possible to simplify it for finite temperatures. Note that the kernel is symmetric around $s = \beta\hbar/2$. Since we only need it in the interval $[0, \beta\hbar]$, we may assume periodicity outside this interval and expand it in a Fourier series

$$K_n(s) = \sum_{l=-\infty}^{\infty} c_l^{(n)} e^{i\nu_l s}, \quad (2.69)$$

where

$$\nu_l := \frac{2\pi l}{\beta\hbar} \quad (2.70)$$

are the so-called **Matsubara frequencies**. The coefficients are given by

$$c_l^{(n)} = \frac{1}{\beta\hbar} \int_0^{\beta\hbar} ds K_n(s) e^{-i\nu_l s} = \frac{c_n^2}{m_n \beta\hbar} \frac{1}{\omega_n^2 + \nu_l^2}. \quad (2.71)$$

Using the result (2.6) we obtain

$$\mathcal{F}_n[x] = \frac{1}{2 \sinh(\beta\hbar \omega_n/2)} \exp\left[-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \int_0^\tau d\tau' k_n(\tau - \tau') x(\tau) x(\tau')\right]. \quad (2.72)$$

Here we have split up the Fourier expansion of the kernel $K_n(s)$ (see Eqs. (2.69, 2.71)) into

$$\begin{aligned} K_n(s) &= \frac{c_n^2}{m_n \omega_n^2 \beta\hbar} \sum_{l=-\infty}^{\infty} e^{i\nu_l s} - \frac{c_n^2}{m_n \omega_n^2 \beta\hbar} \sum_{l=-\infty}^{\infty} \frac{\nu_l^2}{\omega_n^2 + \nu_l^2} e^{i\nu_l s} \\ &=: \frac{c_n^2}{m_n \omega_n^2} \sum_{j=-\infty}^{\infty} \delta(s - j\beta\hbar) - k_n(s). \end{aligned} \quad (2.73)$$

In the interval $[0, \beta\hbar]$ only the $j = 0$ -term contributes to the sum of δ -functions and exactly cancels the last term in Eq. (2.67), i.e. the explicit "potential"-term in the interaction between system and environment (caution:

Due to the integration limits the δ -functions contribute only half of their strength!) It can be shown that the reduced kernel $k_n(s)$ does not contain a local (i.e. one-time) contribution anymore.

The full influence functional therefore is

$$\mathcal{F}[x] = \prod_{n=1}^N \left(\frac{1}{2 \sinh(\beta \hbar \omega_n)} \right) \exp \left[-\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau \int_0^\tau d\tau' k(\tau - \tau') x(\tau) x(\tau') \right], \quad (2.74)$$

with

$$k(s) = \sum_{n=1}^N \frac{c_n^2}{m_n \omega_n^2} \frac{1}{\beta \hbar} \sum_{l=-\infty}^{+\infty} \frac{\nu_l^2}{\nu_l^2 + \omega_n^2} e^{i\nu_l s} \equiv \frac{2}{\pi \beta \hbar} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \sum_{l=-\infty}^{+\infty} \frac{\nu_l^2}{\nu_l^2 + \omega^2} e^{i\nu_l s}. \quad (2.75)$$

In the second line we have used the definition (2.56) of the spectral density of the bath oscillators. As the damping kernel is determined as well by the spectral density via Eq. (2.57) one can express the integrand in Eq. (2.75) also by the Laplace transform of $\gamma(t)$

$$\tilde{\gamma}(z) := \int_0^\infty dt \gamma(t) e^{-zt} = \frac{2}{\pi m} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \frac{z}{z^2 + \omega^2}. \quad (2.76)$$

Thus

$$k(s) = \frac{m}{\beta \hbar} \sum_{l=-\infty}^{+\infty} |\nu_l| \tilde{\gamma}(|\nu_l|) e^{i\nu_l s}. \quad (2.77)$$

The Laplace transform of the Drude damping (2.59) is

$$\tilde{\gamma}^{\text{Drude}}(z) = \gamma \frac{\omega_D}{\omega_D + z}, \quad (2.78)$$

which reduces to $\gamma^{\text{Ohm}}(z) = \gamma$ for pure Ohmic damping.

As in the polaron case we have seen that the influence of the environment can be taken into account by adding a non-local (**two-time**) term to the original action. The properties of the infinitely many bath oscillators can be modelled by simple *ansätze*.

Examples :

a) The Damped Harmonic Oscillator

If the particle moves in a harmonic potential

$$V(x) = \frac{1}{2} m \omega_0^2 x^2 \quad (2.79)$$

all further steps can be done analytically. The partition function of the undamped harmonic oscillator is given by Eq. (2.6), or in the product representation of Eq. (1.73)

$$Z^{\text{h.o.}} = \frac{1}{\beta \hbar \omega_0} \prod_{k=1}^{\infty} \frac{\nu_k^2}{\nu_k^2 + \omega_0^2}. \quad (2.80)$$

If the fluctuations for the damped harmonic oscillator are also expanded in a Fourier series, we may perform the path integral (2.64) with the influence functional (2.74) and obtain a result which is modified by damping

$$Z^{\text{damped h.o.}} = \frac{1}{\beta \hbar \omega_0} \prod_{k=1}^{\infty} \frac{\nu_k^2}{\nu_k^2 + \nu_k \tilde{\gamma}(\nu_k) + \omega_0^2}. \quad (2.81)$$

Which information is contained in Eq. (2.81)? First, we can determine the free energy (2.2) at inverse temperature β

$$F^{\text{damped h.o.}} = \frac{1}{\beta} \ln(\beta \hbar \omega_0) + \frac{1}{\beta} \sum_{k=1}^{\infty} \ln \left(1 + \frac{\tilde{\gamma}(\nu_k)}{\nu_k} + \frac{\omega_0^2}{\nu_k^2} \right) \quad (2.82)$$

In the limit $\beta \rightarrow \infty$ the ground-state energy of the damped harmonic oscillator follows from that

$$E_0^{\text{damped h.o.}} = \frac{\hbar}{2\pi} \int_0^{\infty} d\nu \ln \left(1 + \frac{\tilde{\gamma}(\nu)}{\nu} + \frac{\omega_0^2}{\nu^2} \right), \quad (2.83)$$

since the difference between the Matsubara frequencies shrinks to zero and the sum can then be replaced by an integral. For Ohmic damping with Drude regularization the partition function as well as the ground-state energy can be given in closed analytical form **{Weiss}**. However, it is instructive to consider the results for weak damping:

$$\begin{aligned} E_0^{\text{damped h.o.}} &\rightarrow \frac{\hbar}{2\pi} \int_0^{\infty} d\nu \ln \left(1 + \frac{\omega_0^2}{\nu^2} \right) + \frac{\hbar}{2\pi} \int_0^{\infty} d\nu \frac{\nu}{\nu^2 + \omega_0^2} \tilde{\gamma}(\nu) + \dots \\ &= \frac{1}{2} \hbar \omega_0 + \frac{\hbar}{2\pi m} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega(\omega + \omega_0)}. \end{aligned} \quad (2.84)$$

With the spectral density (2.59) one obtains

$$E_0^{\text{damped h.o.}} = \frac{1}{2} \hbar \omega_0 + \gamma \left[\frac{\hbar}{2\pi} \ln \left(\frac{\omega_D}{\omega_0} \right) + \mathcal{O}(\omega_D^{-1}) \right] + \mathcal{O}(\gamma^2), \quad (2.85)$$

which is in agreement with second-order perturbation theory for the interaction term (2.48) (note that Eq. (2.85) diverges if the cut-off frequency ω_D goes to infinity). Thus, the coupling to the environmental degrees of freedom leads to an energy shift, similar as in the polaron problem or in the interaction of atoms with the radiation field (“Lamb shift”). Actually, the similarity with the latter system is even more pronounced since the excited states also get a finite lifetime by the damping. This can be determined, e.g., from the density of states of the damped system

$$Z(\beta) =: \int_0^{\infty} dE \rho(E) e^{-\beta E} \implies \rho(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta Z(\beta) e^{\beta E}. \quad (2.86)$$

In the inverse Laplace transform one has to choose the constant c such that the path of integration is to the right of all poles of the integrand. The explicit calculations [33] show that instead of a sum of δ -functions for the undamped harmonic oscillator, the density of state of the damped oscillator consists of one δ -function for the ground state and (for small damping) a series of peaks which are slightly shifted from the excitation energies of the pure harmonic oscillator while they become broader and broader for increasing excitation energy until they cannot be resolved as individual peaks anymore. This is in qualitative and quantitative agreement with Fermi’s ”Golden Rule” according to which the width of the n^{th} level is given by

$$\Gamma_n = \frac{2\pi}{\hbar^2} \sum_{j=1}^{\infty} \left| \langle n+1, 1_j | c_j q x_j | n, 0 \rangle \right|^2 \delta(\omega_0 - \omega_j). \quad (2.87)$$

Here we have used that the dipole interaction (2.48) can only connect neighbouring states and that the environment cannot give energy but only can take it. With the help of the matrix element

$$\langle n+1, 1_j | c_j q x_j | n, 0 \rangle = \frac{\hbar}{2\sqrt{m m_j \omega_0 \omega_j}} n^{1/2} \quad (2.88)$$

one finds

$$\Gamma_n = \frac{n}{m\omega_0} J(\omega_0) \stackrel{\text{Ohm}}{=} n \gamma, \quad (2.89)$$

which is particularly simple for Ohmic damping. As expected the width increases with increasing damping γ and level number n .

b) Structure Function of the Damped Harmonic Oscillator

This can also be seen in the structure function (1.251) which we have studied for a harmonically bound particle in **chapter 1.7**. It is possible to apply the formalism used for dissipative quantum systems also to this process either by an analytic continuation of the temperature result to real times [34] or by direct calculation of the Green function

$$G_{\mathcal{O}\mathcal{O}^\dagger}^{\text{damped h.o.}}(T) = \text{const.} \int \mathcal{D}x \exp \left[i \int_{-\infty}^{+\infty} dt \left(\frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega_0^2 x^2 - b(t) \cdot x \right) \right] \prod_{n=1}^N \mathcal{F}_n[x], \quad (2.90)$$

where the "impulse function" $b(t)$ has been defined in Eq. (1.259). The influence functional in real time is now

$$\begin{aligned} \mathcal{F}_n[x] &= \int \mathcal{D}q_n \exp \left\{ i \int_{-\infty}^{+\infty} dt \left[\frac{m}{2} \dot{q}_n^2 - \frac{m_n}{2} \omega_n^2 \left(q_n - \frac{c_n}{m_n \omega_n^2} x \right)^2 \right] \right\} \\ &= \text{const}' \cdot \exp \left\{ -i \frac{c_n^2}{2m_n} \int_{-\infty}^{+\infty} dt dt' x(t) \left(t \left| \frac{1}{-\partial_t^2 - \omega_n^2 + i0^+} + \frac{1}{\omega_n^2} \right| t' \right) x(t') \right\}. \end{aligned} \quad (2.91)$$

Not unexpected the functional integration over the particle coordinate $x(t)$ can be done as a Gaussian integral and with the correct normalization at $q = 0$ one obtains instead of Eq. (1.260)

$$G_{\mathcal{O}\mathcal{O}^\dagger}^{\text{damped h.o.}}(T) = \exp \left[-i \frac{q^2}{2m} \int_{-\infty}^{+\infty} \frac{dE}{\pi} \frac{1 - \cos(ET)}{E^2 - \omega_0^2 - \Sigma(E)} \right]. \quad (2.92)$$

The effect of coupling the particle to additional degrees of freedom shows up as a complex "self-energy"

$$\Sigma(E) = \sum_{n=1}^N \frac{c_n^2}{mm_n} \left(\frac{1}{E^2 - \omega_n^2 + i0^+} + \frac{1}{\omega_n^2} \right) \xrightarrow{N \rightarrow \infty} \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{m\omega} \frac{E^2}{E^2 - \omega^2 + i0^+}, \quad (2.93)$$

where $J(\omega)$ is the (continuous) spectral density of the environmental oscillators defined in Eq. (2.56). One sees that $\Sigma(E)$ is even and vanishes at $E = 0$: Thus the ground state remains a sharp line. Due to the decomposition (1.255) the imaginary part is always negative, i.e. excitations now have a **finite width**. For Ohmic damping (2.58) one finds

$$\Sigma^{\text{Ohm}}(E) = -i\gamma |E|, \quad (2.94)$$

which explains the growing width (2.89) because $E \simeq n\omega_0$.

As in Eq. (1.263) the square of the elastic form factor is given by the T -independent part of Eq. (2.92). A simple calculation gives again a Gaussian dependence on the momentum transfer

$$\left(F_{00}^{\text{damped h.o.}}(q) \right)^2 = \exp \left[-i \frac{q^2}{2m} \int_{-\infty}^{+\infty} \frac{dE}{\pi} \frac{1}{E^2 - \omega_0^2 + i\gamma|E|} \right] = \exp \left[-\frac{q^2}{2m\Omega} \frac{2}{\pi} \arctan \left(\frac{2\Omega}{\gamma} \right) \right], \quad (2.95a)$$

but with the shifted frequency

$$\Omega := \sqrt{\omega_0^2 - \frac{\gamma^2}{4}} \leq \omega_0 \quad (2.95b)$$

(here we only consider the so-called oscillatory case $\gamma \leq 2\omega_0$). The coupling to the bath degrees of freedom thus reduces the target size: The mean square radius which can be measured in the elastic form factor ($F_{00}(q) \rightarrow 1 - q^2 \langle r^2 \rangle / 6 + \dots$ for $q \rightarrow 0$) becomes for small damping

$$\langle r^2 \rangle = \frac{3}{2m\omega_0} \left[1 - \frac{\gamma}{\pi\omega_0} + \mathcal{O}(\gamma^2) \right]. \quad (2.95c)$$

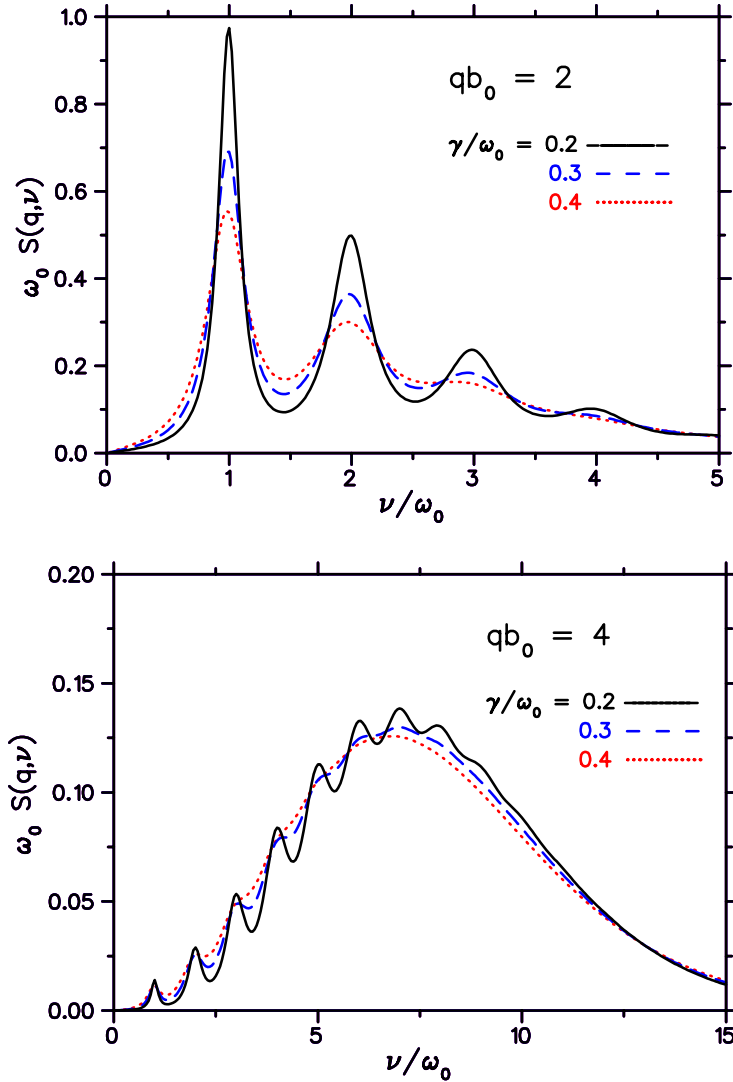


Fig. 13 : Inelastic structure function of the damped harmonic oscillator for several momentum transfers q and Ohmic damping parameters γ [34]. The oscillator frequency of the undamped system is denoted by ω_0 , $b_0 = (m\omega_0)^{-1/2}$ is the oscillator length and serves as unit of length.

Fig. 13 shows the result of a calculation for two different momentum transfers and several values of the Ohmic damping parameter γ . This damping may simulate the coupling to more complicated states like the continuum in which parts of the target have been ejected or the conversion of the struck quark inside the proton into observable hadrons. As can be seen, at high momentum transfer the individual excitation lines merge into a continuous curve, the "quasielastic peak" which has its maximum at $\nu \simeq q^2/(2m)$ and whose width reflects the momentum distribution of the bound particle. Starting from a consistent Hamiltonian for system + environment there are no unphysical excitations with $\nu < 0$: The individual broadened lines are therefore not exact Lorentz- or Breit-Wigner curves which also would extend to negative excitation energies. Therefore

the sum rule obtained by integration over ν from Eq. (1.251)

$$\int_0^\infty d\nu S^{\text{inelast.}}(q, \nu) + F_{00}^2(q) = \langle 0 | e^{-iq \cdot \hat{x}} \sum_n |n\rangle \langle n | e^{iq \cdot \hat{x}} | 0 \rangle = \langle 0 | 0 \rangle = 1 \quad (2.96)$$

is exactly conserved. It is based on the completeness of all target states and is independent of the special form of the Hamiltonian and its eigenstates. Thus, by coupling to other degrees of freedom the spectrum is shifted and distorted but the total strength remains the unchanged.

2.4 Particle-Number Representation and Path Integrals over Coherent States

While in the first chapter of this section the particles always moved in an external potential we now consider a genuine many-body problem: A non-relativistic system of N **identical** particles interacting via two-body forces:

$$\hat{H} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} + \sum_{i<j} \hat{V}_{ij} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij}. \quad (2.97)$$

In systems of identical particles it is a fundamental principle of quantum mechanics⁵¹ that the wave function for bosons (particles with integer spin) should be **symmetric** and the one for fermions (particles with half-integer spin) **antisymmetric** under the exchange of particles

$$\begin{aligned} \hat{H} | \Psi \rangle &= E | \Psi \rangle \\ \Psi(\dots i \dots j \dots) &= \zeta \Psi(\dots j \dots i \dots), \quad \zeta = \begin{cases} +1 & : \text{bosons} \\ -1 & : \text{fermions} \end{cases}. \end{aligned} \quad (2.98)$$

In the usual formulation of quantum mechanics it is cumbersome or difficult to realize this symmetry requirement in every step of the calculation. It is much more convenient to have an formalism at hand which incorporates this requirement automatically. This is the case for the **particle-number representation** (also misleadingly and confusingly called **"second quantization"**), which is already known from treating the harmonic oscillator. Instead of describing the state of the system by a wave function Ψ , which depends on the coordinates and momenta of the particles, one specifies how many particles are in a given state $|\alpha\rangle$ of a chosen complete basis. One then defines annihilation and creation operators, \hat{a}_α , and \hat{a}_α^\dagger , respectively, which annihilate or create a particle in the state $|\alpha\rangle$. The "vacuum" is that state of lowest energy in which there are no particles at all:

$$\hat{a}_\alpha | 0 \rangle = 0 \quad \forall \alpha. \quad (2.99)$$

An one-particle operator, e.g. the kinetic energy, then has the following representation

$$\hat{T} = \sum_{i=1}^N \hat{T}_i \longrightarrow \sum_{\alpha, \beta} \langle \alpha | \hat{T} | \beta \rangle \hat{a}_\alpha^\dagger \hat{a}_\beta, \quad (2.100)$$

and a two-particle operator, e.g. the potential energy,

$$\hat{V} = \frac{1}{2} \sum_{i \neq j}^N \hat{V}_{ij} \longrightarrow \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \langle \alpha \beta | \hat{V} | \gamma \delta \rangle \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\delta \hat{a}_\gamma. \quad (2.101)$$

⁵¹Also called the spin-statistics theorem and proven for local, relativistic quantum field theory by Fierz and Pauli in 1939/40.

Note the different order of the indices in the two-particle matrix element and the annihilation operators. It is also noteworthy that the operators in the particle-number representation do not contain any information about the particle number – the summations are unrestricted and run over all quantum numbers of the basis, not over the number of particles! This is because the operators act in the **Fock space** which is a direct sum of Hilbert spaces with particle number 0, 1, 2 ... In each subspace \mathcal{H}_N they then have the same matrix elements as the operators with which we started. Since both in the kinetic as well as in the potential energy always pairs of $\hat{a}^\dagger \hat{a}$ occur (see Eqs. (2.100, 2.101)), the number of particles remains conserved and the dynamics of the system never carries us outside the chosen Hilbert space. In contrast to this we see single \hat{a}^\dagger 's and \hat{a} 's in the polaron Hamiltonian (2.21) – a typical feature of a field theory is that particle (here: phonon) number may not be conserved.

The particle-number representation is extremely advantageous in many-body physics because the symmetry requirement is automatically built into the commutation relations:

$$\begin{aligned} \left[\hat{a}_\alpha, \hat{a}_\beta^\dagger \right]_{-\zeta} &:= \hat{a}_\alpha \hat{a}_\beta^\dagger - \zeta \hat{a}_\beta^\dagger \hat{a}_\alpha = \delta_{\alpha\beta} \\ \left[\hat{a}_\alpha, \hat{a}_\beta \right]_{-\zeta} &= \left[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger \right]_{-\zeta} = 0, \end{aligned} \quad (2.102)$$

i.e. for bosons one has to use commutators and for fermions anti-commutators. The latter realize the **Pauli principle** in the following way

$$\hat{a}_\alpha^{\dagger 2} |0\rangle = -\hat{a}_\alpha^{\dagger 2} |0\rangle = 0, \quad (2.103)$$

which means that two fermions cannot exist in the same state.

The one-particle basis must be orthonormal and complete

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta}, \quad \sum_{\alpha} | \alpha \rangle \langle \alpha | = \hat{1}, \quad (2.104)$$

but otherwise can be arbitrary. For an electron, e.g., one could use the states of a 3-dimensional harmonic oscillator characterized by n = principal quantum number, l = orbital angular momentum, j = total angular momentum, m_j = magnetic quantum number. For nucleons one would have to add the isospin, for quarks the color etc. Going over to another basis, e.g. to the position basis, is possible by the transformation

$$\hat{a}_{\mathbf{r}} \equiv \hat{\phi}(\mathbf{r}) = \sum_{\alpha} \langle \mathbf{r} | \alpha \rangle \hat{a}_{\alpha} \quad \text{etc.} \quad (2.105)$$

The **field operators** $\hat{\phi}(\mathbf{r})$, $\hat{\phi}^\dagger(\mathbf{r})$ annihilate or create a particle at the point \mathbf{r} (with the other quantum numbers not written out explicitly). It is easily found that they obey the commutation relations

$$\left[\hat{\phi}(\mathbf{r}), \hat{\phi}^\dagger(\mathbf{r}') \right]_{-\zeta} = \delta(\mathbf{r} - \mathbf{r}'). \quad (2.106)$$

For a local potential $\hat{V}_{ij} = V(\hat{x}_i - \hat{x}_j)$ the Hamiltonian then reads

$$\hat{H} = \int d^3r \hat{\phi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta \right) \hat{\phi}(\mathbf{r}) + \frac{1}{2} \int d^3r d^3r' \hat{\phi}^\dagger(\mathbf{r}) \hat{\phi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\phi}(\mathbf{r}') \hat{\phi}(\mathbf{r}). \quad (2.107)$$

If one writes $\hat{H} = \int d^3r \hat{\mathcal{H}}(\mathbf{r})$ then the form of the Hamilton density \mathcal{H} is very similar to that of a ϕ^4 - field theory the only difference being that the interaction is non-local here: The fields are not taken at the same position which is not necessary in a non-relativistic theory with an instantaneous potential.

Due to the great importance of the particle-number representation it is advantageous to choose a basis where the states are no longer eigenstates of the position operator but of the annihilation operator when deriving the path integral ⁵². These are the **coherent states** which are also important in quantum optics (Glauber 1963). This representation goes also under the name "**holomorphic**" or "**Bargmann**" representation. In the following some properties are collected for the case of a particle in a harmonic potential

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right) \tag{2.108}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) , \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^\dagger - \hat{a}) , \quad [\hat{a}, \hat{a}^\dagger] = 1 , \tag{2.109}$$

namely

a) Definition: Coherent states are eigenstates of the annihilation operator ⁵³

$$\hat{a} |z\rangle = z |z\rangle , \quad z \text{ complex .} \tag{2.110}$$

Since \hat{a} is not hermitean, the eigenvalue is necessarily complex.

b) Explicit form:

$$|z\rangle = \exp(z\hat{a}^\dagger) |0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle , \tag{2.111}$$

where $|n\rangle = (\hat{a}^\dagger)^n |0\rangle / \sqrt{n!}$ is the normalized eigenstate of the Hamiltonian (2.108).

c) Coherent states are states of minimal uncertainty (**Problem 12**), i.e. particularly "classical".

d) Overlap:

$$\langle z_2 | z_1 \rangle = \exp(z_2^* z_1) , \tag{2.112}$$

i.e. coherent states are not orthogonal.

e) Representation of unity (closure relation):

$$\hat{1} = \frac{1}{2\pi i} \int dz^* dz |z\rangle\langle z| e^{-|z|^2} . \tag{2.113}$$

Proof : Using polar coordinates for the complex variable z one obtains (the Jacobian is $2i$)

$$\begin{aligned} \frac{1}{2\pi i} \int dz^* dz |z\rangle\langle z| e^{-|z|^2} &= \frac{1}{\pi} \int d(\text{Re } z) d(\text{Im } z) \sum_{n,m} \frac{z^{*n} z^m}{\sqrt{n! m!}} |m\rangle\langle n| e^{-|z|^2} \\ &= \frac{1}{\pi} \sum_{n,m} \frac{|m\rangle\langle n|}{\sqrt{n! m!}} \int_0^\infty dr r e^{-r^2} r^{m+n} \int_0^{2\pi} d\phi e^{-in\phi + im\phi} \\ &= \sum_n \frac{|n\rangle\langle n|}{n!} 2 \int_0^\infty dr r^{2n+1} e^{-r^2} = \sum_n |n\rangle\langle n| = \hat{1} . \end{aligned} \tag{2.114a}$$

⁵² Although the visualization as "sum over all paths" doesn't exist anymore, we will still speak of **path integrals** for convenience. The name "functional integral" is more general but less physical.

⁵³ One can easily see that the creation operator doesn't have eigenstates since it raises the minimal particle number by one.

Because of these properties coherent states are also called “**overcomplete**”: Every state in Fock space can be represented but the basis vectors are linearly dependent:

$$|\psi\rangle = \int \frac{dz^* dz}{2\pi i} e^{-|z|^2} \psi(z^*) |z\rangle, \text{ with } \psi(z^*) = \langle z | \psi \rangle. \quad (2.115)$$

f) Action of \hat{a} and \hat{a}^\dagger :

$$\hat{a} = \frac{\partial}{\partial z^*}, \quad \hat{a}^\dagger = z^*, \quad (2.116)$$

since $\langle z | \hat{a} | \psi \rangle = \langle 0 | \exp(z^* \hat{a}) \hat{a} | \psi \rangle = \partial \psi(z^*) / \partial z^*$ and $\langle z | \hat{a}^\dagger | \psi \rangle = (\hat{a} | z \rangle)^\dagger | \psi \rangle = z^* \psi(z^*)$. In the holomorphic representation the Schrödinger equation for a Hamiltonian $H(\hat{a}^\dagger, \hat{a})$ therefore is $H(z^*, \partial/\partial z^*) \psi(z^*) = E \psi(z^*)$. Indeed, Eq. (2.116) is an explicit representation of the bosonic commutation relations.

g) Matrix elements of operators: These are particularly simple if the operators are **normal ordered**, i.e. if all annihilation operators \hat{a} are to the right of the creation operators \hat{a}^\dagger . Let $\hat{A}(\hat{a}^\dagger, \hat{a})$ be such an operator. From the definition (2.110) it then follows immediately

$$\langle z | \hat{A}(\hat{a}^\dagger, \hat{a}) | z' \rangle = A(z^*, z') \langle z | z' \rangle = A(z^*, z') e^{z^* z'}. \quad (2.117)$$

By inserting the unity operator (2.113) we obtain for the trace of the operator

$$\begin{aligned} \text{tr } \hat{A} &= \sum_n \langle n | \hat{A} | n \rangle = \sum_n \int \frac{dz^* dz}{2\pi i} \langle n | z \rangle \langle z | \hat{A} | n \rangle e^{-|z|^2} \\ &= \int \frac{dz^* dz}{2\pi i} \langle z | \hat{A} \sum_n | n \rangle \langle n | z \rangle e^{-|z|^2} = \int \frac{dz^* dz}{2\pi i} \langle z | \hat{A} | z \rangle e^{-|z|^2}. \end{aligned} \quad (2.118)$$

Going over to **many-body systems** is easy for bosons (fermions will be treated in the next chapter): One only has to replace the complex eigenvalue z by a set of complex numbers $z \rightarrow z_\alpha$ where α denotes the occupied one-particle state and one has to sum over the states. The bosonic coherent state therefore is defined by

$$|z\rangle = \exp\left(\sum_\alpha z_\alpha \hat{a}_\alpha^\dagger\right) |0\rangle, \quad (2.119)$$

where here and in the following we always will characterize the state simply by $z \equiv \{z_\alpha\}$. The unit operator in bosonic Fock space is represented by

$$\hat{1} = \int \prod_\alpha \frac{dz_\alpha^* dz_\alpha}{2\pi i} e^{-\sum_\alpha |z_\alpha|^2} |z\rangle \langle z| \quad (2.120)$$

and all other relations are to be rewritten correspondingly. It should be clear that bosonic coherent states **do not have a fixed particle number** as they are a superposition of states from different Hilbert spaces. Indeed, one finds for the mean particle number

$$\bar{N} = \frac{\langle z | \hat{N} | z \rangle}{\langle z | z \rangle} = \frac{\sum_\alpha \langle z | \hat{a}_\alpha^\dagger \hat{a}_\alpha | z \rangle}{\langle z | z \rangle} = \sum_\alpha |z_\alpha|^2, \quad (2.121)$$

but for the mean-square deviation

$$(\Delta N)^2 = \frac{\langle z | \hat{N}^2 | z \rangle}{\langle z | z \rangle} - \bar{N}^2 = \sum_{\alpha} |z_{\alpha}|^2 = \bar{N}. \quad (2.122)$$

Only in the thermodynamic limit in which $\bar{N} \rightarrow \infty$, the relative deviation $\Delta N / \bar{N} = 1 / \sqrt{\bar{N}}$ goes to zero; then the coherent states are sharply centered around the mean particle number.

After this preliminaries we may begin to derive the path-integral representation of the time-evolution operator for a bosonic many-particle system

$$\hat{U}(t_f, t_i) = \exp\left(-\frac{i}{\hbar} \hat{H}(t_f - t_i)\right) \quad (2.123)$$

in the coherent basis. As in the one-particle case we achieve that goal by splitting the time interval $t_f - t_i$ into M sub-intervals of length ϵ and by inserting the representation (2.120) at $M - 1$ places. Then we obtain

$$\begin{aligned} \langle z_f | \hat{U}(t_f, t_i) | z_i \rangle &\equiv U(z_f^*, t_f; z_i, t_i) = \lim_{M \rightarrow \infty} \mathcal{N} \int \left(\prod_{k=1}^{M-1} \prod_{\alpha} dz_{\alpha,k}^* dz_{\alpha,k} \right) \\ &\cdot \exp\left(-\sum_{k=1}^{M-1} \sum_{\alpha} |z_{\alpha,k}|^2\right) \prod_{k=1}^M \langle z_k | e^{-i\epsilon \hat{H}/\hbar} | z_{k-1} \rangle. \end{aligned} \quad (2.124)$$

Here $z_0 = z_i, z_M = z_f$ and \mathcal{N} is a normalization factor which is of no concern for us. For small time steps ϵ we expand the last factor in Eq. (2.124) and rewrite it then again as exponential function⁵⁴

$$\begin{aligned} \langle z_k | e^{-i\epsilon \hat{H}/\hbar} | z_{k-1} \rangle &= \langle z_k | z_{k-1} \rangle - \frac{i\epsilon}{\hbar} \langle z_k | \hat{H} | z_{k-1} \rangle + \mathcal{O}(\epsilon^2) \\ &= \langle z_k | z_{k-1} \rangle \exp\left(-\frac{i\epsilon \langle z_k | \hat{H} | z_{k-1} \rangle}{\hbar \langle z_k | z_{k-1} \rangle}\right) + \mathcal{O}(\epsilon^2). \end{aligned} \quad (2.125)$$

Assuming that the Hamiltonian is normal-ordered as, e.g. in Eq. (2.107), we then obtain by means of Eqs. (2.112, 2.117)

$$\begin{aligned} U(z_f^*, t_f; z_i, t_i) &= \lim_{M \rightarrow \infty} \mathcal{N} \int \left(\prod_{k=1}^{M-1} \prod_{\alpha} dz_{\alpha,k}^* dz_{\alpha,k} \right) \exp\left(-\sum_{k=1}^{M-1} \sum_{\alpha} |z_{\alpha,k}|^2\right) \\ &\cdot \exp\left[\sum_{k=1}^M \left(\sum_{\alpha} z_{\alpha,k}^* z_{\alpha,k-1} - \frac{i\epsilon}{\hbar} H(z_k^*, z_{k-1})\right)\right]. \end{aligned} \quad (2.126)$$

Now we adopt a continuous (and, of course, more symbolic) notation:

$$\{z_{\alpha,1}, z_{\alpha,2}, \dots, z_{\alpha,M}\} \longrightarrow z_{\alpha}(t) \quad (2.127)$$

and

$$z_{\alpha,k}^* \frac{z_{\alpha,k} - z_{\alpha,k-1}}{\epsilon} \longrightarrow z_{\alpha}^*(t) \frac{\partial}{\partial t} z_{\alpha}(t) \quad (2.128)$$

$$H(z_k^*, z_{k-1}) \longrightarrow H(z^*(t), z(t)). \quad (2.129)$$

⁵⁴A more detailed derivation can be found in Ref. [35].

For velocity-dependent interactions the last equation has to be modified as in the one-particle case. In the continuous notation the argument of all exponential functions in Eq. (2.126) becomes

$$\begin{aligned}
& \sum_{\alpha} z_{\alpha, M}^* z_{\alpha, M-1} - \frac{i\epsilon}{\hbar} H(z_M^*, z_{M-1}) + \frac{i\epsilon}{\hbar} \sum_{k=1}^{M-1} \left[i\hbar \sum_{\alpha} z_{\alpha, k}^* \left(\frac{z_{\alpha, k} - z_{\alpha, k-1}}{\epsilon} \right) - H(z_k^*, z_{k-1}) \right] \\
& \longrightarrow \sum_{\alpha} z_{\alpha}^*(t_f) z_{\alpha}(t_f) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[i\hbar \sum_{\alpha} z_{\alpha}^*(t) \frac{\partial z_{\alpha}(t)}{\partial t} - H(z^*(t), z(t)) \right] \\
& \equiv \sum_{\alpha} z_{\alpha}^*(t_f) z_{\alpha}(t_f) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt L(z^*(t), z(t)) \equiv \sum_{\alpha} z_{\alpha}^*(t_f) z_{\alpha}(t_f) + \frac{i}{\hbar} S[z^*(t), z(t)]. \quad (2.130)
\end{aligned}$$

Here

$$\hat{L} = i\hbar \frac{\partial}{\partial t} - \hat{H} \quad (2.131)$$

is the Lagrange operator of the Schrödinger theory⁵⁵ and S the corresponding classical action. If we omit the index α for the modes or take $z(t) = \{z_{\alpha}(t)\}$ as column vector, $\bar{z} = \{z_{\alpha}^*(t)\}$ as row vector, then the path-integral representation for the time-evolution operator in the coherent basis reads

$$U(\bar{z}_f, t_f; z_i, t_i) = \int_{z(t_i)=z_i}^{\bar{z}(t_f)=\bar{z}_f} \mathcal{D}\bar{z}(t) \mathcal{D}z(t) \exp\left(\bar{z}(t_f)z(t_f) + \frac{i}{\hbar} S[\bar{z}(t), z(t)]\right). \quad (2.132)$$

The term $\bar{z}(t_f)z(t_f)$ in the first exponent is a remainder from collecting the individual terms for the derivative in Eq. (2.128). If we had collected

$$\frac{-z_{\alpha, k+1}^* + z_{\alpha, k}^*}{\epsilon} z_{\alpha, k} \longrightarrow \left(-\frac{\partial}{\partial t} z_{\alpha}^*(t)\right) z_{\alpha}(t) \quad (2.133)$$

then $\bar{z}_1 z_0 \rightarrow \bar{z}(t_i)z(t_i)$ would have been left over. Both results are from the same discrete expression and are thus equivalent. If one wants to have an expression which is symmetric in initial and final time one may average both.

Now we are able to give the path-integral representation of the bosonic partition function. By means of Eq. (2.118) (the remainder is canceled!) and after going over to Euclidean time we obtain

$$Z = \text{tr}\left(e^{-\beta\hat{H}}\right) = \oint_{z(0)=z(\beta\hbar)} \mathcal{D}\bar{z}(\tau) \mathcal{D}z(\tau) \exp\left(-\frac{1}{\hbar} S_E[\bar{z}(\tau), z(\tau)]\right), \quad (2.134)$$

where the Euclidean action is given by

$$S_E[\bar{z}(\tau), z(\tau)] = \int_0^{\beta\hbar} d\tau \left[\hbar \bar{z}(\tau) \frac{\partial z(\tau)}{\partial \tau} + H(\bar{z}(\tau), z(\tau)) \right]. \quad (2.135)$$

⁵⁵Formally Schrödinger's equation is the Euler-Lagrange equation of the action $S[\psi^*, \psi] = \int dt \psi^* \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \psi$. Thus, the operator in the integrand can be considered as Lagrange operator.

What we can treat analytically are systems where the particles move independently in an external or mean potential: In such a case the Hamiltonian (and thus the action) is quadratic in the variables $\bar{z}(\tau)$, $z(\tau)$. We then need to evaluate complex multidimensional Gaussian integrals with hermitean matrices, i.e. need an extension of our toolbox used up to now

Indeed one finds for the **complex Gaussian integral with a hermitean and positive definite $n \times n$ matrix \mathbb{H}**

$$G_{2n}(\mathbb{H}) := \int d^n x d^n y \exp(-\mathbf{z}^\dagger \mathbb{H} \mathbf{z}) = \frac{\pi^n}{\det_n \mathbb{H}}, \quad (2.136)$$

where one integrates over real and imaginary part of the complex vector

$$\mathbf{z} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix}, \quad \mathbf{z}^\dagger = (z_1^*, z_2^* \dots z_n^*), \quad z_j = x_j + i y_j. \quad (2.137)$$

This result is very plausible: If one integrates over the real as well as the imaginary part of the complex vector \mathbf{z} then one obtains the square of the corresponding real-symmetric Gaussian integral (1.89).

Detail 19: Gaussian Complex Integral for Hermitean Matrices

As in Eq. (2.114a) one writes the integral (2.136) also as

$$G_{2n}(\mathbb{H}) = \int d^n z d^n z^* J_{2n} \exp(-\mathbf{z}^\dagger \mathbb{H} \mathbf{z}), \quad (2.138a)$$

where one treats \mathbf{z}, \mathbf{z}^* as independent (real) variables. Because of $\mathbf{x} = (\mathbf{z} + \mathbf{z}^*)/2$, $\mathbf{y} = (\mathbf{z} - \mathbf{z}^*)/(2i)$ the associated Jacobian is

$$J_{2n} = \det_{2n} \begin{pmatrix} \frac{\partial x_i}{\partial z_j} & \frac{\partial x_i}{\partial z_j^*} \\ \frac{\partial y_i}{\partial z_j} & \frac{\partial y_i}{\partial z_j^*} \end{pmatrix} = \det_{2n} \begin{pmatrix} 1/2 & 1/2 \\ 1/(2i) & -1/(2i) \end{pmatrix} = \left(\frac{i}{2}\right)^n. \quad (2.138b)$$

In the last line we have used the identity (see, e.g. <http://en.wikipedia.org/wiki/Determinant>)

$$\det_{2n} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det_n A \cdot \det_n (D - CA^{-1}B) \quad (2.138c)$$

which holds for block matrices (A must be invertible which is trivially fulfilled for the diagonal matrices encountered here). The integral is real since \mathbb{H} is hermitean ($H_{ij}^* = H_{ji}$)

$$(\mathbf{z}^\dagger \mathbb{H} \mathbf{z})^* = (z_i^* H_{ij} z_j)^* = z_j^* (H_{ij})^* z_i = z_j^* H_{ji} z_i \stackrel{i \leftrightarrow j}{=} z_i^* H_{ij} z_j \equiv \mathbf{z}^\dagger \mathbb{H} \mathbf{z}. \quad (2.138d)$$

However, for the convergence of the integral we have to require additionally that \mathbb{H} is positive definite, i.e.

$$z_i H_{ij} z_j > 0, \quad \text{for all } \mathbf{z} \in \mathbb{C}. \quad (2.138e)$$

This can be achieved easily by not considering \mathbb{H} but $\mathbb{H} - E_0 \hat{1}$ where E_0 is the lowest eigenvalue (the ground-state energy).

In many textbooks the calculation of this complex Gaussian integral is performed in close analogy to the real-symmetric case: One uses the fact that a hermitean matrix can be diagonalized by an **unitary transformation**

$$\mathbb{H} = U^\dagger D U, \quad \text{with } U^\dagger U = 1 \quad \text{and } D = (\lambda_1 \dots \lambda_n), \quad \lambda_i > 0 \quad (2.138f)$$

and defines

$$z'_i := U_{ij} z_j \implies z_i = (U^\dagger)_{ij} z'_j. \quad (2.138g)$$

The complex Gaussian integral (2.138a) then becomes

$$G_{2n}(\mathbb{H}) = \left(\frac{i}{2}\right)^n \int d^n z' d^n z'^* J_U \exp(-\mathbf{z}'^\dagger D \mathbf{z}') = \int d^n x' d^n y' J_U \exp\left[-\sum_{i=1}^n \lambda_i (x_i'^2 + y_i'^2)\right], \quad (2.138h)$$

where the Jacobi determinant is

$$J_U = \det_{2n} \begin{pmatrix} \frac{\partial z_i}{\partial z_j'} & \frac{\partial z_i}{\partial z_j'^*} \\ \frac{\partial z_i^*}{\partial z_j'} & \frac{\partial z_i^*}{\partial z_j'^*} \end{pmatrix} = \det_{2n} \begin{pmatrix} U^\dagger & 0 \\ 0 & U^T \end{pmatrix} = \det_n U^\dagger \cdot \det_n U^T = \det_n U^\dagger \cdot \det_n U = \det_n (U^\dagger U) = 1. \quad (2.138i)$$

The remaining integrations over \mathbf{x}', \mathbf{y}' are then trivial and one obtains

$$G_{2n}(\mathbb{H}) = \left(\prod_{i=1}^n \sqrt{\frac{\pi}{\lambda_i}}\right) \cdot \left(\prod_{i=1}^n \sqrt{\frac{\pi}{\lambda_i}}\right) = \frac{\pi^n}{\det_n \mathbb{H}}, \quad (2.138j)$$

i.e. the result (2.136).

However, there is "snag" in this derivation: The unitary transformation (2.138g) distorts the integration path into the complex plane and it is not obvious whether and how one can bring it back to the real axis for integrating over the coordinates x'_i, y'_i (even in the 1-dimensional Fresnel case (1.25a) this requires some effort).

Therefore we will evaluate the integral (2.136) by **real** methods. If we set

$$\mathbb{H} =: \mathbb{A} + i\mathbb{B}, \quad \mathbb{H}^\dagger = \mathbb{H} \implies \mathbb{A}^T = \mathbb{A}, \quad \mathbb{B}^T = -\mathbb{B} \quad (2.138k)$$

then

$$\mathbf{z}^\dagger \mathbb{H} \mathbf{z} = (\mathbf{x}^T - i\mathbf{y}^T) (\mathbb{A} + i\mathbb{B}) (\mathbf{x} + i\mathbf{y}) =: (\mathbf{x}^T, \mathbf{y}^T) \tilde{\mathbb{H}} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}, \quad (2.138l)$$

where

$$\tilde{\mathbb{H}} := \begin{pmatrix} \mathbb{A} & -\mathbb{B} \\ \mathbb{B} & \mathbb{A} \end{pmatrix} \quad (2.138m)$$

is a **symmetric** $2n \times 2n$ matrix. Hence we can utilize the result (1.89) and obtain

$$G_{2n}(\mathbb{H}) = \frac{\pi^{2n/2}}{\sqrt{\det_{2n} \tilde{\mathbb{H}}}}. \quad (2.138n)$$

There only remains the task to calculate the determinant of $\tilde{\mathbb{H}}$. Due to its block form that is easily done by means of the relation (2.138c) and we obtain

$$\det_{2n} \tilde{\mathbb{H}} = \det_{2n} \begin{pmatrix} \mathbb{A} & -\mathbb{B} \\ \mathbb{B} & \mathbb{A} \end{pmatrix} = \det_n \mathbb{A} \cdot \det_n (\mathbb{A} - \mathbb{B}\mathbb{A}^{-1}(-\mathbb{B})) = (\det_n \mathbb{A})^2 \cdot \det_n (1 + \mathbb{A}^{-1}\mathbb{B}\mathbb{A}^{-1}\mathbb{B}). \quad (2.138o)$$

This can be related to the determinant of the original hermitean matrix \mathbb{H} which is real and positive (as are the eigenvalues of \mathbb{H} by assumption). Hence we get

$$\begin{aligned} \det_n \mathbb{H} &= \det_n \mathbb{A} \cdot \det_n (1 + i\mathbb{A}^{-1}\mathbb{B}), \quad \det_n \mathbb{H}^T = \det_n \mathbb{H} = \det_n \mathbb{A} \cdot \det_n (1 - i\mathbb{A}^{-1}\mathbb{B}) \\ \implies (\det_n \mathbb{H})^2 &= \det_n \mathbb{H} \cdot \det_n \mathbb{H}^T = (\det_n \mathbb{A})^2 \cdot \det_n (1 + \mathbb{A}^{-1}\mathbb{B}\mathbb{A}^{-1}\mathbb{B}) \equiv \det_{2n} \tilde{\mathbb{H}}. \end{aligned} \quad (2.138p)$$

As the integral is real and poitive we have to take the positive root and thereby obtain the same result (2.138j) as was derived before (by somehow doubtful methods).

By completing the square one obtains for the extended integral

$$\int d^n x d^n y \exp(-\mathbf{z}^\dagger \mathbb{H} \mathbf{z} + \mathbf{z}^\dagger \mathbf{b} + \mathbf{b}^\dagger \mathbf{z}) = \frac{\pi^n}{\det_n \mathbb{H}} \exp(\mathbf{b}^\dagger \mathbb{H}^{-1} \mathbf{b}), \quad (2.139)$$

where $\mathbf{b}, \mathbf{b}^\dagger$ are n -dimensional complex vectors.

2.5 Description of Fermions : Grassmann Variables

If we want to describe fermions (obeying anticommutation relations) by coherent states which are eigenstates of the annihilation operator

$$\hat{a}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle, \tag{2.140}$$

then we see that the eigenvalues ξ_α cannot be ordinary numbers: $(\hat{a}_\alpha \hat{a}_\beta + \hat{a}_\beta \hat{a}_\alpha) |\xi\rangle = 0$ requires that the eigenvalues ξ_α should be **anticommuting** quantities. Algebras of anticommuting numbers are known as **Grassmann** algebras and are defined by a set of generators which fulfill

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0, \quad \alpha, \beta = 1, 2, \dots, m. \tag{2.141}$$

(Here and below Grassmann-valued quantities are always denoted by a blue-green color). If we have an even number of generators $m = 2n$ one can define a conjugation (also called an involution): We choose a set of n generators and to each Generator ξ_α we assign a generator which we call $\bar{\xi}_\alpha$. If λ is a complex number, then one has

$$\overline{(\lambda \xi_\alpha)} = \lambda^* \bar{\xi}_\alpha, \tag{2.142}$$

and for a product of generators

$$\overline{(\xi_{\alpha_1} \dots \xi_{\alpha_n})} = \bar{\xi}_{\alpha_n} \dots \bar{\xi}_{\alpha_1}. \tag{2.143}$$

Similar as for ordinary complex functions one can define a differentiation (acting to the right) for functions of Grassmann variables. It is defined as for ordinary functions with the difference that the variable ξ_α in the function in question has to be anticommutated until it is in front of the differential operator. For example,

$$\frac{\partial}{\partial \xi_\beta} \bar{\xi}_\alpha \xi_\beta = \frac{\partial}{\partial \xi_\beta} (-\xi_\beta \bar{\xi}_\alpha) = -\bar{\xi}_\alpha.$$

More uncommon is integration over Grassmann variables: Berezin has shown **{Berezin}** that

$$\int d\xi_\alpha 1 = 0, \quad \int d\xi_\alpha \xi_\alpha = 1 \tag{2.144}$$

$$\int d\bar{\xi}_\alpha 1 = 0, \quad \int d\bar{\xi}_\alpha \bar{\xi}_\alpha = 1 \tag{2.145}$$

leads to a consistent description. This "integration" actually behaves more like a differentiation – the power of a variable in integrand is decreased by one. For our purposes it is sufficient to consider these definitions as a clever design to obtain the the diverse minus signs which are connected with the anti-symmetry of fermionic systems without trying to inject too much physical intuition in it. Since Gaussian integrals played a dominant role in the previous treatment of the path integrals, it is quite natural to investigate the corresponding Gaussian Grassmann integral. Let us do that, first, for the case $n = 1$, i.e. for two generators of a Grassmann algebra: Because the square of a Grassmann variable vanishes the exponential series for the Gaussian integrand terminates after the second term; after anticommutating and applying the integration rules (2.144, 2.145) one finds

$$\int d\bar{\xi} d\xi \exp(-\lambda \bar{\xi} \xi) = \int d\bar{\xi} d\xi (1 - \lambda \bar{\xi} \xi) = \lambda \int d\bar{\xi} d\xi \xi \bar{\xi} = \lambda. \tag{2.146}$$

This **Gaussian Grassmann integral** can be easily generalized to an arbitrary even number of Grassmann generators and for a **hermitean matrix** \mathbb{H} :

$$\int \left(\prod_{\alpha=1}^n d\bar{\xi}_\alpha d\xi_\alpha \right) \exp \left(- \sum_{\alpha,\beta} \bar{\xi}_\alpha \mathbb{H}_{\alpha,\beta} \xi_\beta \right) = \det \mathbb{H}. \quad (2.147)$$

Detail 20: Gaussian Grassmann Integral

The proof of Eq. (2.147) is straightforward as we do not have to consider boundary conditions: We diagonalize \mathbb{H} by an unitary matrix so that

$$U^\dagger \mathbb{H} U = \text{diag} (\lambda_1, \dots, \lambda_n). \quad (2.148a)$$

A crucial difference compared to ordinary integrals is that in integrals over Grassmann variables the inverse of the absolute value of the Jacobian is to be used if a linear transformation of the variables is performed. This can already be seen in Eq. (2.146) by setting $\xi = \xi' / \sqrt{\lambda}$, $\bar{\xi} = \bar{\xi}' / \sqrt{\lambda}$: The Jacobian is

$$\mathcal{J} = \det \begin{pmatrix} \frac{\partial \xi}{\partial \xi'} & \frac{\partial \bar{\xi}}{\partial \bar{\xi}'} \\ \frac{\partial \bar{\xi}}{\partial \xi'} & \frac{\partial \xi}{\partial \bar{\xi}'} \end{pmatrix} = \det \begin{pmatrix} 1/\sqrt{\lambda} & 0 \\ 0 & 1/\sqrt{\lambda} \end{pmatrix} = \frac{1}{\lambda}, \quad (2.148b)$$

but the integral has the value

$$\lambda \stackrel{!}{=} \int d\bar{\xi}' d\xi' C \exp(-\bar{\xi}' \xi') = C \implies C = \lambda \equiv \mathcal{J}^{-1}. \quad (2.148c)$$

However, in the case under discussion the Jacobian is one and hence one obtains for the Gaussian Grassmann integral directly

$$\begin{aligned} \int \left(\prod_{\alpha=1}^n d\bar{\xi}_\alpha d\xi_\alpha \right) \exp \left(- \sum_{\alpha,\beta} \bar{\xi}_\alpha \mathbb{H}_{\alpha,\beta} \xi_\beta \right) &= \int \left(\prod_{\alpha=1}^n d\bar{\xi}'_\alpha d\xi'_\alpha \right) \exp \left(- \sum_{\alpha} \bar{\xi}'_\alpha \lambda_\alpha \xi'_\alpha \right) \\ &= \int \left(\prod_{\alpha=1}^n d\bar{\xi}'_\alpha d\xi'_\alpha [1 - \bar{\xi}'_\alpha \lambda_\alpha \xi'_\alpha] \right) = \prod_{\alpha=1}^n \lambda_\alpha = \det \mathbb{H}. \end{aligned} \quad (2.148d)$$

In most applications the Gaussian integral (2.147) is the only result which is needed when integrating over Grassmann variables. Slightly exaggerating one could say: In general, Grassmann variables are introduced only to get rid of them as fast as possible...

Comparison with the bosonic case in Eq. (2.136) shows that – apart from the irrelevant normalization constants – fermionic Gaussian integrals just give the inverse of the bosonic integrals. Using $\det \mathbb{H} = \exp(\text{tr} \ln \mathbb{H})$ (**Problem 13**) one can combine the bosonic and fermionic cases for the extended Gaussian integral

$$\int d\bar{z} dz \exp(-\bar{z} \mathbb{H} z + \bar{z} b + \bar{b} z) = \text{const} \cdot \exp(-\zeta \text{tr} \ln \mathbb{H} + \bar{b} \mathbb{H}^{-1} b) \quad (2.149)$$

where z, b and \bar{z}, \bar{b} are complex or Grassmann-valued variables depending on whether bosonic or fermionic systems are considered. The different sign in the exponent of Eq. (2.149) leads to the important property that in perturbation theory fermion loops get a minus sign relative to boson loops.

In close analogy to the bosonic case, fermionic coherent states can now be defined by

$$|\xi\rangle = \exp \left(- \sum_{\alpha} \xi_{\alpha} \hat{a}_{\alpha}^{\dagger} \right) |0\rangle. \quad (2.150)$$

It is convenient to require (i.e. to define) that Grassmann variables also anticommute with creation and annihilation operators. Then $\xi_{\alpha} \hat{a}_{\alpha}^{\dagger}$ is **Grassmann even**, i.e. it commutes with all other $\xi_{\beta} \hat{a}_{\beta}^{\dagger}$ in the expansion of the exponential function and one obtains

$$|\xi\rangle = \prod_{\alpha} (1 - \xi_{\alpha} \hat{a}_{\alpha}^{\dagger}) |0\rangle. \quad (2.151)$$

Fermionic coherent states practically have the same properties as the bosonic coherent states studied in the previous chapter – with some small, but crucial differences. For example, the overlap is

$$\langle \xi | \xi' \rangle = \exp \left(\sum_{\alpha} \bar{\xi}_{\alpha} \xi'_{\alpha} \right), \quad (2.152)$$

and the unit operator in fermionic Fock space is represented by

$$\hat{1} = \int \left(\prod_{\alpha} d\bar{\xi}_{\alpha} d\xi_{\alpha} \right) \exp \left(- \sum_{\alpha} \bar{\xi}_{\alpha} \xi_{\alpha} \right) | \xi \rangle \langle \xi |. \quad (2.153)$$

As in the bosonic case the trace of a operator is given by

$$\text{tr } \hat{A} = \int \left(\prod_{\alpha} d\bar{\xi}_{\alpha} d\xi_{\alpha} \right) \exp \left(- \sum_{\alpha} \bar{\xi}_{\alpha} \xi_{\alpha} \right) \sum_n \langle n | \xi \rangle \langle \xi | \hat{A} | n \rangle. \quad (2.154)$$

However, since the matrix elements $\langle n | \xi \rangle$ and $\langle \xi | m \rangle$ between states $| n \rangle, | m \rangle$ in Fock space and coherent states also contain Grassmann numbers linearly (cf. Eq. (2.151)), it follows from the anticommutation rules that

$$\langle n | \xi \rangle \langle \xi | m \rangle = \langle -\xi | m \rangle \langle n | \xi \rangle \quad (2.155)$$

holds. With that Eq. (2.154) becomes

$$\begin{aligned} \text{tr } \hat{A} &= \int \left(\prod_{\alpha} d\bar{\xi}_{\alpha} d\xi_{\alpha} \right) \exp \left(- \sum_{\alpha} \bar{\xi}_{\alpha} \xi_{\alpha} \right) \langle -\xi | \hat{A} \sum_n | n \rangle \langle n | \xi \rangle \\ &= \int \left(\prod_{\alpha} d\bar{\xi}_{\alpha} d\xi_{\alpha} \right) \exp \left(- \sum_{\alpha} \bar{\xi}_{\alpha} \xi_{\alpha} \right) \langle -\xi | \hat{A} | \xi \rangle. \end{aligned} \quad (2.156)$$

This change compared to the bosonic form (2.118) entails that in the path-integral representation of the fermionic partition function the boundary condition is

$$\boxed{\xi(0) = -\xi(\beta\hbar)}, \quad (2.157)$$

i.e. that fermions have to obey **antiperiodic** boundary conditions.

It is now possible to give an unified path-integral representation for the partition function of a many-body system

$$\boxed{Z(\beta) = \int_{z(\beta\hbar)=\zeta z(0)} \mathcal{D}\bar{z}(\tau) \mathcal{D}z(\tau) \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[\hbar \bar{z}(\tau) \frac{\partial z(\tau)}{\partial \tau} + H(\bar{z}(\tau), z(\tau)) \right] \right\}}. \quad (2.158)$$

For the two-particle interaction (2.101) the Hamiltonian contains terms up to $\bar{z}z z z$ and hence this path integral is not a Gaussian functional integral anymore which can be solved exactly. However, Eq. (2.158) serves as a starting point for an unified perturbation theory in powers of these terms, both for bosons and fermions.

2.6 Perturbation Theory and Diagrams

We now want to calculate the partition function for a bosonic or fermionic system in a systematic way in order to deduce or predict its macroscopic properties from the microscopic Hamiltonian. For simplicity of notation we will use a system of units in which $\hbar = 1$. When using coherent states without fixed particle number it seems best to adopt the **grand-canonical ensemble** for the description of the system, where it is in contact with a particle and heat bath. The probability to observe it with energy E and particle number N is proportional to $\exp[-(E - \mu N)/(k_B T)]$ (the chemical potential μ controls the mean particle number). Therefore we will use the partition function

$$Z = \text{tr} \left[e^{-\beta(\hat{H} - \mu\hat{N})} \right] =: e^{-\beta\Omega} \quad (2.159)$$

to describe the macroscopic thermodynamics of the system.

Similarly as for the free energy one obtains the pressure or the entropy from the **thermodynamic** (grand-canonical) **potential** $\Omega(\mu, V, T)$ by differentiation w.r.t. the volume V or the temperature T , respectively, and by differentiation w.r.t. the chemical potential the mean particle number

$$\bar{N} = -\frac{\partial\Omega}{\partial\mu} = \frac{1}{Z} \text{tr} \left[\hat{N} e^{-\beta(\hat{H} - \mu\hat{N})} \right]. \quad (2.160)$$

More generally, the thermodynamic average of an operator \hat{O} is given by

$$\langle \hat{O} \rangle_\beta = \frac{1}{Z} \text{tr} \left[\hat{O} e^{-\beta(\hat{H} - \mu\hat{N})} \right]. \quad (2.161)$$

This can be expressed by the corresponding n -particle Green function

$$G^{(n)}(\alpha_1\tau_1 \dots \alpha_n\tau_n | \alpha_{n+1}\tau_{n+1} \dots \alpha_{2n}\tau_{2n}) = \frac{1}{Z} \text{tr} \left\{ \mathcal{T} e^{-\beta(\hat{H} - \mu\hat{N})} \hat{a}_{\alpha_1}^{(H)}(\tau_1) \dots \hat{a}_{\alpha_n}^{(H)}(\tau_n) \cdot \hat{a}_{\alpha_{n+1}}^{(H)\dagger}(\tau_{n+1}) \dots \hat{a}_{\alpha_{2n}}^{(H)\dagger}(\tau_{2n}) \right\}, \quad (2.162)$$

where

$$\begin{aligned} \hat{a}_\alpha^{(H)}(\tau) &= e^{\tau(\hat{H} - \mu\hat{N})} \hat{a}_\alpha e^{-\tau(\hat{H} - \mu\hat{N})} \\ \hat{a}_\alpha^{(H)\dagger}(\tau) &= e^{\tau(\hat{H} - \mu\hat{N})} \hat{a}_\alpha^\dagger e^{-\tau(\hat{H} - \mu\hat{N})} \end{aligned} \quad (2.163)$$

are the Heisenberg operators in imaginary time and \mathcal{T} orders in imaginary time (note that \hat{a}_α and \hat{a}_α^\dagger are not hermitean adjugated anymore).

The path-integral representation of the grand-canonical partition function is a simple generalization of Eq. (2.158):

$$Z = \int_{z(\beta)=\zeta z(0)} \mathcal{D}(\bar{z}(\tau) z(\tau)) \exp \left\{ -\int_0^\beta d\tau \left[\bar{z}(\tau) \left(\frac{\partial}{\partial\tau} - \mu \right) z(\tau) + H(\bar{z}(\tau), z(\tau)) \right] \right\}, \quad (2.164)$$

as one only has to replace the Hamiltonian by $\hat{H} - \mu \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$. Similarly the $(2n)$ -point function is given by

$$\begin{aligned}
 G^{(n)}(\alpha_1 \tau_1 \dots \alpha_n \tau_n \mid \alpha_{n+1} \tau_{n+1} \dots \alpha_{2n} \tau_{2n}) \\
 = \frac{1}{Z} \int_{z(\beta)=\zeta z(0)} \mathcal{D}(\bar{z}(\tau) z(\tau)) z_{\alpha_1}(\tau_1) \dots z_{\alpha_n}(\tau_n) \bar{z}_{\alpha_{n+1}}(\tau_{n+1}) \dots \bar{z}_{\alpha_{2n}}(\tau_{2n}) \\
 \cdot \exp \left\{ - \int_0^\beta d\tau \left[\bar{z}(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) z(\tau) + H(\bar{z}(\tau), z(\tau)) \right] \right\}.
 \end{aligned} \tag{2.165}$$

Since we cannot perform the path integrals exactly, we will combine the single-particle part of $H(\bar{z}, z)$ together with the other quadratic terms and develop the many-body part of the Hamiltonian in a Taylor series. This will lead to functional integrals over Gaussian functions times polynomials which can be evaluated directly. The resulting perturbative series will be discussed for **finite temperature** as this is somehow easier to handle than the direct treatment of the system at zero temperature.

As a warm-up (pun intended) we will calculate the partition function and the one-particle Green function for a system of **non-interacting** particles which is described by a one-body Hamiltonian

$$\hat{H}_0 = \sum_{\alpha} \epsilon_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}. \tag{2.166}$$

In Eq. (2.166) we have chosen a basis in which \hat{H}_0 is diagonal – including the case of an external potential as well as the case of a mean potential acting between the particles. The “free” partition function is

$$\begin{aligned}
 Z_0 &= \int_{z(\beta)=\zeta z(0)} \mathcal{D}(\bar{z}(\tau) z(\tau)) \exp \left\{ - \int_0^\beta d\tau \sum_{\alpha} \left[\bar{z}_{\alpha}(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) z_{\alpha}(\tau) + \epsilon_{\alpha} \bar{z}_{\alpha}(\tau) z_{\alpha}(\tau) \right] \right\} \\
 &= \text{const.} \prod_{\alpha} \text{Det}^{-\zeta} \left[\frac{\partial}{\partial \tau} - \mu + \epsilon_{\alpha} \right].
 \end{aligned} \tag{2.167}$$

As usual we calculate the determinant as product of the eigenvalues of the corresponding operator with the given boundary conditions. In this way one obtains for the eigenvalues $\epsilon_{\alpha} - \mu + i\omega_n$ with $n = 0, \pm 1, \pm 2, \dots$, where

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} & : \text{ bosons } (\zeta = 1) \\ \frac{(2n+1)\pi}{\beta} & : \text{ fermions } (\zeta = -1) \end{cases} \tag{2.168}$$

are the **Matsubara frequencies**. As in the treatment of the harmonic oscillator in **chapter 1.2** we use Euler’s formula $\prod_{n=1}^{\infty} [1 + x^2/(n^2\pi^2)] = \sinh x/x$ to obtain the well-known expression

$$Z_0 = \prod_{\alpha} \left[1 - \zeta e^{-\beta(\epsilon_{\alpha} - \mu)} \right]^{-\zeta}. \tag{2.169}$$

By means of Eq. (2.160) one then obtains $N = \prod_{\alpha} n_{\alpha}$ where

$$n_{\alpha} = \frac{1}{\exp[\beta(\epsilon_{\alpha} - \mu)] - \zeta} \tag{2.170}$$

is the occupation probability of the state α . For free fermions ($\zeta = -1$) the occupation probability is depicted schematically in Fig.14 as a function of the energy.

Although the expressions for bosons and fermions differ ”only” by a sign this has far-reaching consequences: For example, the expression in the square bracket of Eq. (2.169) can vanish for $\mu \leq 0$ if we consider bosons

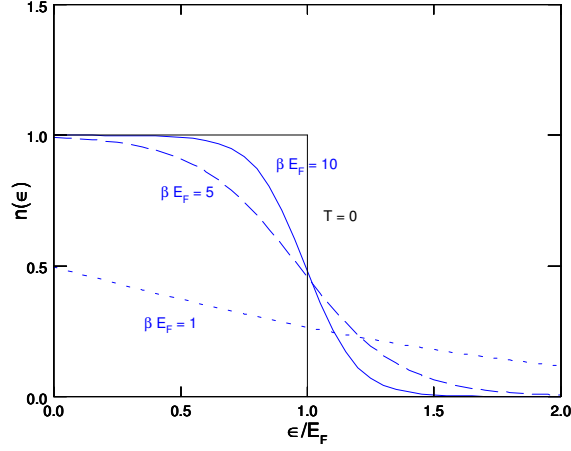


Fig. 14 : Distribution functions of an ideal Fermi gas at different temperatures and constant density N/V . The Fermi energy $E_F = k_F^2/(2m)$ from Eq. (2.180) is used as an energy scale. For $\beta E_F = 10, 5, 1$ the corresponding chemical potential has been calculated numerically as $\mu/E_F = 9.916, 4.823, -0.0214$. The occupation probability for $T = 0$, i.e. $\beta = \infty$ is also depicted.

but not for fermions. This is the phenomenon of **Bose-Einstein condensation** which already shows up for non-interacting particles⁵⁶.

Similarly we calculate the one-particle Green function:

$$G(\alpha\tau | \alpha'\tau') = \frac{\delta^2}{\delta J_\alpha(\tau) \delta \bar{J}_{\alpha'}(\tau')} \ln \int \mathcal{D}(\bar{z}, z) \exp \left\{ -S[\bar{z}, z] + (\bar{J}, z) + (\bar{z}, J) \right\} \Big|_{\bar{J}=J=0}, \quad (2.171)$$

where we use again a compact notation as in **chapter 1.7**. For instance, the "free" action may be written as

$$S_0[\bar{z}, z] = \int_0^\beta dt \sum_\gamma \bar{z}_\gamma(t) \left(\frac{\partial}{\partial t} + \epsilon_\gamma - \mu \right) z_\gamma(t) \equiv \left(\bar{z}, \left(\frac{\partial}{\partial t} + \epsilon - \mu \right) z \right). \quad (2.172)$$

Completing the square in the generating functional gives

$$\begin{aligned} G_0(\alpha\tau | \alpha'\tau') &= \frac{\delta^2}{\delta J_\alpha(\tau) \delta \bar{J}_{\alpha'}(\tau')} \ln \exp \left\{ \left(\bar{J}, \frac{1}{\partial/\partial t + \epsilon - \mu} J \right) \right\} \\ &= \delta_{\alpha\alpha'} \left\langle \tau \left| \frac{1}{\partial/\partial t + \epsilon_\alpha - \mu} \right| \tau' \right\rangle, \end{aligned} \quad (2.173)$$

as the operator to be inverted is diagonal in the chosen basis. As can be seen the "free" one-particle Green function is solution of the equation

$$\left(\frac{\partial}{\partial \tau} + \epsilon_\alpha - \mu \right) G_0(\alpha\tau | \alpha'\tau') = \delta_{\alpha\alpha'} \delta(\tau - \tau') \quad (2.174)$$

with boundary condition

$$G_0(\alpha\beta | \alpha'\tau') = \zeta G_0(\alpha 0 | \alpha'\tau'). \quad (2.175)$$

⁵⁶See, e.g., **{Fetter-Walecka}**, p. 39 - 44 .

In the discretized formulation the calculation is more cumbersome but this is compensated by the advantage of getting an unambiguous result for equal times $\tau = \tau'$ which is not the case in the continuous (and more symbolic) notation. The final result is

$$G_0(\alpha\tau | \alpha'\tau') = \delta_{\alpha\alpha'} e^{-(\epsilon_\alpha - \mu)(\tau - \tau')} \left[\Theta(\tau - \tau' - 0^+) (1 + \zeta n_\alpha) + \zeta \Theta(\tau' - \tau + 0^+) n_\alpha \right]. \quad (2.176)$$

From the one-particle Green function the thermal expectation value of an arbitrary one-particle operator

$$\hat{A} = \sum_{\alpha, \alpha'} \langle \alpha' | \hat{A} | \alpha \rangle \hat{a}_{\alpha'}^\dagger \hat{a}_\alpha, \quad (2.177)$$

can be calculated easily with the help of Eq. (2.161)

$$\langle \hat{A} \rangle_\beta = \zeta \lim_{\tau' \rightarrow \tau^+} \sum_{\alpha, \alpha'} \langle \alpha' | \hat{A} | \alpha \rangle G(\alpha\tau | \alpha'\tau'). \quad (2.178)$$

This is because the infinitesimally greater time τ' in the Green function exactly gives the correct ordering of creation and annihilation operators required in Eq. (2.177).

Example : Mean Particle Number and Energy of a Free Fermi Gas

The basis is made up of plane waves $\exp(i\mathbf{k} \cdot \mathbf{x})/\sqrt{V}$ normalized to one in the volume V . From Eq. (2.176) we find for $\zeta = -1$, $\lim_{\tau' \rightarrow \tau^+} G_0 = -n_{\mathbf{k}}$ and hence

$$\begin{aligned} \langle N \rangle_\beta &= 2 \sum_{\mathbf{k}} \frac{1}{\exp[\beta(k^2/(2m) - \mu)] + 1} \\ \langle E \rangle_\beta &= 2 \sum_{\mathbf{k}} \frac{k^2}{2m} \frac{1}{\exp[\beta(k^2/(2m) - \mu)] + 1}, \end{aligned} \quad (2.179)$$

where the factor of 2 comes from the summation over the spin 1/2 of the particles. In the continuous limit $\sum_{\mathbf{k}}$ turns again into $V \int d^3k/(2\pi)^3$. The integrals are particularly simple for $T = 0$ since the occupation probability then becomes a step function cutting off the momenta at the Fermi momentum k_F ($\mu = E_F = k_F^2/(2m)$), see Fig. 14. We then obtain

$$N \equiv \langle N \rangle_{\beta=\infty} = \frac{2V}{(2\pi)^3} \frac{4\pi}{3} k_F^3 \quad (2.180)$$

$$\bar{E} \equiv \langle E \rangle_{\beta=\infty} = \frac{2V}{(2\pi)^3} \frac{4\pi}{5} \frac{k_F^5}{2m} = N \frac{3}{5} E_F. \quad (2.181)$$

Eq. (2.180) provides the relation between density N/V and Fermi momentum and Eq. (2.181) expresses the mean energy of the particles by the Fermi energy.

Let us now return to the problem of calculating the partition function for a system whose Hamiltonian contains many-body interactions:

$$\hat{H} = \hat{H}_0 + V(\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger \dots; \hat{a}_\gamma, \hat{a}_\delta \dots). \quad (2.182)$$

Obviously one can expand

$$\begin{aligned} Z &= Z_0 \left\langle \exp \left\{ - \int_0^\beta d\tau V(\bar{z} \dots; z \dots) \right\} \right\rangle_{0,\beta} \\ &= Z_0 \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\beta d\tau_1 \dots d\tau_n \langle V(\bar{z}(\tau_1) \dots) \dots V(\bar{z}(\tau_n) \dots) \rangle_{0,\beta} \end{aligned} \quad (2.183)$$

in a series containing powers of the perturbative potential. In each term of this series the expectation value is to be taken w.r.t. the "free" action S_0 and at inverse temperature β . Let us assume that the perturbation potential is a polynomial in creation and annihilation operators (e.g. a two-body potential). Then in Eq. (2.183) one has to evaluate functional integrals over polynomials multiplied by Gaussian functions. This is done with the help of **Wick's theorem** which is based on the following identity

$$\frac{\int \mathcal{D}(\bar{z}z) z_{i_1} \dots z_{i_n} \bar{z}_{j_1} \dots \bar{z}_{j_n} \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j \right]}{\int \mathcal{D}(\bar{z}z) \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j \right]} = \sum_{\text{permutations}} \eta^P M_{i_{Pn}, j_{Pn}}^{-1} \dots M_{i_{P1}, j_{P1}}^{-1}. \quad (2.184)$$

Here the index i denotes the time and state and η is the parity of the permutation, i.e. ± 1 for an even/odd number of permutations.

Detail 21: Proof of Wick's Theorem

This can be verified by differentiating the corresponding generating functional

$$\begin{aligned} W(\bar{J}, J) &= \frac{\int \mathcal{D}(\bar{z}z) \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j + \sum_i (\bar{J}_i z_i + z_i J_i) \right]}{\int \mathcal{D}(\bar{z}z) \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j \right]} \\ &= \exp \left[\sum_{i,j} \bar{J}_i M_{ij}^{-1} J_j \right] \end{aligned} \quad (2.185a)$$

w.r.t. to the external sources:

$$\left. \frac{\delta^{2n} W}{\delta \bar{J}_{i_1} \dots \delta \bar{J}_{i_n} \delta J_{j_1} \dots \delta J_{j_n}} \right|_{J=J=0} = \eta^n \frac{\int \mathcal{D}(\bar{z}z) z_{i_1} \dots z_{i_n} \bar{z}_{j_1} \dots \bar{z}_{j_n} \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j \right]}{\int \mathcal{D}(\bar{z}z) \exp \left[-\sum_{i,j} \bar{z}_i M_{ij} z_j \right]}. \quad (2.185b)$$

Indeed, if one performs the derivatives in Eq. (2.185a) carefully (taking into account order and sign), one obtains Wick's theorem (2.184).

The usual formulation is obtained by defining a **contraction**

$$\underbrace{\hat{a}_\alpha^{(H)}(\tau) \hat{a}_{\alpha'}^{(H)\dagger}(\tau')}_{\text{contraction}} := \left\langle \mathcal{T} \hat{a}_\alpha^{(H)}(\tau) \hat{a}_{\alpha'}^{(H)\dagger}(\tau') \right\rangle_{0\beta} = G_0(\alpha\tau | \alpha'\tau') \equiv \delta_{\alpha\alpha'} g_\alpha(\tau - \tau'). \quad (2.186)$$

Contractions of $\hat{a}\hat{a}$ and $\hat{a}^\dagger\hat{a}^\dagger$ are defined to be zero. Then the identity (2.184) for the Gaussian integrals is equivalent to

$$\left\langle \mathcal{T} \hat{b}_{\alpha_1}^{(H)}(\tau_1) \dots \hat{b}_{\alpha_n}^{(H)}(\tau_n) \right\rangle_{0\beta} = \sum_{\hat{b} = \hat{a}, \hat{a}^\dagger} (\text{all complete contractions}). \quad (2.187)$$

For a two-body interaction

$$V(\bar{z}(\tau), z(\tau)) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle \bar{z}_\alpha(\tau) \bar{z}_\beta(\tau) z_\delta(\tau) z_\gamma(\tau) \quad (2.188)$$

the n^{th} term in the perturbative expansion (2.183) reads

$$\begin{aligned} \left(\frac{Z}{Z_0} \right)^{(n)} &= \frac{(-)^n}{n! 2^n} \sum_{\substack{\alpha_1 \beta_1 \\ \gamma_1 \delta_1}} \dots \sum_{\substack{\alpha_n \beta_n \\ \gamma_n \delta_n}} \langle \alpha_1 \beta_1 | V | \gamma_1 \delta_1 \rangle \dots \langle \alpha_n \beta_n | V | \gamma_n \delta_n \rangle \\ &\cdot \int_0^\beta d\tau_1 \dots d\tau_n \left\langle \bar{z}_{\alpha_1}(\tau_1) \bar{z}_{\beta_1}(\tau_1) z_{\delta_1}(\tau_1) z_{\gamma_1}(\tau_1) \dots \right. \\ &\quad \left. \dots \bar{z}_{\alpha_n}(\tau_n) \bar{z}_{\beta_n}(\tau_n) z_{\delta_n}(\tau_n) z_{\gamma_n}(\tau_n) \right\rangle_{0\beta}, \end{aligned}$$

(2.189)

for which Wick's theorem (2.187) has to be applied when evaluating its expectation value.

For "book keeping" it is very helpful to have a graphical representation for the individual terms:

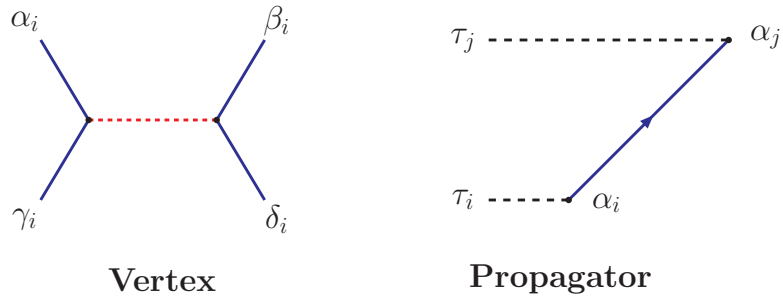


Fig. 15 : Graphical representation of a vertex for a two-body interaction and of a propagator in "labeled" Feynman diagrams.

A **vertex** represents

$$\text{vertex} \hat{=} \langle \alpha_i \beta_i | V | \gamma_i \delta_i \rangle , \tag{2.190}$$

and a **propagator**

$$\begin{aligned} \text{propagator} &\hat{=} \delta_{\alpha_i \alpha_j} g_{\alpha_i} (\tau_j - \tau_i) \\ &= \delta_{\alpha_i \alpha_j} e^{-(\epsilon_{\alpha_i} - \mu)(\tau_j - \tau_i)} \left[(1 + \zeta n_{\alpha_i}) \Theta(\tau_j - \tau_i) + \zeta n_{\alpha_i} \Theta(\tau_i - \tau_j) \right] . \end{aligned} \tag{2.191}$$

In n^{th} order the rules for these "labeled" Feynman diagrams are then as follows:

1. : Draw all **distinct** labeled diagrams with n vertices (diagrams are distinct if they cannot be deformed in such a way that they are identical – including all time labels, left-right-labels and the direction of arrows).
2. : Assign a single-particle index to each directed line and give it the factor (2.191).
3. : Give each vertex the factor (2.190).
4. : Sum over all single-particle indices and integrate over all times in the interval $[0, \beta]$.
5. : Multiply the result by $(-)^n \zeta^{n_L} / (n! 2^n)$ where n_L is the number of closed loops of single-particle propagators in the diagram.

Example : 1st-Order Perturbation Theory

For $n = 1$ there are two diagrams (see Fig. 16):

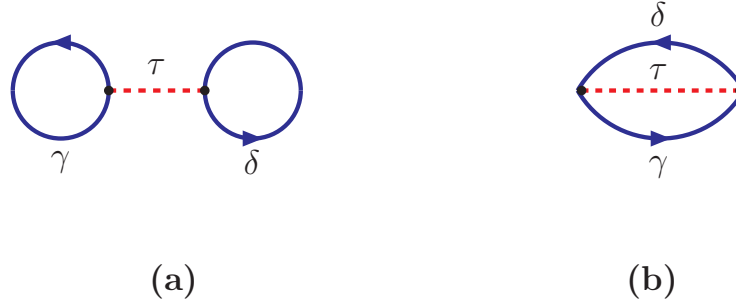


Fig. 16 : Diagrams for the partition function in 1st-order perturbation theory at finite temperature.

Diagram (a) is given by

$$\begin{aligned}
 (a) &= -\frac{1}{2} \int_0^\beta d\tau \sum_{\alpha\beta\gamma\delta} \underbrace{\bar{z}_\alpha(\tau) \bar{z}_\beta(\tau) z_\delta(\tau) z_\gamma(\tau)}_{\langle \gamma\delta|V|\gamma\delta \rangle} \\
 &= -\frac{1}{2} \int_0^\beta d\tau \sum_{\gamma\delta} g_\gamma(0) g_\delta(0) \langle \gamma\delta|V|\gamma\delta \rangle .
 \end{aligned} \tag{2.192}$$

Diagram (b) results from contracting $\bar{z}_\alpha(\tau)$ with $z_\delta(\tau)$ and $\bar{z}_\beta(\tau)$ with $z_\gamma(\tau)$. It has the value

$$(b) = -\frac{1}{2} \zeta \int_0^\beta d\tau \sum_{\gamma\delta} g_\gamma(0) g_\delta(0) \langle \delta\gamma|V|\gamma\delta \rangle . \tag{2.193}$$

By means of the explicit expression (2.191) we thus obtain

$$\frac{Z}{Z_0} = 1 - \frac{\beta}{2} \sum_{\gamma\delta} n_\gamma n_\delta \left[\langle \gamma\delta|V|\gamma\delta \rangle + \zeta \langle \delta\gamma|V|\gamma\delta \rangle \right] + \mathcal{O}(V^2) \tag{2.194}$$

and from that for the thermodynamic potential

$$\frac{Z}{Z_0} = e^{-\beta(\Omega - \Omega_0)} = 1 - \beta(\Omega_1 - \Omega_0) + \dots \tag{2.195}$$

$$\Omega_1 = \Omega_0 + \frac{1}{2} \sum_{\gamma\delta} n_\gamma n_\delta \left[\langle \gamma\delta|V|\gamma\delta \rangle + \zeta \langle \delta\gamma|V|\gamma\delta \rangle \right] . \tag{2.196}$$

For fermions ($\zeta = -1$) we can determine the ground-state energy by the limit $T \rightarrow 0$, i.e. $\beta \rightarrow \infty$

$$\boxed{E_1 = E_0 + \frac{1}{2} \sum_{\gamma\delta < F} \left[\langle \gamma\delta|V|\gamma\delta \rangle - \langle \delta\gamma|V|\gamma\delta \rangle \right]} . \tag{2.197}$$

In this expression the summation over single-particle states extends up to the Fermi energy since at zero temperature the occupation number becomes a step-function. The first term is the direct or “**Hartree**” term, the second one the exchange or “**Fock**” term for the energy ⁵⁷.

The number of “labeled” Feynman diagrams grows dramatically with the order of perturbation theory. As many have the same numerical value, it is useful to introduce “unlabeled” diagrams which are weighted by a **symmetry factor**. The modified Feynman rules for these types of diagrams are derived in the book of **Negele & Orland** and are not presented here. Likewise, it is obvious that in **homogeneous systems** further simplifications of the rules can be achieved by going over to energy and/or momentum representation.

2.7 Auxiliary Fields and Hartree Approximation

Perturbation theory, of course, fails at strong coupling and then the famous question arises “**What Is to Be Done?**” {**Lenin**}. Apart from a numerical evaluation of the (Euclidean) path integral there also exist analytical methods which are helpful in this case. These are based on the introduction of a **mean field** which is generated by the particles themselves and in which they move independently in lowest approximation. This approximation is physically plausible and the fundament for the successful description of atoms and nuclei by shell models.

In the path-integral formalism one derives these approaches most easily by transforming Eq. (2.132) for the time-evolution operator in the coherent basis. For a local (spinless) two-body interaction $V(\mathbf{x} - \mathbf{x}')$ this formula reads in position representation

$$U(\Phi_f^* t_f; \Phi_i t_i) = \int_{\Phi(t_i)=\Phi_i}^{\Phi(t_f)=\Phi_f^*} \mathcal{D}\Phi^*(\mathbf{x}, t) \mathcal{D}\Phi(\mathbf{x}, t) \exp\left(\int d^3x \Phi_f^*(\mathbf{x}) \Phi_f(\mathbf{x}) + \frac{i}{\hbar} S[\Phi^*, \Phi]\right) \quad (2.198)$$

with the action (see Eq. (2.107))

$$S[\Phi^*, \Phi] = \int_{t_i}^{t_f} dt \int d^3x \left[\Phi^*(\mathbf{x}, t) \left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \Delta}{2m} \right) \Phi(\mathbf{x}, t) - \frac{1}{2} \int d^3x' \Phi^*(\mathbf{x}, t) \Phi^*(\mathbf{x}', t) V(\mathbf{x} - \mathbf{x}') \Phi(\mathbf{x}', t) \Phi(\mathbf{x}, t) \right]. \quad (2.199)$$

As is well-known the last (quadri-linear) term prevents an evaluation of the path integral by analytical means. However, it is possible to express this interaction term formally by a term which is quadratically in the fields. This is based on the following identity for the (one-dimensional) Gaussian integral which we already have used in Eq. (1.167) (replace there $a \rightarrow -V/2$, $x \rightarrow ix$)

$$\exp\left(-\frac{i}{2} V x^2\right) = \frac{1}{\sqrt{2\pi i V}} \int_{-\infty}^{\infty} dy \exp\left(\frac{i}{2V} y^2 - iyx\right). \quad (2.200)$$

This is called “**undoing the square**” because on the r.h.s. the variable x now only appears linearly. As always such Gaussian integrals can be generalized to the multi-dimensional, even infinite-dimensional case – in many-body physics the corresponding identity is usually called the **Hubbard-Stratonovich transformation**. If we introduce the density

$$\rho(\mathbf{x}, t) := \Phi^*(\mathbf{x}, t) \Phi(\mathbf{x}, t) \quad (2.201)$$

⁵⁷In general this designation is not fully correct as the basis here is arbitrary and not optimal (selfconsistent), see the next chapter. However, for homogeneous systems plane waves are also the selfconsistent states.

then we may write the interaction term for bosons as well as for fermions (anticommute twice) in the form ⁵⁸

$$\frac{1}{2} \int d^3x d^3x' \Phi^*(\mathbf{x}, t) \Phi^*(\mathbf{x}', t) V(\mathbf{x} - \mathbf{x}') \Phi(\mathbf{x}', t) \Phi(\mathbf{x}, t) = \frac{1}{2} \int d^3x d^3x' \rho(\mathbf{x}, t) V(\mathbf{x} - \mathbf{x}') \rho(\mathbf{x}', t). \quad (2.202)$$

The functional generalization of Eq. (2.200) is then (we now set $\hbar = 1$)

$$\exp \left[-\frac{i}{2} \int dt \int d^3x d^3x' \rho(\mathbf{x}, t) V(\mathbf{x} - \mathbf{x}') \rho(\mathbf{x}', t) \right] = \text{const. } \mathcal{D}\text{et}^{-1/2}(V) \int \mathcal{D}\sigma(\mathbf{x}, t) \cdot \exp \left\{ i \int dt \left[\frac{1}{2} \int d^3x d^3x' \sigma(\mathbf{x}, t) (V^{-1})(\mathbf{x}, \mathbf{x}') \sigma(\mathbf{x}', t) - \int d^3x \rho(\mathbf{x}, t) \sigma(\mathbf{x}, t) \right] \right\}. \quad (2.203)$$

With that the matrix element (2.198) of the time-evolution operator assumes the form

$$U(\Phi_f^* t_f; \Phi_i t_i) = \exp \left(\int d^3x \Phi_f^*(\mathbf{x}) \Phi_f(\mathbf{x}) \right) \int \mathcal{D}\sigma(\mathbf{x}, t) W[\sigma] \int_{\Phi(t_i)=\Phi_i}^{\Phi(t_f)=\Phi_f^*} \mathcal{D}\Phi^*(\mathbf{x}, t) \mathcal{D}\Phi(\mathbf{x}, t) \cdot \exp \left[i \int dt \int d^3x \left(i \Phi^*(\mathbf{x}, t) \frac{\partial \Phi(\mathbf{x}, t)}{\partial t} - \mathcal{H}_\sigma(\Phi^*, \Phi) \right) \right], \quad (2.204)$$

where

$$\mathcal{H}_\sigma(\Phi^*, \Phi) = \Phi^*(\mathbf{x}, t) \left(-\frac{\Delta}{2m} \right) \Phi(\mathbf{x}, t) + \sigma(\mathbf{x}, t) \Phi^*(\mathbf{x}, t) \equiv \Phi^*(\mathbf{x}, t) \hat{H}_\sigma \Phi(\mathbf{x}, t) \Phi(\mathbf{x}, t) \quad (2.205)$$

is the Hamilton density of particles moving independently in the auxiliary field $\sigma(\mathbf{x}, t)$ and thus a **single-particle** operator (c.f. Eq. (2.100)). However, one has to integrate functionally over this auxiliary field with the weight

$$W[\sigma] = \text{const. } \exp \left[\frac{i}{2} \int dt \int d^3x d^3x' \sigma(\mathbf{x}, t) (V^{-1})(\mathbf{x}, \mathbf{x}') \sigma(\mathbf{x}', t) \right] \quad (2.206)$$

which contains the information about the actual two-body interaction $V(\mathbf{x} - \mathbf{x}')$. Note that this weight does not have a kinetic term for the auxiliary field $\sigma(\mathbf{x}, t)$ with the consequence that the σ -configurations can be very "rough", i.e. discontinuous, similar as in the phase-space path integral.

The Hubbard-Stratonovich transform gives the exact expression (2.204) in which we can calculate the single-particle problem in the auxiliary field but not the subsequent functional integral over $\sigma(\mathbf{x}, t)$ – which illustrates the well-known principle of conservation of difficulties ... However, if we apply the **stationary phase approximation** to the σ -functional integral we get a meaningful approximation which can be improved systematically. The auxiliary field which makes the action in Eq. (2.204) stationary is obtained by variation of the σ -dependent exponents w.r.t. $\sigma(\mathbf{x}, t)$:

$$\int d^3x (V^{-1})(\mathbf{x}, \mathbf{x}') \sigma(\mathbf{x}', t) - \rho(\mathbf{x}, t) \stackrel{!}{=} 0, \quad (2.207)$$

i.e. the stationary auxiliary field is the average of the two-body interaction over the density of the particles:

$$\sigma_0(\mathbf{x}, t) = \int d^3x' V(\mathbf{x} - \mathbf{x}') \rho(\mathbf{x}, t), \quad (2.208)$$

⁵⁸In the treatment by **Negele & Orland**, ch. 7 unphysical selfenergy terms arise which are canceled in higher orders.

and thus the expected mean field. If we consider a fermionic system with N particles we may expand w.r.t. eigenfunctions $\varphi_k(\mathbf{x}, t)$ of the single-particle time-evolution operator. The ground state wave function in the (fixed) auxiliary field $\sigma_0(\mathbf{x}, t)$ is a **Slater determinant**

$$\Psi_H(\mathbf{x}_1 \dots \mathbf{x}_N, t) = \frac{1}{\sqrt{N!}} \det_{j,k} [\varphi_k(\mathbf{x}_j, t)] \quad (2.209)$$

built from this complete, orthonormal single-particle basis and the density is given by the sum over all occupied single-particle states

$$\rho(\mathbf{x}, t) = \sum_{k=1}^N |\varphi_k(\mathbf{x}, t)|^2. \quad (2.210)$$

Due to the Hubbard-Stratonovich transformation the remaining functional integral over φ^*, φ is a Gaussian integral to which we may apply the stationary-phase method as well (which gives the exact result in this case). By variation w.r.t. $\varphi_k^*(\mathbf{x}, t)$ we then obtain the Schrödinger equation

$$i \frac{\partial \varphi_k(\mathbf{x}, t)}{\partial t} = -\frac{\Delta}{2m} \varphi_k(\mathbf{x}, t) + \sigma_0(\mathbf{x}, t) \varphi_k(\mathbf{x}, t) \quad (2.211)$$

for the motion in the mean field $\sigma_0(\mathbf{x}, t)$. Eqs. (2.208-2.211) are coupled equations and define the well-known **Hartree approximation**.

If we assume a time-independent mean field $\sigma(\mathbf{x})$ the time dependence of the single-particle wave functions can be separated, i.e. we can set $\varphi_k(\mathbf{x}, t) = \varphi_k(\mathbf{x}) \exp(-i\epsilon_k t)$ and then has to solve the non-linear Schrödinger equation

$$\left[-\frac{\Delta}{2m} + \sum_{l=1}^N \int d^3x' V(\mathbf{x} - \mathbf{x}') |\varphi_l(\mathbf{x}')|^2 \right] \varphi_k(\mathbf{x}) = \epsilon_k \varphi_k(\mathbf{x}). \quad (2.212)$$

If this would be a normal Schrödinger equation then the total energy would be

$$\sum_{k=1}^N \epsilon_k = \sum_{k=1}^N \left\langle \varphi_k \left| -\frac{\Delta}{2m} \right| \varphi_k \right\rangle + \sum_{k,l} \left\langle \varphi_k \varphi_l | \hat{V} | \varphi_k \varphi_l \right\rangle,$$

where the last relation follows from Eq. (2.212) after multiplying with $\varphi_k^*(\mathbf{x})$, integrating over \mathbf{x} and using the orthonormality of the eigenfunctions. Obviously, the potential energy has been counted twice in this procedure. The correct relation is obtained from the resolvent

$$G(E) = \text{tr} \left(\frac{1}{E - \hat{H} + i0^+} \right) = -i \int_0^\infty dT e^{iET} \text{tr} \hat{U}(T, 0), \quad (2.213)$$

which in the N -particle sector in a fixed basis of Slater determinants Ψ_k takes the form

$$G_N(E) = -i \sum_{k_1 \dots k_N} \int_0^\infty dT e^{iET} \int \mathcal{D}\sigma \exp \left[\frac{i}{2} \int_0^T \int d^3x d^3x' \sigma(\mathbf{x}) V^{-1}(\mathbf{x}, \mathbf{x}') \sigma(\mathbf{x}') + \ln \left\langle \Psi_k | \hat{U}_\sigma(T, 0) | \Psi_k \right\rangle \right] \quad (2.214)$$

where $\hat{U}_\sigma(T, 0) = \mathcal{T} \exp \left(-i \int_0^T dt \hat{H}_\sigma \right)$ is the time-evolution operator for independent particles in the potential $\sigma(\mathbf{x}, t)$. In static Hartree approximation this becomes

$$G_N(E) \simeq -i \sum_{k_1 \dots k_N} \int_0^\infty dT e^{iET} \exp \left[\frac{iT}{2} \int d^3x d^3x' \sigma_0(\mathbf{x}) V^{-1}(\mathbf{x}, \mathbf{x}') \sigma_0(\mathbf{x}') - iT \sum_{i=1}^N \epsilon_{k_i} \right]. \quad (2.215)$$

The pole of the resolvent gives us the total energy

$$E_H = \sum_{k=1}^N \epsilon_k - \frac{1}{2} \int d^3x d^3x' \sigma_0(\mathbf{x}) V^{-1}(\mathbf{x}, \mathbf{x}') \sigma_0(\mathbf{x}') = \sum_{k=1}^N \left\langle \varphi_k \left| -\frac{\Delta}{2m} \right| \varphi_k \right\rangle + \frac{1}{2} \sum_{k,l} \left\langle \varphi_k \varphi_l | \hat{V} | \varphi_k \varphi_l \right\rangle, \quad (2.216)$$

in which the potential energy between the particles has been counted correctly. In contrast to the perturbation theory considered in the last chapter, now the single-particle wave functions are not specified anymore but have to be determined **self-consistently** from Eq. (2.212) which contains the interaction potential as well. This is essential for finite systems (electrons in an atom, nucleons in a nucleus).

An obvious disadvantage of this approximation is the violation of translational invariance: While the two-body potential $V(\mathbf{x} - \mathbf{x}')$ is unchanged by a shift of coordinates, the mean field $\sigma_0(\mathbf{x})$ has a fixed origin (for which one usually takes the center of mass of the system).

It is clear that one can calculate systematic corrections to the lowest order stationary-phase approximation. Taking into account the quadratic fluctuations leads to the so-called **RPA**⁵⁹ corrections to the Hartree approximation.

Detail 22: RPA Corrections

Following **Negele & Orland**, p. 344 - 348 (beware of misprints!) we make the change of variables $\sigma(\mathbf{x}, t) = \sigma_0(\mathbf{x}) + \eta(\mathbf{x}, t)$ where $\sigma_0(\mathbf{x})$ is the Hartree solution and expand the exponential in the resolvent of Eq. (2.214) up to second order in η . This gives

$$G_N(E) = \mathcal{N} \sum_{k_1 \dots k_N} (-i) \int_0^\infty dT e^{i(E-E_H)T} \int \mathcal{D}\eta \exp \left\{ -\frac{1}{2} \int d1 d2 \eta(1) \underbrace{\left[-iv^{-1}(1,2) - \frac{\delta^2 \ln \langle \Psi_k | U_\sigma | \Psi_k \rangle}{\delta\sigma(1)\delta\sigma(2)} \Big|_{\sigma=\sigma_0} \right]}_{=: \Gamma^{-1}(1,2)} \eta(2) + \mathcal{O}(\eta^3) \right\} \quad (2.217a)$$

because the terms independent of η generate the Hartree energy E_H and the first-order term vanishes due to the stationary-phase approximation. To simplify the notation we abbreviate $1 \equiv (\mathbf{x}_1, t_1)$ etc. and set $v^{-1}(1,2) := \delta(t_1 - t_2)(V^{-1})(\mathbf{x}_1, \mathbf{x}_2)$. Time integrations run from zero to T . In quadratic approximation the η -integral gives

$$\mathcal{Z} = \mathcal{N} \left[\mathcal{D}\text{et}(\Gamma^{-1}) \right]^{-1/2} = \left[\frac{\mathcal{D}\text{et}(\Gamma^{-1})}{\mathcal{D}\text{et}(-iv^{-1})} \right]^{-1/2} = \left[\mathcal{D}\text{et}(iv\Gamma^{-1}) \right]^{-1/2} \quad (2.217b)$$

where we normalize to the case of first-order interaction. Evaluation of the derivative appearing in Γ leads to

$$\frac{\delta^2 \ln \langle \Psi_H | U_\sigma | \Psi_H \rangle}{\delta\sigma(1)\delta\sigma(2)} \Big|_{\sigma=\sigma_0} = - \langle \Psi_H | \mathcal{T}(\hat{\psi}^\dagger(1)\hat{\psi}(2)) | \Psi_H \rangle \langle \Psi_H | \mathcal{T}(\hat{\psi}(1)\hat{\psi}^\dagger(2)) | \Psi_H \rangle \quad (2.217c)$$

where

$$\hat{\psi}^\dagger(1) = \exp(ih_{\sigma_0} t_1) \hat{\psi}^\dagger(\mathbf{x}_1) \exp(-ih_{\sigma_0} t_1) \quad (2.217d)$$

is the creation operator for a particle at space-time "1" in the Heisenberg representation for the Hartree Hamiltonian. Introducing the Hartree Green function $G(1,2) := -i \langle \Psi_H | \mathcal{T}(\hat{\psi}(1)\hat{\psi}^\dagger(2)) | \Psi_H \rangle$ and the Hartree particle-hole propagator (depicted graphically in Fig. 17 (a))

$$iD_0(1,2) := G(1,2)G(2,1) \quad (2.217e)$$

one obtains for the quadratic fluctuations

$$\mathcal{Z} = \left[\mathcal{D}\text{et}(1 - vD_0) \right]^{-1/2} = \exp \left[\frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{n} \text{tr}((vD_0)^n) \right]. \quad (2.217f)$$

The n th term in the exponent reads

$$\frac{1}{2n} \int_0^T dt_1 d^3x_1 d^3x'_1 \dots dt_n d^3x_n d^3x'_n V(\mathbf{x}_1 - \mathbf{x}_2) D_0(\mathbf{x}'_1 t_1, \mathbf{x}_2 t_2) \dots V(\mathbf{x}'_n - \mathbf{x}_n) D_0(\mathbf{x}'_n t_n, \mathbf{x}_1 t_1) \quad (2.217g)$$

and can be represented by a **ring** diagram as shown in Fig. 17 (b).

Writing $\mathcal{Z} \sim \exp(-iET)$ for $T \rightarrow \infty$ one can read off the contributions to the energies from the quadratic fluctuations: The $n = 1$ -term provides the exchange energy which was absent in the Hartree approximation and the higher terms give the RPA-energy

$$E_{\text{RPA}} = \lim_{T \rightarrow \infty} \frac{i}{2T} \sum_{n=2}^{\infty} \frac{1}{n} \text{tr}(D_0 V)^n. \quad (2.217h)$$

As already mentioned the RPA correction also contains the exchange ("Fock") term (2.197) for the energy. One may wonder why this term does not appear already in the lowest order; in the case of nuclear forces, for

⁵⁹for "**Random Phase Approximation**", the name traditionally given for this approximation although it is not very illuminating in the present context ...

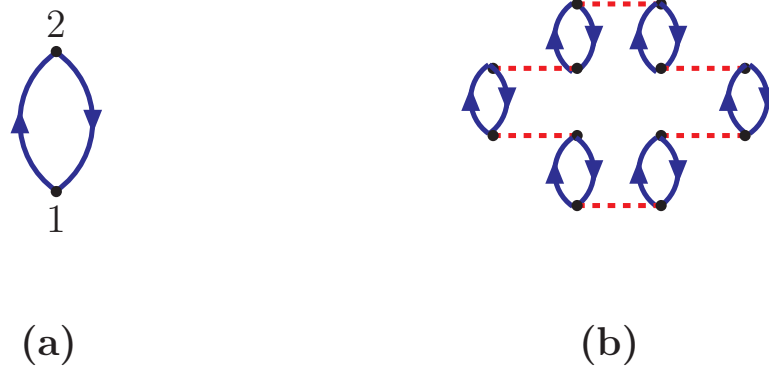


Fig. 17 : (a) Graphical representation of the particle-hole propagator $D_0(1, 2)$.
 (b) Graphical representation of the $n = 6$ term in the expansion (2.217f) for the RPA corrections.

example, it is much more attractive than the direct ("Hartree") term which does not even bind the nucleons if realistic interactions are used. As a matter of fact one has considerable freedom to modify the lowest order result by a different grouping of fields than used in Eq. (2.202) and it is indeed possible to obtain the Hartree-Fock approximation or more advanced approximations as lowest-order result of the stationary-phase method ⁶⁰. This is due to a lack of a systematic expansion parameter: Since Planck's elementary quantum \hbar also shows up in the action (2.199) the stationary-phase method is not a semi-classical approximation anymore. Different choices of the zeroth approximation for which one then calculates corrections correspond to an arbitrary split-up of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$ and must be justified by the physics of the particular problem.

2.8 Asymptotic Expansion of a Class of Path Integrals

In contrast to perturbation theory for weak coupling a general expansion for strong coupling is not available. This is due to the (much deplored) inability to calculate non-gaussian functional integrals by analytic methods. However, following a work of Luttinger [36] it is possible to evaluate a particular class of path integrals asymptotically. This will be presented in this chapter and applied to the polaron problem. Although only the single-particle problem is treated here, methods of many-body physics are used and the polaron problem (a single-particle problem after integrating out the phonons) really belongs to "infinite-particle" physics, i.e. to field theory.

We begin with the expression (2.4) for the partition function of a particle moving (in 3 dimensions) under the influence of an external potential (in the following we set $\hbar = 1$)

$$Z(\beta) = \text{tr} \left(e^{-\beta \hat{H}} \right) = \oint_{\mathbf{x}(0)=\mathbf{x}(\beta)} \mathcal{D}^3 x \exp \left[- \int_0^\beta d\tau \left(\frac{m}{2} \dot{\mathbf{x}}^2 + V(\mathbf{x}) \right) \right], \quad (2.218)$$

From the partition function we may determine the ground-state energy by taking the limit $\beta \rightarrow \infty$:

$$E_0 = \lim_{\beta \rightarrow \infty} \left\{ -\frac{1}{\beta} \ln Z(\beta) \right\}. \quad (2.219)$$

⁶⁰For example, the nuclear pairing force can be included via the so-called Hartree-Fock-Bogoliubov approximation [40].

It can be shown that the partition function (2.218) can also be represented by the following path integral over bosonic fields $\Phi(\mathbf{x}), \Phi^*(\mathbf{x})$ and fermionic (Grassmann-valued) fields $\eta(\mathbf{x}), \bar{\eta}(\mathbf{x})$:

$$Z(\beta) = \int \mathcal{D}\Phi^* \mathcal{D}\Phi \mathcal{D}\bar{\eta} \mathcal{D}\eta \int d^3x \bar{\eta}(\mathbf{x}) \eta(\mathbf{x}) \delta\left((\Phi^*, \Phi) + (\bar{\eta}, \eta) - 1\right) \cdot \exp\left\{-\beta\left[(\Phi^*, H\Phi) + (\bar{\eta}, H\eta)\right]\right\}. \quad (2.220)$$

Here we have used the abbreviations

$$(\Phi^*, \mathcal{O}\Phi) := \int d^3x d^3y \Phi^*(\mathbf{x}) \langle \mathbf{x} | \hat{\mathcal{O}} | \mathbf{y} \rangle \Phi(\mathbf{y}), \quad (\bar{\eta}, \eta) := \int d^3x d^3y \bar{\eta}(\mathbf{x}) \langle \mathbf{x} | \hat{\mathcal{O}} | \mathbf{y} \rangle \eta(\mathbf{y}) \quad (2.221)$$

for the operators $\hat{\mathcal{O}} = \hat{1}, \hat{H}$ and the bosonic path integral has been normalized to

$$\int \mathcal{D}\Phi^* \mathcal{D}\Phi \exp[-(\Phi^*, \Phi)] = 1. \quad (2.222)$$

Detail 23: Luttinger's Path-Integral Relation

Due to the constraint by the δ -function we can also write Eq. (2.220) as

$$Z(\beta) = e^{-\beta E_0} \int \mathcal{D}\Phi^* \mathcal{D}\Phi \mathcal{D}\bar{\eta} \mathcal{D}\eta \int d^3x \bar{\eta}(\mathbf{x}) \eta(\mathbf{x}) \delta\left((\Phi^*, \Phi) + (\bar{\eta}, \eta) - 1\right) \cdot \exp\left\{-\beta\left[(\Phi^*, h\Phi) + (\bar{\eta}, h\eta)\right]\right\} \quad (2.223a)$$

where $h := H - E_0$ has only positive eigenvalues. If we use the Fourier representation of the δ -function

$$\delta\left((\Phi^*, \Phi) + (\bar{\eta}, \eta) - 1\right) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega \exp\left\{-i\omega\left[(\Phi^*, \Phi) + (\bar{\eta}, \eta)\right] + i\omega\right\} \quad (2.223b)$$

then we can perform the integrations over bosonic and fermionic auxiliary fields by means of Eq. (2.149) :

$$\begin{aligned} \int \mathcal{D}\Phi^* \mathcal{D}\Phi \exp[-(\Phi^*, (i\omega + \beta h)\Phi)] &= \frac{1}{\mathcal{D}\text{et}(i\omega + \beta \hat{h})} \\ \int \mathcal{D}\bar{\eta} \mathcal{D}\eta \int \underbrace{d^3x \bar{\eta}(\mathbf{x}) \eta(\mathbf{x})}_{\equiv (\bar{\eta}, \eta)} \exp[-(\bar{\eta}, (i\omega + \beta h)\eta)] &= i \frac{\partial}{\partial \omega} \int \mathcal{D}\bar{\eta} \mathcal{D}\eta \exp[-(\bar{\eta}, (i\omega + \beta h)\eta)] \\ &= i \frac{\partial}{\partial \omega} \mathcal{D}\text{et}(i\omega + \beta \hat{h}) \\ &= -\text{tr}\left((i\omega + \beta \hat{h})^{-1}\right) \mathcal{D}\text{et}(i\omega + \beta \hat{h}). \end{aligned} \quad (2.223c)$$

In the last line the result of **Problem 13 b)** for the differentiation of a determinant w.r.t. a parameter has been used. We see that the inverse determinant from the bosonic and the determinant from the fermionic integration cancel. With the theorem of residues we then indeed obtain

$$Z(\beta) = -e^{-\beta E_0} \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{i\omega} \text{tr}\left(\frac{1}{i\omega + \beta \hat{h}}\right) = e^{-\beta E_0} \frac{i}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{i\omega} \text{tr}\left(\frac{1}{\omega - i\beta(\hat{H} - E_0)}\right) = \text{tr}\left(e^{-\beta \hat{H}}\right), \quad (2.223e)$$

as we have to close the integration contour in the upper half plane where all the poles are located.

On first sight the representation (2.220) looks like an unnecessary complication of the “simple” path integral over **trajectories**: Now one integrates over bosonic and fermionic **fields**! However, as we will see shortly, this representation has some advantages:

If we express on the l.h.s. the term

$$\int_0^\beta d\tau V(\mathbf{x}(\tau)) = \beta \int d^3x L_\beta(\mathbf{x}) V(\mathbf{x}) \quad (2.224)$$

by the “local time”

$$L_\beta(\mathbf{x}) := \frac{1}{\beta} \int_0^\beta d\tau \delta(\mathbf{x} - \mathbf{x}(\tau)) \quad (2.225)$$

then the interaction term has the same form as on the r.h.s. where

$$\begin{aligned} (\Phi^*, H\Phi) + (\bar{\eta}, H\eta) &= \underbrace{\int d^3x \Phi^*(\mathbf{x}) \left(-\frac{\Delta}{2m} \right) \Phi(\mathbf{x})}_{=(\Phi^*, H_0\Phi)} + \int d^3x \Phi^*(\mathbf{x}) V(\mathbf{x}) \Phi(\mathbf{x}) \\ &+ (\bar{\eta}, H_0\eta) + \int d^3x \bar{\eta}(\mathbf{x}) V(\mathbf{x}) \eta(\mathbf{x}) \end{aligned} \quad (2.226)$$

show up. We thus see that going from a description by paths to a description by fields amounts to the replacement

$$L_\beta(\mathbf{x}) \longrightarrow \Phi^*(\mathbf{x}) \Phi(\mathbf{x}) + \bar{\eta}(\mathbf{x}) \eta(\mathbf{x}). \quad (2.227)$$

Now one can multiply both sides by an arbitrary functional of V (let’s call it $\Gamma[V]$) and functionally integrate over both sides; in this way we extend the class of simple path integrals over one-time actions to more general forms. If the functional $F_\beta[L_\beta]$ is defined by

$$\exp(-\beta F_\beta[L_\beta]) := \int \mathcal{D}V \Gamma[V] \exp\left(-\beta \int d^3x L_\beta(\mathbf{x}) V(\mathbf{x})\right) \quad (2.228)$$

then the relation

$$\begin{aligned} \oint \mathcal{D}^3x \exp\{-S_0[x] - \beta F_\beta[L_\beta]\} &= \int \mathcal{D}\Phi^* \mathcal{D}\Phi \mathcal{D}\bar{\eta} \mathcal{D}\eta \int d^3x \bar{\eta}(\mathbf{x}) \eta(\mathbf{x}) \delta(\Phi^*, \Phi) + (\bar{\eta}, \eta) - 1 \\ &\cdot \exp\left\{-\beta[(\Phi^*, H_0\Phi) + (\bar{\eta}, H_0\eta)] - \beta F_\beta[\Phi^*\Phi + \bar{\eta}\eta]\right\} \end{aligned} \quad (2.229)$$

follows. This means that we can “translate” path integrals over more general functionals into functional integrals over fields – but unfortunately, in general we also cannot “do” the latter ones... However, in the limit $\beta \rightarrow \infty$ the r.h.s. of Eq. (2.229) simplifies: If one scales $\eta \rightarrow \eta/\beta$, $\bar{\eta} \rightarrow \bar{\eta}/\beta$ then we know that the fermionic “measure” transforms with the inverse Jacobian, i.e. all $\bar{\eta}, \eta$ -integrals remain invariant. This means that the fermionic parts in the integrand are suppressed and that asymptotically the partition function is determined solely by the bosonic integral

$$\begin{aligned} \lim_{\beta \rightarrow \infty} \oint \mathcal{D}^3x \exp\{-S_0[x] - \beta F_\beta[L_\beta]\} &= \int \mathcal{D}\Phi^* \mathcal{D}\Phi \int d^3x \bar{\eta}(\mathbf{x}) \eta(\mathbf{x}) \delta(\Phi^*, \Phi) - 1 \\ &\cdot \exp\left\{-\beta(\Phi^*, H_0\Phi) - \beta F_{\beta \rightarrow \infty}[\Phi^*\Phi]\right\}. \end{aligned} \quad (2.230)$$

The leading term of this integral may be determined by **Laplace’s method** (see Eq. (1.130c)): Recall that for large values of a parameter in the exponential function of the integral only the minimum of the function (here: of the functional) contributes which is multiplied by this parameter. Therefore we obtain from Eq. (2.219)

$$\boxed{E_0 = \min_{(\Phi^*, \Phi)=1} \left\{ (\Phi^*, H_0\Phi) + F_\infty[\Phi^*\Phi] \right\}.} \quad (2.231)$$

Applications:

a) Quantum Mechanics : If $F_\beta[L_\beta] = \int d^3x L_\beta(\mathbf{x}) U(\mathbf{x})$, then Eq. (2.231) is nothing else than the Rayleigh-Ritz variational principle for the motion of a non-relativistic particle in the potential $U(\mathbf{x})$. Unconstraint variation w.r.t. the normalized (wave) function $\Phi^*(\mathbf{x})$ gives the usual time-independent **linear Schrödinger equation**.

b) Polaron in the Limit of Strong Coupling : For arbitrary coupling constants the interaction term in the effective action of the polaron (after integrating out the phonons) does **not** have a form so that it can be expressed solely in terms of the “local time” (2.225). However, this is the case for large coupling constants as can be seen by scaling [37]

$$\begin{aligned} \bar{\tau} &= \lambda\tau, & \bar{\mathbf{x}}(\bar{\tau}) &= \sqrt{\lambda}\mathbf{x}(\tau) & \lambda > 0 \\ \Rightarrow \frac{1}{2} \int_0^\beta d\tau \left(\frac{\mathbf{x}(\tau)}{d\tau} \right)^2 &\longrightarrow \frac{1}{2} \int_0^{\lambda\beta} d\bar{\tau} \left(\frac{\bar{\mathbf{x}}(\bar{\tau})}{d\bar{\tau}} \right)^2 \\ -\frac{\alpha}{\sqrt{2}} \int_0^\beta d\tau d\tau' \frac{G_\beta(\tau - \tau')}{|\mathbf{x}(\tau) - \mathbf{x}(\tau')|} &\longrightarrow -\frac{\alpha}{\sqrt{2}} \frac{1}{\lambda^{3/2}} \int_0^{\lambda\beta} d\bar{\tau} d\bar{\tau}' \frac{G_\beta((\tau - \tau')/\lambda)}{|\bar{\mathbf{x}}(\bar{\tau}) - \bar{\mathbf{x}}(\bar{\tau}')|}. \end{aligned} \quad (2.232)$$

Here (cf. Eq. (2.27k))

$$G_\beta(t) = \frac{\cosh(\beta/2 - |t|)}{2 \sinh(\beta/2)}$$

is the polaron retardation function for finite β . If we choose

$$\lambda = (\kappa \alpha \beta)^2 \quad (2.233)$$

(with an arbitrary numerical factor κ), then we see that for fixed β the retardation vanishes for $\alpha \rightarrow \infty$ and that in this case the polaron self-interaction can indeed be written as a functional of the local time. Replacing the primed quantities by unprimed ones we get

$$\begin{aligned} -\frac{\alpha}{\sqrt{2}} \frac{1}{\lambda} \frac{G_\beta(0)}{\kappa \alpha \beta} \int_0^{\lambda\beta} d\tau d\tau' \frac{1}{|\mathbf{x}(\tau) - \mathbf{x}(\tau')|} &= -\frac{G_\beta(0)}{\kappa \sqrt{2}} \frac{1}{T} \int_0^T d\tau d\tau' \frac{1}{|\mathbf{x}(\tau) - \mathbf{x}(\tau')|} \\ &\equiv T \int d^3x d^3y L_T(\mathbf{x}) \left(-\frac{G_\beta(0)}{\kappa \sqrt{2}} \frac{1}{|\mathbf{x} - \mathbf{y}|} \right) L_T(\mathbf{y}). \end{aligned} \quad (2.234)$$

Instead of the Euclidean time β we now have the quantity

$$T = \lambda \beta \quad (2.235)$$

which also becomes asymptotically large in the limit of strong coupling and finite β . Hence we can apply Luttinger’s method and from Eq. (2.231) and the choice (2.233) we obtain for the free energy

$$F(\beta, \alpha) \xrightarrow{\alpha \rightarrow \infty} \frac{\alpha^2 \beta^2}{\beta} G_\beta(0) \gamma_P = \beta \frac{1}{2} \coth(\beta/2) \gamma_P \alpha^2 \quad (2.236)$$

with

$$\gamma_P = \kappa^2 \min_{(\Phi^*, \Phi)=1} \left\{ \int d^3x \Phi^*(\mathbf{x}) \left(-\frac{\Delta}{2} \right) \Phi(\mathbf{x}) - \frac{1}{\kappa \sqrt{2}} \int d^3x d^3y \frac{\Phi^{*2}(\mathbf{x}) \Phi^2(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \right\}. \quad (2.237)$$

The free energy should tend to the ground-state energy for small temperature (large β). Unfortunately, we cannot perform the limit $\beta \rightarrow \infty$ in Eq. (2.236) anymore as essential parts of the action have been removed by the ($\alpha \rightarrow \infty$) - limit - obviously, both limits do not commute. The general property that the

free energy is always smaller than the ground-state energy and grows monotonically with β (**Problem 16**) comes to our rescue. In the limit $\beta \rightarrow 0$ we have

$$\beta \frac{1}{2} \coth(\beta/2) \xrightarrow{\beta \rightarrow 0} \beta \frac{1}{\beta} = 1, \quad (2.238)$$

so that $F(0) = \gamma_P \alpha^2$ is a **lower bound** for the ground-state energy of the strong-coupling polaron. Exactly the same result had been derived much earlier by Pekar by a quantum-mechanical *ansatz* for the total wave function of electron + phonon system [38] in a Rayleigh-Ritz variational calculation. Since it is basic knowledge that the variational principle leads to an **upper bound** for the true ground-state energy, the equality of these two bounds allows the conclusion that indeed the ground-state energy of the polaron at strong coupling is given by ⁶¹

$$\boxed{E_0 \xrightarrow{\alpha \rightarrow \infty} \gamma_P \alpha^2.} \quad (2.239)$$

Independent variation of the functional (2.237) w.r.t. Φ^* and Φ gives

$$-\frac{\Delta}{2} \Phi(\mathbf{r}) + \int d^3 y \Phi^2(\mathbf{y}) V(\mathbf{r}, \mathbf{y}) \cdot \Phi^*(\mathbf{r}) - \epsilon_0 \Phi(\mathbf{r}) = 0 \quad (2.240)$$

$$-\frac{\Delta}{2} \Phi^*(\mathbf{r}) + \int d^3 x \Phi^{*2}(\mathbf{x}) V(\mathbf{x}, \mathbf{r}) \cdot \Phi(\mathbf{r}) - \epsilon_0 \Phi^*(\mathbf{r}) = 0, \quad (2.241)$$

where the constraint $(\Phi^*, \Phi) = 1$ has been incorporated into the functional by a Lagrange multiplier $\epsilon_0 ((\Phi^*, \Phi) - 1)$. We see that $\Phi^* = \Phi$ is a solution since the interaction has the property

$$V(\mathbf{x}, \mathbf{y}) := -\frac{\sqrt{2}}{\kappa} \frac{1}{|\mathbf{x} - \mathbf{y}|} = V(\mathbf{y}, \mathbf{x}). \quad (2.242)$$

Therefore we can write Eq. (2.237) also as

$$\gamma_P = \kappa^2 \min_{(\Phi, \Phi)=1} \left\{ \int d^3 x \Phi(\mathbf{x}) \left(-\frac{\Delta}{2} \right) \Phi(\mathbf{x}) + \frac{1}{2} \int d^3 x d^3 y \Phi^2(\mathbf{x}) V(\mathbf{x}, \mathbf{y}) \Phi^2(\mathbf{y}) \right\}. \quad (2.243)$$

The numerical value of $\kappa > 0$ is irrelevant because the scaling behaviour of the Coulomb-like interaction (2.242) compensates other values. Usually one chooses $\kappa = 1$ [37] but one also could take the value $\kappa = \sqrt{2}$ which simplifies the interaction (2.242).

Pekar's *ansatz* which leads to the exact result for strong coupling, is built on the intuitive picture that in this limit the ‘bare’ electron moves so fast ⁶² that the phonons only feel a mean field $\Phi^2(\mathbf{x})$. Actually Eq. (2.243) is identical with the **Hartree approximation** of the previous chapter and the variational equation

$$-\frac{\Delta}{2} \Phi(\mathbf{r}) + \int d^3 x V(\mathbf{r}, \mathbf{x}) \Phi^2(\mathbf{x}) \cdot \Phi(\mathbf{r}) = \epsilon_0 \Phi(\mathbf{r}), \quad (2.244)$$

a **non-linear** Schrödinger equation, is identical with the Hartree equation (2.212). If we multiply Eq. (2.244) with $\Phi(\mathbf{r})$ and integrate over \mathbf{r} , then we obtain by means of the normalization and by comparison with Eq. (2.243)

$$\epsilon_0 = (\Phi, H_0 \Phi) + (\Phi^2, V \Phi^2) = \frac{E_0}{\kappa^2 \alpha^2} + \frac{1}{2} (\Phi^2, V \Phi^2), \quad (2.245)$$

in agreement with the result (2.216) of the Hartree approximation.

⁶¹Rigorously proven by Lieb and Thomas [39].

⁶²In contrast, at fixed momentum the ‘dressed’ electron = polaron moves slower and slower since its effective mass grows $\propto \alpha^4$.

Choosing simple *ansätze* for $\Phi(\mathbf{x})$ the minimal principle (2.243) can be evaluated and one finds (**Problem 18 a) b)**)

$$\gamma_P = -\frac{25}{256} = -0.0977 \quad \text{for} \quad \Phi(\mathbf{x}) = C e^{-r/a} \quad (2.246)$$

$$\gamma_P = -\frac{1}{3\pi} = -0.1061 \quad \text{for} \quad \Phi(\mathbf{x}) = C e^{-r^2/a^2}. \quad (2.247)$$

The result (2.247) is exactly the same as obtained by Feynman's quadratic retarded trial action at large coupling (see **Problem 11 b)**). This is not surprising since we have seen that in this limit the retardation does not play a role and since we know that quadratic (local) actions correspond to oscillator-like wave functions.

How can we determine the exact value for the Pekar constant γ_P , i.e. for the polaron ground-state energy at large coupling? One option is to use better and better variational functions in the minimum principle (2.243), another possibility is to determine γ_P numerically from the Hartree equation (2.244). Since this equation is a non-linear one, we have to solve it iteratively until the wave function, which also determines the interaction, is obtained **selfconsistently**.

Here we choose the first option and determine the Pekar coefficient γ_P by variation of the coefficient in a suitable *ansatz* for the S-wave⁶³

$$\Phi(\mathbf{r}) = \frac{y(r)}{r} \frac{1}{\sqrt{4\pi}}, \quad r \equiv |\mathbf{r}|. \quad (2.248)$$

This projects the monopole part out of the Coulomb interaction

$$\int d\Omega_x d\Omega_y \frac{1}{|\mathbf{x} - \mathbf{y}|} = \frac{(4\pi)^2}{\max(|\mathbf{x}|, |\mathbf{y}|)}, \quad (2.249)$$

so that the minimal functional reads (we choose $\kappa = 1$)

$$\gamma_P = \min_{(y,y)=1} \left[\langle T \rangle + \langle V \rangle \right] \quad (2.250)$$

with

$$\int_0^\infty dr y^2(r) = 1, \quad \langle T \rangle = \frac{1}{2} \int_0^\infty dr y'^2(r), \quad \langle V \rangle = -\frac{1}{\sqrt{2}} \int_0^\infty dr y^2(r) \int_0^\infty ds \frac{y^2(s)}{\max(r, s)}. \quad (2.251)$$

Detail 24: Numerical Treatment and FORTRAN Program

The simplest *ansatz* which generalizes the trial wave function in **Problem 18 b)** and represents a complete function system for $N \rightarrow \infty$, is

$$y(r) = C r \sum_{i=0}^N c_i \left(\frac{r}{a} \right)^i e^{-r/a}, \quad c_0 \equiv 1. \quad (2.252a)$$

With the help of the integral

$$\int_x^\infty dt t^n e^{-\lambda t} = \frac{n!}{\lambda^{n+1}} e^{-\lambda x} \sum_{j=0}^n \frac{(\lambda x)^j}{j!}, \quad \text{in particular: } \int_0^\infty dt t^n e^{-\lambda t} = \frac{n!}{\lambda^{n+1}} \quad (2.252b)$$

(which can be obtained by subsequent integrations by parts) one easily finds the normalization of the trial wave function (2.252a)

$$C^{-2} = a^3 \sum_{i,j=0}^N c_i c_j d_{i+j+2}, \quad \text{with } d_n := \frac{n!}{2^{n+1}}, \quad (2.252c)$$

⁶³We assume that the ground-state wave function is spherically symmetric which is always the case for rotationally symmetric problems in quantum mechanics.

the expectation value of the kinetic energy

$$\langle T \rangle = \frac{1}{2} C^2 a \sum_{i,j=0}^N c_i c_j \left[(i+1)(j+1) d_{i+j} - d_{i+j+2} \right], \quad (2.252d)$$

and of the potential (self-)energy

$$\langle V \rangle = -\sqrt{2} C^4 a^5 \sum_{i,j,k,l=0}^N c_i c_j \frac{1}{2^{i+j+3}} c_k c_l d_{k+l+1} \sum_{m=0}^{k+l+1} \frac{d_{i+j+m+2}}{m!}. \quad (2.252e)$$

Due to the simple scaling properties ($C^2 \sim a^{-3}$, $\langle T \rangle \sim a^{-2}$, $\langle V \rangle \sim a^{-1}$) the variation w.r.t. the scaling parameter a can be performed analytically:

$$\frac{\partial}{\partial a} \left[\frac{1}{a^2} \langle T \rangle_{a=1} + \frac{1}{a} \langle V \rangle_{a=1} \right] = 0 \implies a_{\text{optimal}} = -2 \frac{\langle T \rangle}{\langle V \rangle} \Bigg|_{a=1}, \quad \left[\langle T \rangle + \langle V \rangle \right]_{\text{optimal}} = -\frac{1}{4} \frac{\langle V \rangle^2}{\langle T \rangle} \Bigg|_{a=1} \quad (2.252f)$$

and one “only” has to vary the energy functional (which is now given completely analytically) w.r.t. the remaining coefficients $c_1, c_2 \dots c_N$. However, “there is no free lunch”, as non-linear multi-dimensional minimalization is a difficult numerical problem in need of an efficient, robust method.

We will use the AMOEBA program in the (freely available) Fortran77 version of the book **{Num. Recipes}** to perform numerically the minimalization over the coefficients $c_1, c_2 \dots c_N$. This procedure may be slow as the “amoeba” only crawls down the hills but is applicable to general functions. It is based on the “downhill”- simplex method and not only needs a starting value but $N+1$ points defining an initial simplex and the corresponding function values. A simplex is a geometrical figure consisting of $N+1$ points (or vertices) in N dimensions. We determine these points from an initial point $\mathbf{P}_1 = (c_1, c_2 \dots c_N)$ and generate additional points simply by

$$\mathbf{P}_i = \mathbf{P}_1 + \left(c_1, c_2, \dots, \underbrace{c_j + \lambda^j}_{j=i-1}, \dots c_N \right) \quad i = 2, 3 \dots N+1, \quad (2.252g)$$

where λ is a suitably chosen constant (in the example below we take $\lambda = 0.3$). Of course, with $N = 0$ one just obtains the result (2.246) from **Problem 18 b**) and we increase step-by-step the number of coefficients to be varied. As initial point we take the minimalization result from the previous run with $(N-1)$ coefficients and set the additional coefficient $c_N = 0$ at the point \mathbf{P}_1 . By this procedure it is guaranteed that at each N we obtain at least the previous result. The big risk is that during iteration one gets stuck in a local minimum; therefore it is recommended (at each N) to start again with the obtained minimum as new starting point.

The AMOEBA program stops if a prescribed accuracy (with single precision we take $\text{FTOL} = 10^{-6}$) has been achieved and presents $N+1$ points as result which lie inside the precision bound around the discovered minimum. In the program presented below we average over the function values of this final simplex.

```

c+++++ MAIN PROGRAM ++++++
c
c Program minimizes the Pekar functional for the polaron problem
c in the limit of strong coupling
c using the ansatz for the S-wave function
c
c y(r) = C r [ 1 + sum_{i=1}^N c_i r^i exp(-r/a) ] ;
c int_0^{infinity} dr y^2(r) = 1 .
c
c The scale a is determined analytically by variation.
c Minimization by "downhill simplex method" for the coefficients c_i;
c program from NUMERICAL RECIPES, ch. 10.4
c
c Loop over N = 0,1, ... NMAX-1 = 9 coefficients
c
c EXTERNAL ENERGIE
c PARAMETER (NMAX = 10, FTOL=1.E-6, ALAM=0.3)
c COMMON N,D(0:4*NMAX+3)
c DIMENSION P(NMAX+1,NMAX), X(NMAX), Y(NMAX), XNEU(NMAX), XALT(NMAX+1)
C
C tabellation of n!/2^(n+1)
C
c NHOCH = 4*NMAX + 3
c D(0) = 0.5
c DO 10 I = 1,NHOCH
c D(I) = I*D(I-1)*0.5
10 CONTINUE
C
C WRITE(6,9) FTOL
9 FORMAT(// ' rel. accuracy = ',e10.3/)
c
c DO 100 NN = 1,NMAX ! loop over different number of coefficients
c
c N = NN - 1
c
c ISTART = 0 ! initial start
C

```

```

C  N+1 start simplices for minimization routine AMOEBA
C
50  CONTINUE
      DO 20 I = 1,NN
        DO 25 J = 1,N
          IF(ISTART .EQ. 0) P(I,J) = XALT(J)
          IF(ISTART .EQ. 1) P(I,J) = XNEU(J)
          IF(J .EQ. (I-1)) P(I,J) = P(I,J) + ALAM**J
25  CONTINUE
20  CONTINUE
C
      DO 30 I = 1,NN
        DO 35 J = 1,N
          X(J) = P(I,J)
35  CONTINUE
      Y(I) = ENERGIE(X)
30  CONTINUE
C
      CALL AMOEBA(P,Y,NMAX+1,NMAX,N,FTOL,ENERGIE,ITER)
C
      DO 38 J = 1,N          ! store first simplex for restart
        XNEU(J) = P(1,J)
        XALT(J) = XNEU(J)   ! store first simplex for next N
38  CONTINUE
      XALT(NN) = 0.        ! and add c(N+1)=0 as last coefficient
C
C  minimal value averaged over the simplices
C
      YMIT = 0.
      DO 40 I = 1,NN
        YMIT = YMIT + Y(I)
40  CONTINUE
      YMIT = YMIT/NN
C
      IF(ISTART .EQ. 0) WRITE(6,98) N
98  FORMAT(// ' N = ',I3/)
      IF(ISTART .EQ. 1) WRITE (*,*) 'restart:'
      WRITE(6,99) ITER,YMIT
99  FORMAT(' iterations = ',I4,10X,
&        'mean minimal value = ',F10.7)
C
      ISTART = ISTART + 1
      IF(ISTART .EQ. 1) GO TO 50
100 CONTINUE
      STOP
      END

C+++++ SUBPROGRAM ENERGIE +++++
      FUNCTION ENERGIE(X)
C
      PARAMETER (NMAX=10)
      COMMON N,D(0:4*NMAX+3)
      DIMENSION X(NMAX),C(0:NMAX)
      DATA WU2 /1.414213562/          ! square root from 2
C
      C(0) = 1.                      ! fixed
      DO 10 I = 1,N
        C(I) = X(I)
10  CONTINUE
C
C  normalization
C
      ANORM = 0.
      DO 20 I = 0,N
        DO 25 J = 0,N
          ANORM = ANORM + C(I)*C(J)*D(I+J+2)
25  CONTINUE
20  CONTINUE
      ANORM = 1./ANORM
C
C  kinetic energy
C
      T = 0.
      DO 30 I = 0,N
        DO 35 J = 0,N
          DT = (I+1.)*(J+1.)*D(I+J) - D(I+J+2)
          T = T + DT*C(I)*C(J)
35  CONTINUE
30  CONTINUE
      T = 0.5*ANORM*T
C
C  potential energy
C
      V = 0.
      DO 40 I = 0,N
        DO 45 J = 0,N
          ISUM = I + J + 2
          DO 50 K = 0,N

```

```

DO 55 L = 0,N
  KSUM = K + L + 1
  HILF = C(I)*C(J)/(2**(ISUM+1))
  HILF = HILF*C(K)*C(L)*D(KSUM)
  V1 = 0.
  FAK = 1. ! 0!
DO 60 M = 0,KSUM
  MSUM = ISUM + M
  V1 = V1 + D(MSUM)/FAK
  FAK = (M+1.)*FAK ! (M+1)!
60 CONTINUE
  V = V + HILF*V1
55 CONTINUE
50 CONTINUE
45 CONTINUE
40 CONTINUE
  V = -WU2*V*ANORM*ANORM
C
C energy after variation of scale parameter
C
  ENERGIE = -0.25*V*V/T
C
  RETURN
  END

C+++++ SUB PROGRAM AMOEBA ++++++

SUBROUTINE AMOEBA(P,Y,MP,NP,NDIM,FTOL,FUNK,ITER)
C
C *****
C from: W. H.Press et al. "Numerical Recipes in Fortran 77" , ch. 10.4
C Cambridge University Press, 2nd ed. (1992)
C *****
C Multidimensional minimization of the function FUNK(X) where X is an
C NDIM-dimensional vector, by the downhill simplex method of Nelder and Mead.
C
C Input is a matrix P whose NDIM+1 rows are NDIM-dimensional vectors which
C are the vertices of the starting simplex.
C [Logical dimensions of P are P(NDIM+1,NDIM); physical dimensions are input as P(MP,NP)].
C Also input is the vector Y of length NDIM+1, whose components must be
C pre-initialized to the values of FUNK evaluated at the NDIM+1 vertices (rows) of P;
C and FTOL the fractional convergence tolerance to be achieved in the
C function value (n.b.!).
C On output, P and Y will have been reset to NDIM+1
C new points all within FTOL of a minimum function value,
C and ITER gives the number of iterations taken.
C
  PARAMETER (NMAX=10,ALPHA=1.0,BETA=0.5,GAMMA=2.0,ITMAX=1000)
C
C Expected maximum number of dimensions, three parameters which define
C the expansions and contractions, and maximum allowed number of iterations.
C
  DIMENSION P(MP,NP),Y(MP),PR(NMAX),PRR(NMAX),PBAR(NMAX)
C
  MPTS = NDIM + 1 ! Note that MP is the physical dimension
                  ! corresponding to the logical dimension
                  ! MPTS, NP to NDIM
  ITER = 0
  ILO = 1 ! First we must determine which point is the
          ! highest (worst), next-highest, and
          ! lowest (best).
  IF(Y(1) .GT. Y(2)) THEN
    IHI = 1
    INHI = 2
  ELSE
    IHI = 2
    INHI = 1
  ENDIF
C
DO 11 I = 1,MPTS ! by looping over the points in the simplex
  IF(Y(I) .LT. Y(ILO)) ILO = I
  IF(Y(I) .GT. Y(IHI)) THEN
    INHI = IHI
    IHI = I
  ELSE IF(Y(I) .GT. Y(INHI)) THEN
    IF(I .NE. IHI) INHI = I
  ENDIF
11 CONTINUE
C
C Compute the fractional range from highest to lowest and return if satisfactory
C
  RTOL = 2.*ABS(Y(IHI)-Y(ILO))/(ABS(Y(IHI))+ABS(Y(ILO)))
  IF(RTOL .LT. FTOL) RETURN
  IF(ITER .EQ. ITMAX) PAUSE 'Amoeba exceeding maximum iterations.'

```

```

ITER = ITER + 1
DO 12 J = 1,NDIM
  PBAR(J) = 0.
12 CONTINUE
      ! Begin a new iteration. Compute the vector average
      ! of all points except the highest, i.e. the center
      ! of the "face" of the simplex across from the high
      ! point. We will subsequently explore along the ray
      ! from the high point through that center.

DO 14 I = 1,MPTS
  IF(I .NE. IHI) THEN
    DO 13 J = 1,NDIM
      PBAR(J) = PBAR(J) + P(I,J)
13 CONTINUE
    ENDIF
14 CONTINUE
DO 15 J = 1,NDIM
      ! Extrapolate by a factor ALPHA through the
      ! face, i.e. reflect the simplex from the
      ! high point.

  PBAR(J) = PBAR(J)/NDIM
  PR(J) = (1.+ ALPHA)*PBAR(J) - ALPHA*P(IHI,J)
15 CONTINUE
  YPR = FUNK(PR)
  IF(YPR .LE. Y(ILO)) THEN
      ! Evaluate the function at the reflected point.
      ! Gives a result better than the best point,
      ! so try an additional extrapolation by a
      ! factor GAMMA,

    DO 16 J = 1,NDIM
      PRR(J) = GAMMA*PR(J) + (1.-GAMMA)*PBAR(J)
16 CONTINUE
    YPRR = FUNK(PRR)
    IF(YPRR .LT. Y(ILO)) THEN
      ! check out the function there.
      ! The additional extrapolation succeeded,
      ! and replaces the high point.

      DO 17 J = 1,NDIM
        P(IHI,J) = PRR(J)
17 CONTINUE
      Y(IHI) = YPRR
    ELSE
      ! The additional extrapolation failed,
      ! but we can still use the reflected point

      DO 18 J = 1,NDIM
        P(IHI,J) = PR(J)
18 CONTINUE
      Y(IHI) = YPR
    ENDIF
  ELSE IF(YPR .GE. Y(INHI)) THEN
      ! The reflected point is worse than
      ! the second-highest
      ! If it's better than the highest,
      ! then replace the highest,

    DO 19 J = 1,NDIM
      P(IHI,J) = PR(J)
19 CONTINUE
      Y(IHI) = YPR
    ENDIF
  DO 21 J = 1,NDIM
      ! but look for an intermediate lower point

      PRR(J) = BETA*P(IHI,J) + (1.-BETA)*PBAR(J)

21 CONTINUE
      ! in other words, perform a contraction
      ! of the simplex along one dimension.
      ! Then evaluate the function.

      YPRR = FUNK(PRR)
      IF(YPRR .LT. Y(IHI)) THEN
          ! Contraction gives an improvement,
          ! so accept it.
          DO 22 J = 1,NDIM
            P(IHI,J) = PRR(J)
22 CONTINUE
            Y(IHI) = YPRR
          ELSE
            ! Can't seem to get rid of that high point.
            ! Better contract around the lowest (best)
            ! point.

            DO 24 I = 1,MPTS
              IF(I .NE. ILO) THEN
                DO 23 J = 1,NDIM
                  PR(J) = 0.5*(P(I,J) + P(ILO,J))
                  P(I,J) = PR(J)
23 CONTINUE
                  Y(I) = FUNK(PR)
                ENDIF
              CONTINUE
            ENDIF
          ELSE
            ! We arrive here if the original reflection gives
            ! a middling point.
            ! Replace the old high point and continue

            DO 25 J = 1,NDIM
              P(IHI,J) = PR(J)
25 CONTINUE
              Y(IHI) = YPR
            ENDIF
          GO TO 1
          ! for the test of doneness and the next
          ! iteration.

END

```

After running this program we obtain the following print-out:

```

rel. accuracy = .100E-05

N = 0
iterations = 1           mean minimal value = -.0976562
restart:
iterations = 0           mean minimal value = -.0976562

N = 1
iterations = 8           mean minimal value = -.1080244
restart:
iterations = 4           mean minimal value = -.1080244

N = 2
iterations = 16          mean minimal value = -.1085069
restart:
iterations = 12          mean minimal value = -.1085069

N = 3
iterations = 12          mean minimal value = -.1085069
restart:
iterations = 12          mean minimal value = -.1085069

N = 4
iterations = 21          mean minimal value = -.1085092
restart:
iterations = 65          mean minimal value = -.1085098

N = 5
iterations = 81          mean minimal value = -.1085106
restart:
iterations = 82          mean minimal value = -.1085114

N = 6
iterations = 117         mean minimal value = -.1085121
restart:
iterations = 96          mean minimal value = -.1085124

N = 7
iterations = 136         mean minimal value = -.1085123
restart:
iterations = 134         mean minimal value = -.1085125

N = 8
iterations = 154         mean minimal value = -.1085124
restart:
iterations = 154         mean minimal value = -.1085124

N = 9
iterations = 171         mean minimal value = -.1085125
restart:
iterations = 152         mean minimal value = -.1085126

```

The numerical value of Pekar's coefficient for the polaron energy at strong coupling therefore is

$$\gamma_P = -0.108513(1) \quad (2.253)$$

with an estimated error of (1) in the last digit. A more precise value can be obtained by taking a smaller accuracy parameter (FTOL) and a larger number of coefficients (NMAX) but then double-precision arithmetic is required (**Problem 18 c**).

3. Path Integrals in Field Theory

3.1 Generating Functionals and Perturbation Theory

The transition from many-body quantum physics to field theory is a transition from a finite number of degrees of freedom to an infinite number. We will perform this transition **formally** thus omitting in a first step all subtleties like renormalization, even ignoring the question of the sheer existence of an interacting theory.

In the beginning we consider for simplicity a system of particles of mass m which is described by a neutral scalar field $\Phi(x)$. Let the Lagrange density (Lagrangian) be ⁶⁴

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \Phi \partial^\mu \Phi - m^2 \Phi^2) - V(\Phi), \quad (3.1)$$

where $V(\Phi)$ denotes the self-interaction of the field ⁶⁵.

If one requires the theory to be renormalizable (in 1 time and 3 space dimensions) this interaction can only be a polynomial of the field up to degree four; a typical example is

$$V(\Phi) = \frac{\lambda}{4!} \Phi^4, \quad (3.2)$$

which is of great importance in superconductivity (Ginzburg-Landau theory) and particle physics (Higgs mechanism).

As in the quantum-mechanical case we consider the transition matrix element

$$\langle \Phi_f | e^{-i\hat{H}(t_f - t_i)} | \Phi_i \rangle \quad (3.3)$$

of the time-evolution operator between field configurations Φ_i and Φ_f . $\hat{H} = \int d^3x \hat{\mathcal{H}}$ is the Hamilton operator of the systems. The classical Hamilton density follows from Eq. (3.1) by the usual Legendre transformation

$$\mathcal{H} = \pi \dot{\Phi} - \mathcal{L} = \frac{1}{2} \pi^2 + \frac{1}{2} (\nabla \Phi)^2 + \frac{1}{2} m^2 \Phi^2 + V(\Phi), \quad (3.4)$$

where $\pi = \partial \mathcal{L} / \partial \dot{\Phi} = \dot{\Phi}$ is the canonically conjugated momentum (density) of the field. We divide the (finite) space volume L^3 into N small cells with volume $v = L^3/N$ and the time interval $t_f - t_i$ in M intervals of length ϵ . If we use the completeness for the fields $\Phi(t, \mathbf{x}) = \Phi_j^l$, $l = 1 \dots M-1$, $j = 1 \dots N$ at each time and space point

$$\int d\Phi_j^l | \Phi_j^l \rangle \langle \Phi_j^l | = 1 \quad (3.5)$$

then we obtain

$$\begin{aligned} \langle \Phi_f | e^{-i\hat{H}(t_f - t_i)} | \Phi_i \rangle &= \lim_{N, M \rightarrow \infty} \int \prod_{j=1}^N \left\{ d\Phi_j^{M-1} \dots d\Phi_j^1 \langle \Phi_j^M | e^{-i\epsilon v \hat{\mathcal{H}}} | \Phi_j^{M-1} \rangle \right. \\ &\quad \left. \dots \langle \Phi_j^1 | e^{-i\epsilon v \hat{\mathcal{H}}} | \Phi_j^0 \rangle \right\}. \end{aligned} \quad (3.6)$$

As before we have set $\Phi_j^M = \Phi_f(\mathbf{x}_j)$ and $\Phi_j^0 = \Phi_i(\mathbf{x}_j)$ as abbreviation. Exactly as in the quantum-mechanical case one finds for small times

$$\langle \Phi_j^{l+1} | e^{-i\epsilon v \hat{\mathcal{H}}} | \Phi_j^l \rangle \simeq \int \frac{dp_j^l}{2\pi} \exp [ip_j^l (\Phi_j^{l+1} - \Phi_j^l) - i\epsilon v \mathcal{H}_j^l]. \quad (3.7)$$

⁶⁴Charged scalar particles are represented by complex fields in whose Lagrangian the factor 1/2 is missing, see **Problem 20**.

⁶⁵In this chapter we set $\hbar = 1$. Here and in the following we always choose a system of units with $c = 1$, employ the metric $(+, - - -)$, i.e. $a \cdot b = a_0 b_0 - \mathbf{a} \cdot \mathbf{b}$, and sum over identical indices.

If we write $p_j^l = v\pi_j^l$, we obtain

$$\begin{aligned} \langle \Phi_f | e^{-i\hat{H}(t_f-t_i)} | \Phi_i \rangle &= \lim_{N,M \rightarrow \infty} \int \prod_{j=1}^N \left(\prod_{l=1}^{M-1} \frac{d\Phi_j^l v d\pi_j^l}{2\pi} \right) \int \frac{v d\pi_j^M}{2\pi} \\ &\cdot \exp \left\{ i\epsilon \sum_{l=0}^{M-1} v \sum_{j=1}^N \left(\pi_j^l \frac{\Phi_j^{l+1} - \Phi_j^l}{\epsilon} - \mathcal{H}_j^l \right) \right\} \\ &\equiv \int \frac{\mathcal{D}\Phi(x) \mathcal{D}\pi(x)}{2\pi} \exp \left\{ i \int_{t_i}^{t_f} dt \int d^3x \left[\pi \dot{\Phi} - \mathcal{H}(\pi, \Phi) \right] \right\}. \end{aligned} \quad (3.8)$$

This is the path integral in Hamilton form (note footnote 52). By completing the square ($\pi \dot{\Phi} - \pi^2/2 = -(\pi - \dot{\Phi})^2/2 + \dot{\Phi}^2/2$) we can transform the π -integral into a Gaussian integral and we then obtain the path integral in Lagrange form

$$\langle \Phi_f | e^{-i\hat{H}(t_f-t_i)} | \Phi_i \rangle = \text{const.} \cdot \int \mathcal{D}\Phi(x) e^{iS[\Phi]}. \quad (3.9)$$

Again we have the (classical) action in the exponent because

$$\begin{aligned} &\int_{t_i}^{t_f} dt \int d^3x \left[\frac{1}{2} \dot{\Phi}^2 - \frac{1}{2} (\nabla \Phi)^2 - \frac{1}{2} m^2 \Phi^2 - V(\Phi) \right] \\ &= \int_{t_i}^{t_f} dt \int d^3x \left[\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 - V(\Phi) \right] = \int_{t_i}^{t_f} dt \int d^3x \mathcal{L}(\Phi(x), \partial_\mu \Phi(x)) \equiv S[\Phi]. \end{aligned} \quad (3.10)$$

However, this representation of the transition matrix element between field configurations is only an intermediate step as this is not the relevant quantity in field theory. Actually, all observables in field theory can be obtained from the **n-point functions** or **Green functions**

$$G_n(x_1 \dots x_n) = \langle 0 | \mathcal{T} [\hat{\Phi}(x_1) \dots \hat{\Phi}(x_n)] | 0 \rangle \quad (3.11)$$

(as can be seen below in the example of scattering of two scalar particles). Here $|0\rangle$ is the exact ground state of the theory (the “vacuum”), \mathcal{T} the time-ordering operator and $\hat{\Phi}(x)$ are the exact field operators in the Heisenberg picture. What we need therefore is a path-integral representation for the Green functions.

Fortunately, this already has been done in quantum mechanics (in **chapter 1.7**): The ground state can be projected out by the unphysical limit⁶⁶ $t_i \rightarrow i\infty, t_f \rightarrow -i\infty$ and one has

$$G_n(x_1 \dots x_n) = \lim_{\substack{t_i \rightarrow i\infty \\ t_f \rightarrow -i\infty}} \frac{\int \mathcal{D}\Phi \Phi(x_1) \dots \Phi(x_n) \exp(iS[\Phi])}{\int \mathcal{D}\Phi \exp(iS[\Phi])}. \quad (3.12)$$

The set of all n -point functions can be obtained from the **generating functional**

$$Z[J] = \int \mathcal{D}\Phi \exp \left(iS[\Phi] + i \int d^4x J(x) \Phi(x) \right) \quad (3.13)$$

⁶⁶As a reminder: $e^{-i\hat{H}(t_f-t_i)} = |0\rangle\langle 0| e^{-iE_0(t_f-t_i)} + |1\rangle\langle 1| e^{-iE_1(t_f-t_i)} + \dots$. Also, one doesn't have to take purely imaginary times but can go to infinity along a suitable ray in the complex plane – the essential point is that the excited states are sufficiently damped in this limit.

by functional differentiation:

$$G_n(x_1 \dots x_n) = \left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J(x_1) \dots \delta J(x_n)} \frac{Z[J]}{Z[0]} \Big|_{J=0} . \quad (3.14)$$

As one can see the normalization of the functional integral cancels. Eq. (3.13) can also be considered as functional Fourier transform of $\exp(iS[\Phi])$ and thus the artificially introduced source $J(x)$ can be seen as variable conjugate to the field $\Phi(x)$.

In most cases the generating functional can be calculated only for vanishing self-interaction V :

$$\begin{aligned} Z_0[J] &= \int \mathcal{D}\Phi \exp \left[i \int d^4x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 + J\Phi \right) \right] \\ &= \int \mathcal{D}\Phi \exp \left[\frac{i}{2} \int d^4x \Phi(x) (-\square - m^2) \Phi(x) + i \int d^4x J(x) \Phi(x) \right] . \end{aligned} \quad (3.15)$$

In the second line an integration by parts has been performed under the assumption that boundary terms vanish. The functional integration in Eq. (3.15) can be done since the exponent

$$\begin{aligned} &\frac{i}{2} \int d^4x d^4y \Phi(x) K_0(x, y) \Phi(y) + i \int d^4x J(x) \Phi(x) \\ &= \frac{i}{2} \int d^4x d^4y (\Phi K_0 + J)(x) K_0^{-1}(x, y) (K_0 \Phi + J)(y) - \frac{i}{2} \int d^4x d^4y J(x) K_0^{-1}(x, y) J(y) \end{aligned} \quad (3.16)$$

is quadratic in the fields. The Gaussian integral over Φ thus gives

$$Z_0[J] = \text{const.} \cdot \exp \left[-\frac{i}{2} \int d^4x d^4y J(x) K_0^{-1}(x, y) J(y) \right] \equiv Z_0[0] \exp \left[-\frac{i}{2} (J, K_0^{-1} J) \right] , \quad (3.17)$$

where the constant does not depend on the source. In addition, we have used a convenient short-hand notation. The inverse of the kernel

$$K_0(x, y) = (-\square_x - m^2) \delta^4(x - y) \quad (3.18)$$

is calculated most easily in momentum space as – due to translational invariance – K_0 only depends on the difference $x - y$:

$$\Delta(x, y) \equiv K_0^{-1}(x, y) = \int \frac{d^4k}{(2\pi)^4} \tilde{\Delta}(k) e^{ik \cdot (x - y)} . \quad (3.19)$$

The equation $(-\square_x - m^2) \Delta(x, y) = \delta^4(x - y)$ then just becomes an algebraic equation $(k^2 - m^2) \tilde{\Delta}(k) = 1$ with the solution

$$\tilde{\Delta}_F(k) = \frac{1}{k^2 - m^2 + i0^+} . \quad (3.20)$$

This is the **Feynman propagator** in momentum space. Of course, one has to specify how to treat the pole at $k^2 = m^2$.

As in **Detail 12** this can be achieved by a more careful treatment of the limit $t_i \rightarrow i\infty, t_f \rightarrow -i\infty$ in the path-integral representation (3.12) for the Green functions, or simpler by introducing a **convergence factor**

$$\exp \left[-\frac{\epsilon}{2} \int d^4x \Phi^2(x) \right], \quad \epsilon > 0 \tag{3.21}$$

into the path integral. By combining this term with the mass term in the Lagrangian this leads to the replacement

$$\boxed{m^2 \longrightarrow m^2 - i0^+} \tag{3.22}$$

analogous to the rule (1.240) in the case of the harmonic oscillator. ($i0^+$ is a short-hand for a small, postive imaginary part $i\epsilon, \epsilon > 0$ which at the end of the calculation is set to zero.).

From Eq. (3.17) one thus finds that the 2-point function (or the **propagator**) in lowest order is given by

$$G_2^{(0)}(x_1, x_2) = i\Delta_F(x_1, x_2). \tag{3.23}$$

The generating functional **with** interaction can be obtained formally from $Z_0[J]$ by functional differentiation. As functional differentiation w.r.t. the source $J(x)$ generates the field $\Phi(x)$ we thus have

$$\boxed{\begin{aligned} Z[J] &= \int \mathcal{D}\Phi \exp \left[-i \int d^4x V \left(\frac{1}{i} \frac{\delta}{\delta J(x)} \right) \right] \exp \left[i \int d^4y (\mathcal{L}_0 + J(y)\Phi(y)) \right] \\ &= \exp \left[-i \int d^4x V \left(\frac{1}{i} \frac{\delta}{\delta J(x)} \right) \right] Z_0[J]. \end{aligned}} \tag{3.24}$$

Detail 25: A Functional Equation for the Generating Functional

The representation of the generating functional as a functional integral offers many possibilities for transformations known from usual integral calculus. For instance, we may perform an infinitesimal shift of the integration variable

$$\Phi(x) = \varphi(x) + \epsilon f(x) \tag{3.25a}$$

in the path integral (3.13) (**Itzykson & Zuber**, p. 447). As the Jacobian obviously is "1", we have

$$Z[J] = \int \mathcal{D}\varphi \left\{ 1 + i\epsilon \int d^4x f(x) \frac{\delta}{\delta \varphi(x)} \exp \left(iS[\varphi] + i \int d^4x J(x) \varphi(x) \right) \right\}. \tag{3.25b}$$

Since the function $f(x)$ is totally arbitrary, the (functional) integral over a total (functional) derivative must vanish (as in ordinary integral calculus):

$$0 = \int \mathcal{D}\varphi \frac{\delta}{\delta \varphi(x)} \exp \left(iS[\varphi] + i \int d^4x J(x) \varphi(x) \right) = i \int \mathcal{D}\varphi \left\{ \frac{\delta S[\varphi]}{\delta \varphi(x)} + J(x) \right\} \exp \left(iS[\varphi] + i \int d^4x J(x) \varphi(x) \right). \tag{3.25c}$$

We may pull out the terms, which contain φ in the curly bracket, from the functional integral if we replace $\varphi(x)$ by $\delta/(i\delta J(x))$ (acting on the generating functional) in these terms. Then we obtain

$$\left\{ \frac{\delta S}{\delta \varphi(x)} \left[\frac{\delta}{i\delta J(x)} \right] + J(x) \right\} Z[J] = 0, \tag{3.25d}$$

which for the scalar theory (3.1) explicitly reads

$$\left\{ \left(\square + m^2 \right) \frac{\delta}{i\delta J(x)} + V' \left(\frac{\delta}{i\delta J(x)} \right) - J(x) \right\} Z[J] = 0. \tag{3.25e}$$

This so-called **Schwinger equation** therefore connects different n -point functions.

3.1.1 Perturbation Theory

The connection (3.24) between the functional with and without interaction is a purely formal relation which only can be made concrete by an expansion in powers of the interaction. This will be illustrated in the case of the Φ^4 -Theorie (3.2). In lowest orders of a power series expansion w.r.t. the coupling constant λ we obtain

$$Z[J] = Z_0[J] \left\{ 1 + \lambda \omega_1[J] + \lambda^2 \omega_2[J] + \dots \right\} \quad (3.26)$$

with

$$\omega_1[J] = -\frac{i}{4!} \frac{1}{Z_0[J]} \int d^4x \left(\frac{\delta}{\delta J(x)} \right)^4 Z_0[J]. \quad (3.27)$$

Doing the differentiations gives

$$\omega_1[J] = -\frac{i}{4!} \int d^4x \left\{ 3(-i)^2 \Delta_F(x, x) \Delta_F(x, x) \right. \quad (A1)$$

$$+ 6(-i)^3 \int d^4y_1 d^4y_2 \Delta_F(x, y_1) J(y_1) \Delta_F(x, x) \Delta_F(x, y_2) J(y_2) \quad (B1) \quad (3.28)$$

$$\left. + (-i)^4 \int d^4y_1 d^4y_2 d^4y_3 d^4y_4 \prod_{j=1}^4 \Delta_F(x, y_j) J(y_j) \right\}. \quad (C1)$$

The different terms can be ordered according to the number of sources J and represented graphically: Each propagator $\Delta_F(x, y)$ is symbolized by a line leading from y to x and each interaction vertex by a point into which 4 lines are going in or out (see Fig. 18).

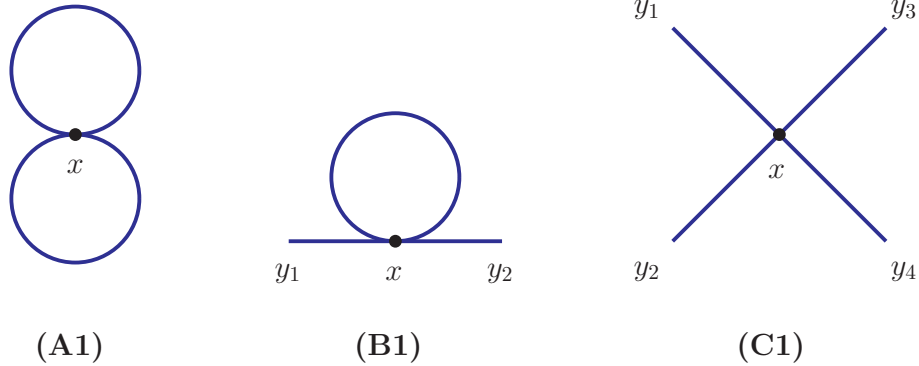


Fig. 18 : Graphical representation of first-order perturbation theory ω_1 for the generating functional in Φ^4 -theory.

The first line of Eq. (3.28) – the term (A1) – describes so-called "vacuum graphs" which do not have any sources and which cancel by division with $Z_0[0]$ in Eq. (3.14) for the Green function⁶⁷. Note that the different terms carry different numerical factors ("multiplicities") making up the **symmetry factors** – these are the numbers with which one has to divide the particular diagram according to the Feynman rules. Considering that functional differentiation w.r.t. $2j$ sources gives an additional factor $(2j)!$ for the particular diagram, Eq.

⁶⁷ If normalized to the free generating functional $Z_0[0]$, this term determines the vacuum-energy density produced in 1st order perturbation theory by the self-interaction.

(3.28) gives multiplicities for the graphs (A1), (B1), (C1) which are in agreement with the ones listed in tables I – III of Ref. [41].

In second-order perturbation theory one finds

$$\omega_2[J] = \frac{1}{2}\omega_1^2[J] + \tilde{\omega}_2[J], \tag{3.29}$$

where the first contribution on the r.h.s. contains **disconnected graphs** in which two parts are not connected by a common line (see, e.g. Fig.19 where the first-order graphs (A1) and (B1) are taken together without connection).

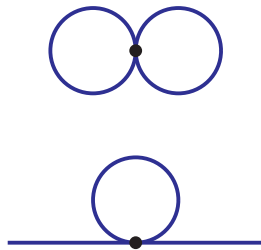


Fig. 19 : A disconnected graph in 2nd order perturbation theory for the Φ^4 -theory.

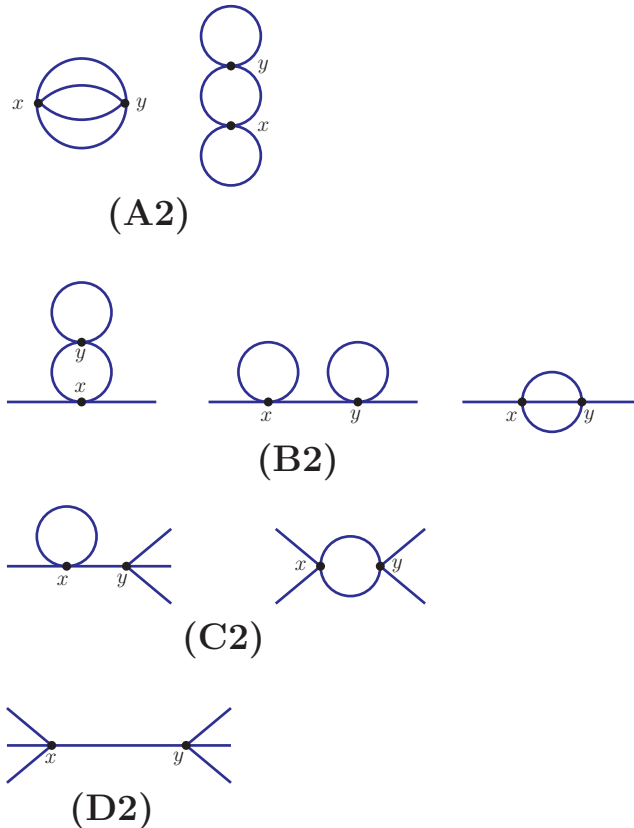


Fig. 20 : Graphical representation of the 2nd order perturbation theory $\tilde{\omega}_2$ for the generating functional of the Φ^4 -theory (see Eq. (3.30b)).

Detail 26: Generating Functional of the Φ^4 -Theory in 2nd Order

The direct calculation of

$$\omega_2[J] = \frac{(-i)^2}{2(4!)^2} \frac{1}{Z_0[J]} \int d^4x d^4y \left(\frac{\delta}{\delta J(y)} \right)^4 \left(\frac{\delta}{\delta J(x)} \right)^4 Z_0[J] =: \frac{1}{2} \omega_1^2[J] + \frac{(-i)^2}{2(4!)^2} \sum_{j=0}^3 (-i)^{4+j} \tilde{\omega}_2^{(2j)}[J] \quad (3.30a)$$

is a little bit cumbersome but feasible when using Leibniz's rule. It gives the multiplicities for the individual graphs without combinatorics. In doing so it is recommended to use a condensed notation: Δ_{12} for $\Delta_F(y_1, y_2)$, J_1 for $J(y_1)$ etc. and integration over repeated indices: $\Delta_{xx} \equiv \int d^4x \Delta_F(x, x)$, $\Delta_{xy}^4 \equiv \int d^4x d^4y (\Delta_F(x, y))^4$ etc. With $\Delta_F(x, y) = \Delta_F(y, x)$ one obtains the following contributions with $2j$ external sources

$$\tilde{\omega}_2^{(0)}[J] = 24 \Delta_{xy}^4 + 72 \Delta_{xx} \Delta_{xy}^2 \Delta_{yy} \quad (A2)$$

$$\tilde{\omega}_2^{(2)}[J] = 144 \Delta_{xy}^2 \Delta_{yy} (\Delta_{x1} J_1)^2 + 144 \Delta_{xx} \Delta_{xy} \Delta_{yy} \Delta_{x1} J_1 \Delta_{y2} J_2 + 96 \Delta_{xy}^3 \Delta_{x1} J_1 \Delta_{y2} J_2 \quad (B2)$$

(3.30b)

$$\tilde{\omega}_2^{(4)}[J] = 96 \Delta_{xx} \Delta_{xy} (\Delta_{y2} J_2)^3 \Delta_{x1} J_1 + 72 (\Delta_{x1} J_1)^2 \Delta_{xy}^2 (\Delta_{y2} J_2)^2 \quad (C2)$$

$$\tilde{\omega}_2^{(6)}[J] = 16 (\Delta_{x1} J_1)^3 \Delta_{xy} (\Delta_{y2} J_2)^3. \quad (D2)$$

After multiplication with $(2j)!$ the numerical factors agree with those given in Ref. [41]. In this reference and elsewhere [42], one can find general procedures and computer programs which give the symmetry factors for all graphs in arbitrary order and for different interactions.

The second part $\tilde{\omega}_2[J]$ in Eq. (3.29) is graphically represented in Fig. 20.

3.1.2 Connected and Amputated Green Functions

It is obvious that the disconnected graphs from the first term on the r.h.s. of Eq. (3.29) do not contribute to physical processes. They are canceled if we define

$$G_c(x_1 \dots x_n) = \left(\frac{1}{i} \right)^n \frac{\delta^n}{\delta J(x_1) \dots \delta J(x_n)} \ln Z[J] \Big|_{J=0} \quad (3.31)$$

as “**connected**” Green functions. Indeed, one finds

$$\begin{aligned} \ln Z[J] &= \ln Z_0[J] + \ln \left\{ 1 + \frac{Z[J] - Z_0[J]}{Z_0[J]} \right\} = \ln Z_0[J] + \ln \{ 1 + \lambda \omega_1[J] + \lambda^2 \omega_2[J] + \dots \} \\ &= -\frac{i}{2} \int d^4x d^4y J(x) \Delta(x, y) J(y) + \lambda \omega_1[J] + \lambda^2 \omega_2[J] - \frac{1}{2} \lambda^2 \omega_1^2[J] + \mathcal{O}(\lambda^3), \end{aligned} \quad (3.32)$$

so that the disconnected part in $\omega_2[J]$ is taken away exactly. One can show that this happens in all orders and that therefore

$$W[J] := -i \ln Z[J] \quad (3.33)$$

is the generating functional for the connected Green functions. The expansion of $Z[J]$ w.r.t. these connected functions is a **cumulant expansion**, which is also important in other areas, for example in statistics (see **Problem 21**).

If the system exhibits translation invariance it is more convenient to employ (connected) Green functions in momentum space where a δ -function can be split off which expresses the total energy-momentum conservation:

$$G_n(p_1 \dots p_n) = \prod_{i=1}^n \left(\int d^4x_i e^{-ip_i \cdot x_i} \right) G_n(x_1 \dots x_n) =: (2\pi)^4 \delta^4 \left(\sum_{i=1}^n p_i \right) \bar{G}_n(p_1 \dots p_n). \quad (3.34)$$

Example: Φ^4 -Theory

The first correction to the propagator (3.23) follows from the second line of Eq. (3.28), i.e. the term (B1)

$$G_2^{(1)}(x_1, x_2) = -\frac{\lambda}{2} \int d^4x \Delta_F(x_1, x) \Delta_F(x, x) \Delta_F(x, x_2). \quad (3.35)$$

This is a loop correction which after Fourier transform and use of the expression (3.19, 3.20) takes the following form

$$\begin{aligned} G_2^{(1)}(p_1, p_2) &= -\frac{\lambda}{2} \int d^4x d^4x_1 d^4x_2 \prod_{j=1}^3 \left(\int \frac{d^4k_j}{(2\pi)^4} \frac{1}{k_j^2 - m^2 + i0^+} \right) e^{-ip_1 \cdot x_1 - ip_2 \cdot x_2} \cdot e^{ik_1 \cdot (x_1 - x) + ik_3 \cdot (x - x_2)} \\ &= -\frac{\lambda}{2} (2\pi)^4 \delta(p_1 + p_2) \Delta_F(p_1) \Delta_F(p_2) \int \frac{d^4k_2}{(2\pi)^4} \frac{1}{k_2^2 - m^2 + i0^+}. \end{aligned} \quad (3.36)$$

After separation of the four-momentum δ -function the total propagator (which, by translation invariance only depends on p^2) therefore reads

$$\begin{aligned} \bar{G}_2(p) &= \frac{i}{p^2 - m^2 + i0^+} + i \left(\frac{1}{p^2 - m^2 + i0^+} \right)^2 \left(i \frac{\lambda}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - m^2 + i0^+} \right) + \mathcal{O}(\lambda^2) \\ &\simeq \frac{i}{p^2 - m^2 + i0^+ - \Sigma^{(1)}} + \mathcal{O}(\lambda^2), \end{aligned} \quad (3.37)$$

where

$$\Sigma^{(1)} := i \frac{\lambda}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - m^2 + i0^+} \quad (3.38)$$

is called (first-order) “**selfenergy**”. In the present case it simply is a (divergent) constant – independent of the external momentum p – which can be combined with the parameter m^2 . This gives the physical mass which can be defined as pole of the propagator:

$$[\bar{G}_2(p^2 = m_{\text{phys}}^2)]^{-1} = 0 \implies m_{\text{phys}}^2 = m^2 + i \frac{\lambda}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - m^2 + i0^+} + \mathcal{O}(\lambda^2). \quad (3.39)$$

In **Problem 19** the divergence of the first-order mass shift is investigated in more detail.

In the general case, the exact 2-point function can be written in the same manner as in Eq. (3.37) but the selfenergy is a function of the square of the external momentum and can be expanded around $p^2 = m_{\text{phys}}^2$

$$\Sigma(p^2) = \Sigma(m_{\text{phys}}^2) + (p^2 - m_{\text{phys}}^2) \Sigma'(m_{\text{phys}}^2) + \dots, \quad (3.40)$$

where the prime indicates the derivative w.r.t. p^2 . With that we have in the vicinity of the pole

$$\begin{aligned} \bar{G}_2(p)(p^2) &= \frac{i}{p^2 - m^2 - \Sigma(p^2) + i0^+} \xrightarrow{p^2 \rightarrow m_{\text{phys}}^2} \frac{i}{p^2 - m^2 - \Sigma(m_{\text{phys}}^2) - (p^2 - m_{\text{phys}}^2) \Sigma'(m_{\text{phys}}^2)} \\ &\equiv \frac{iZ_\Phi}{p^2 - m_{\text{phys}}^2 + i0^+}, \end{aligned} \quad (3.41)$$

with

$$m_{\text{phys}}^2 = m^2 + \Sigma(m_{\text{phys}}^2), \quad Z_\Phi = [1 - \Sigma'(m_{\text{phys}}^2)]^{-1}. \quad (3.42)$$

Since in Φ^4 -theory the first-order selfenergy is a constant it follows that $Z_\Phi = 1 + \mathcal{O}(\lambda^2)$.

By means of the geometric series in Eq. (3.37) one has summed up a lot of recurring corrections for the full propagator; hence the selfenergy is the sum of a particular (smaller) class of diagrams, the **proper** or **one-particle irreducible** graphs, which we will consider in the next **chapter 3.2**.

In contrast to the propagator the connected 4-point function only gets its first contribution in first-order perturbation theory, simply because it needs interaction. From the third line – the term (C1) – of Eq. (3.28) one obtains

$$G_4^{(1)}(x_1, x_2, x_3, x_4) = -i\lambda \int d^4x \prod_{j=1}^4 [\Delta(x, x_j)] \quad (3.43)$$

and thereby after Fourier transformation

$$G_4^{(1)}(p_1, p_2, p_3, p_4) = (2\pi)^4 \delta(p_1 + p_2 + p_3 + p_4) (-i\lambda) \prod_{j=1}^4 \left(\frac{1}{p_j^2 - m^2 + i0^+} \right). \quad (3.44)$$

The term (C1) describes a **tree graph** while (C2) denotes the first loop correction for the 4-point function. Correspondingly, the perturbation theory for the 6-point function starts with the tree graph (D2) of second order.

As **amputated** Green functions one denotes those n -point functions where the external "legs" have been removed

$$G_n^{\text{amp}}(p_1 \dots p_n) = \prod_{i=1}^n \left[\frac{1}{i\tilde{\Delta}_F(p_i)} \right] G_n(p_1 \dots p_n) \quad (3.45)$$

with

$$\tilde{\Delta}_F(p) := \frac{1}{p^2 - m_{\text{phys}}^2 + i0^+}. \quad (3.46)$$

Note that here the **physical**, i.e. measured **mass** of the in- and out-going particles enters, but not the parameter m in the Lagrangian (3.1). This is because the "bare" mass is modified by quantum corrections as we already have seen in the above example in first-order perturbation theory. This is an essential difference to a non-relativistic theory with finite particle number in which the particle properties are **not** modified by the interaction⁶⁸.

The amputated Green functions are of particular importance since they are directly proportional to the scattering amplitudes and thus to the physical observables. This relation is provided by the **reduction formulas**⁶⁹. For instance the S -matrix element for the scattering of 2 scalar particles of mass m_{phys} with initial momenta k_1, k_2 and final momenta k'_1, k'_2 is given by

$$\begin{aligned} \langle k'_1 k'_2 | \hat{S} | k_1 k_2 \rangle = & \text{disconnected terms} + \left(\frac{i}{\sqrt{Z_\Phi}} \right)^4 \int d^4x_1 d^4x_2 d^4y_1 d^4y_2 \exp [i (k'_1 \cdot y_1 + k'_2 \cdot y_2)] \\ & \cdot \exp [-i (k_1 \cdot x_1 + k_2 \cdot x_2)] \cdot [\square_{y_1} + m_{\text{phys}}^2] [\square_{y_2} + m_{\text{phys}}^2] \\ & \cdot [\square_{x_1} + m_{\text{phys}}^2] [\square_{x_2} + m_{\text{phys}}^2] \langle 0 | \mathcal{T} \left(\hat{\Phi}(y_1) \hat{\Phi}(y_2) \hat{\Phi}(x_1) \hat{\Phi}(x_2) \right) | 0 \rangle_c, \end{aligned} \quad (3.47)$$

⁶⁸Due to a "superselection rule" in Galilei-invariant quantum mechanics found by Bargmann in 1954.

⁶⁹See, e.g. z. B., **Itzykson & Zuber**, ch. 5-1, or **Peskin & Schroeder** ch. 7.2. In honor of the authors Lehmann, Symanzik, Zimmermann they are also called LSZ formulas.

where the index “c” shall indicate the connected parts and Z_Φ is the so-called ”wave function renormalization constant” which in lowest order has the value one. Possible bound states of the two-particle system show up as poles of the S matrix below the square of the total energy $(k_1 + k_2)^2 = 4m_{\text{phys}}^2$.

Detail 27: More about the Reduction Formulas

The S -matrix element for the scattering of two scalar particles is given by

$$S_{12 \rightarrow 1'2'} = \langle f \text{ out} | i \text{ in} \rangle \quad (3.48a)$$

where $\Phi_{\text{out}}(x)$ is the field operator for a free state with the quantum numbers of the out/in-going particles. We will now show that this S -matrix element can be expressed by the full Green functions. For that purpose we use

$$\begin{aligned} |k_1, k_2, \text{in}\rangle &= \hat{a}_{\text{in}}(k_1)^\dagger \hat{a}_{\text{in}}(k_2)^\dagger |0\rangle \\ \langle k'_1, k'_2, \text{out}| &= \langle 0 | \hat{a}_{\text{out}}(k'_1) \hat{a}_{\text{out}}(k'_2) \end{aligned} \quad (3.48b)$$

where $\hat{a}^\dagger(k_n)$ generates a particle with four-momentum k_n ($k_n^2 = k_n'^2 = m_{\text{phys}}^2$).

We can ”take out” the initial state $|k_1, \text{in}\rangle$ from the matrix element. This is possible since the ”in”-field is a free field and has the expansion

$$\hat{\phi}_{\text{free}}(x) = \int \frac{d^3k}{(2\pi)^3 2E_k} \left[\hat{a}(k) e^{-ik \cdot x} + \hat{a}^\dagger(k) e^{ik \cdot x} \right], \quad E_k = \sqrt{\mathbf{k}^2 + m_{\text{phys}}^2}. \quad (3.48c)$$

The inverse relations read

$$\hat{a}(k) = i \int d^3x e^{ik \cdot x} \overleftrightarrow{\partial}_0 \hat{\phi}_{\text{free}}(x) \Big|_t, \quad \hat{a}^\dagger(k) = -i \int d^3x e^{-ik \cdot x} \overleftrightarrow{\partial}_0 \hat{\phi}_{\text{free}}(x) \Big|_t \quad (3.48d)$$

and are valid for any time $t \equiv x_0$. Here the operator $\overleftrightarrow{\partial}_0$ is defined in such a way that it acts like

$$f(t) \overleftrightarrow{\partial}_t g(t) := f(t) \left(\frac{\partial g(t)}{\partial t} \right) - \left(\frac{\partial f(t)}{\partial t} \right) g(t). \quad (3.48e)$$

We can use Eq. (3.48d) to get

$$S_{11' \rightarrow 22'} = \int d^3x_1 e^{-ik_1 \cdot x_1} (-i) \overleftrightarrow{\partial}_{t_1} \left\langle k'_1, k'_2 | \hat{\phi}_{\text{in}}(x_1) \Big|_{t_1} | k_2 \right\rangle. \quad (3.48f)$$

The “**adiabatic hypothesis**” is the assumption that the fully-interacting field operator agrees with the ”in”-field in the distant past (where the particle is prepared for the scattering process) up to a constant

$$\hat{\phi}(x_1) \xrightarrow{t_1 \rightarrow -\infty} \sqrt{Z_\Phi} \hat{\phi}_{\text{in}}(x_1). \quad (3.48g)$$

As discussed in all field-theory textbooks this cannot be understood as an operator equation but is only valid for matrix elements. Here Z_Φ is a constant which takes into account that acting with $\hat{\phi}$ on the vacuum not only generates one-particle states but also states with additional particles and antiparticles (if the Lagrangian is even in ϕ). According to this argument one expects that Z_Φ has a value between zero and one (the case without interaction) but it turns out that Z_Φ diverges in higher orders ... Disregarding this (general field-theoretical) problem we can replace at $t_1 = -\infty$

$$\hat{\phi}_{\text{in}}(x_1) \longrightarrow \lim_{t_1 \rightarrow -\infty} \frac{1}{\sqrt{Z_\Phi}} \hat{\phi}(x_1) \quad (3.48h)$$

so that we obtain

$$S_{11' \rightarrow 22'} = \frac{-i}{\sqrt{Z_\Phi}} \lim_{t_1 \rightarrow -\infty} \int d^3x_1 e^{-ik_1 \cdot x_1} \overleftrightarrow{\partial}_{t_1} \left\langle k'_1, k'_2, \text{out} | \hat{\phi}(x_1) | k_2, \text{in} \right\rangle \quad (3.48i)$$

This process can be repeated for the remaining ”in”-state of the second particle and for both ”out”-states. In the latter case one relies on the hypothesis that in the far future

$$\hat{\phi}_{\text{out}}(x'_n) \longrightarrow \lim_{t'_n \rightarrow +\infty} \frac{1}{\sqrt{Z_\Phi}} \hat{\phi}(x'_n), \quad n = 1, 2. \quad (3.48j)$$

The final result is

$$S_{11' \rightarrow 22'} = \frac{1}{Z_\Phi^2} \prod_{n=1}^2 \left\{ \lim_{\substack{t_n \rightarrow -\infty \\ t'_n \rightarrow +\infty}} \int d^3x_n d^3x'_n e^{-ik_n \cdot x_n} e^{+ik'_n \cdot x'_n} \overleftrightarrow{\partial}_{t_n} \overleftrightarrow{\partial}_{t'_n} \right\} \cdot \langle 0 | \mathcal{T} \left(\hat{\phi}(x_1) \hat{\phi}(x_2) \hat{\phi}(x'_1) \hat{\phi}(x'_2) \right) | 0 \rangle \quad (3.48k)$$

where \mathcal{T} is the time-ordering operator. One sees that the last factor is nothing but the 4-point Green function. The last step is to convert the limits $t_n, t'_n \rightarrow \pm\infty$ into integrals over a total time derivative:

$$\begin{aligned} \int d^4x \partial_0 \left[e^{\pm ip \cdot x} \overleftrightarrow{\partial}_0 f(x) \right] &= \int d^4x \left[\partial_0^2 f(x) + p_0^2 f(x) \right] e^{\pm ip \cdot x} = \int d^4x \left[\partial_0^2 f(x) + f(x) \underbrace{\left(m^2 + \mathbf{p}^2 \right)}_{=(m_{\text{phys}}^2 - \Delta)} \right] e^{\pm ip \cdot x} \\ &= \int d^4x e^{\pm ip \cdot x} \left[\partial_0^2 - \Delta + m_{\text{phys}}^2 \right] f(x), \end{aligned} \quad (3.48l)$$

where x stands for each x_n, x'_n , p stands for each k_n, k'_n and Δ is Laplace's operator. In the last line we have performed an integration by parts in the spatial coordinates which does not produce boundary terms if wave packets instead of plane waves would have been used in the very first beginning. This gives Eq. (3.47).

After an integration by parts (assuming that the fields vanish at infinity) one obtains for the r.h.s. of this equation

$$\frac{1}{Z_{\Phi}^2} \left(m_{\text{phys}}^2 - k_1^2 \right) \left(m_{\text{phys}}^2 - k_2^2 \right) \left(m_{\text{phys}}^2 - k_1'^2 \right) \left(m_{\text{phys}}^2 - k_2'^2 \right) \int d^4 x_1 d^4 x_2 d^4 y_1 d^4 y_2 \exp [i (k_1 \cdot y_1 + k_2 \cdot y_2 - k_1' \cdot x_1 - k_2' \cdot x_2)] \cdot \langle 0 | \mathcal{T} \left(\hat{\Phi}(y_1) \hat{\Phi}(y_2) \hat{\Phi}(x_1) \hat{\Phi}(x_2) \right) | 0 \rangle_c \equiv Z_{\Phi}^{-2} G_4^{\text{amp}} (-k_1, -k_2, k_1', k_2') , \quad (3.48\text{m})$$

i.e., essentially the amputated, connected 4-point function⁷⁰. The T matrix is defined via $\hat{S} = 1 + i\hat{T}$ and we can split off the four-momentum conservation

$$\langle k_1', k_2' | \hat{T} | k_1, k_2 \rangle = (2\pi)^4 \delta^{(4)} (k_1 + k_2 - k_1' - k_2') \langle k_1', k_2' | \mathcal{M} | k_1, k_2 \rangle . \quad (3.48\text{n})$$

In the center-of-mass (CM) system the scattering cross section for equal-mass particles is then simply given by

$$\left(\frac{d\sigma}{d\Omega} \right)_{CM} = \frac{1}{64\pi^2 E_{CM}^2} |\mathcal{M}|^2 . \quad (3.48\text{o})$$

(see, e.g., [Peskin & Schroeder](#), eq. (4.85)).

The perturbative calculation of the amputated n -point functions can be summarized by a set of [Feynman rules](#):

1. Draw all possible, connected, topologically distinctive diagrams with n vertices.
2. To each internal line belongs a propagator $i\tilde{\Delta}_F(k) = i/(k^2 - m_{\text{phys}}^2 + i0^+)$, to each vertex (in Φ^4 -theory) a factor $-i\lambda$.
3. For each internal momentum k , which is not fixed by momentum conservation perform an integration $\int d^4 k / (2\pi)^4$.
4. Each graph has to be divided by a symmetry factor S which corresponds to the number of permutations of internal lines which leave the diagram unchanged with fixed vertices.
5. There is an additional vertex connecting two lines which corresponds to the mass-shift factor $\frac{1}{2}\delta m^2 = \frac{1}{2}(m_{\text{phys}}^2 - m^2)$.

As the measured mass enters the amputated Green functions, it is convenient to do that also for all quantities which are altered ("renormalized" as one says) by the interaction. To these belong the coupling constant and the normalization of the field operator. Therefore one defines (here for the Φ^4 -theory)

$$\Phi_{\text{phys}} := Z_{\Phi}^{-1/2} \Phi \quad (3.49)$$

$$m_{\text{phys}}^2 := m^2 + \delta m^2, \quad \text{or} \quad m_{\text{phys}}^2 = Z_m^{-1} Z_{\Phi} m^2 \quad (3.50)$$

$$\lambda_{\text{phys}} := Z_{\lambda}^{-1} Z_{\Phi}^2 \lambda \quad (3.51)$$

and writes the Lagrangian (3.1) with the self-interaction (3.2) as

$$\begin{aligned} \mathcal{L} = & \frac{1}{2} \left[(\partial_{\mu} \Phi_{\text{phys}})^2 - m_{\text{phys}}^2 \Phi_{\text{phys}}^2 \right] - \frac{\lambda_{\text{phys}}}{4!} \Phi_{\text{phys}}^4 \\ & + (Z_{\Phi} - 1) \frac{1}{2} \left[(\partial_{\mu} \Phi_{\text{phys}})^2 - m_{\text{phys}}^2 \Phi_{\text{phys}}^2 \right] - (Z_{\lambda} - 1) \frac{\lambda_{\text{phys}}}{4!} \Phi_{\text{phys}}^4 - \frac{1}{2} (Z_m - 1) m_{\text{phys}}^2 \Phi_{\text{phys}}^2 . \end{aligned} \quad (3.52)$$

⁷⁰Roughly speaking, the reduction formula "fishes" for poles of the Green function corresponding to the external particles and uses the residues of these poles as physical observables.

The additional terms which have been generated by splitting $Z_i = 1 + (Z_i - 1)$, $i = \Phi, \lambda, m$ are called “**counterterms**”. Having the same form as those in the original Lagrangian, they are determined such that in each order of perturbation theory the emerging divergences are compensated. In a renormalizable theory their number is finite. This “**renormalized perturbation theory**” is just a convenient re-organization of the original perturbation theory which used “bare” parameters. In any case, one has to specify how (or at which energy) the physical parameters are measured (renormalization conditions). One has considerable freedom to do so, which, however, only leads to different results in higher orders of perturbation theory than considered.

That **all** divergences in **all** orders of perturbation theory can be subsumed in the constants Z_Φ, Z_λ, Z_m is highly non-trivial and expresses the fact that the Φ^4 -theory is (perturbatively) **renormalizable**. A necessary condition for that is the property that the coupling constant in 4 space-time dimensions is dimensionless or, more generally in arbitrary dimension d , has mass dimension ≥ 0 (**{Le Bellac}**, ch. 6.1). As the action has to be dimensionless (we have $\exp(iS)$ in the path integral) one finds

$$\dim \left[\int d^d x m^2 \Phi^2 \right] = -d + 2 + 2 \dim \Phi = 0, \implies \dim \Phi = \frac{d}{2} - 1 \tag{3.53}$$

$$\dim \left[\int d^d x \lambda \Phi^n \right] = -d + \dim \lambda + n \frac{d}{2} - n = 0, \implies \dim \lambda = n - d \left(\frac{n}{2} - 1 \right). \tag{3.54}$$

While in quantum mechanics the potential can be arbitrary to a large extent (e.g. $V(x) = g x^6$), in quantum field theory the requirement of renormalizability does not allow $g \Phi^6$ -terms in the four-dimensional Lagrangian: The coupling constant g would then have the mass dimension $6 - 2d = -2$.

How can one prove that a particular theory is renormalizable? For this lecture we adopt the attitude “... das ist ein zu weites Feld” **{Fontane}**⁷¹ and refer to more specialized monographs, e.g. **{Collins}** or **{Muta}**.

Detail 28: Additional Generating Functionals

Instead of the formal representation (3.24) one can derive the (equally formal) expression

$$Z[J] = \text{const.} \exp \left[-\frac{i}{2} (J, \Delta_F J) \right] \left\{ \exp \left[\frac{i}{2} \left(\frac{\delta}{\delta \Phi}, \Delta_F \frac{\delta}{\delta \Phi} \right) \right] \exp \left(-i \int d^4 x V(\Phi) \right) \right\}_{\Phi = \Delta_F J} \tag{3.55a}$$

(**Problem 24***) which sometimes is more convenient.

Instead of coupling the source $J(x)$ to **one** field one may introduce **bi-linear** sources, e.g.

$$\tilde{Z}[K] := \text{const.} \int \mathcal{D}\Phi \exp \left[i \int d^4 x \left(\mathcal{L} - \frac{1}{2} K(x) \Phi^2(x) \right) \right] \tag{3.55b}$$

for a single scalar field. In **Problem 25** this is generalized to a N -component field with $O(N)$ -symmetry.

More interesting is to write down a **generating functional for amputated Green functions**⁷²: Starting from the definition (3.45) and from Eq. (3.14) we define

$$\varphi := -\Delta_F J, \quad \text{d.h.} \quad \varphi(x) = - \int d^4 y \Delta_F(x, y) J(y). \tag{3.55c}$$

As the free part of the action can be written as

$$\frac{1}{2} (\Phi, (-\square - m^2)\Phi) = \frac{1}{2} (\Phi, (-\square - m_{\text{phys}}^2)\Phi) + \frac{1}{2} \delta m^2(\Phi, \Phi) \equiv \frac{1}{2} (\Phi, \Delta_F^{-1}\Phi) + \frac{1}{2} \delta m^2(\Phi, \Phi) \tag{3.55d}$$

we have

$$G^{\text{amp}}(1 \dots n) = \frac{1}{Z[0]} \frac{\delta^n}{\delta \varphi_1 \dots \delta \varphi_n} \int \mathcal{D}\Phi \exp \left[\frac{i}{2} (\Phi, \Delta_F^{-1}\Phi) - i (\varphi, \Delta_F^{-1}\Phi) + i S_{\text{int}}[\Phi] \right] \Bigg|_{\varphi=0}, \tag{3.55e}$$

⁷¹”... that is too wide a field”.

⁷²See, e.g., the appendix of Ref. [43] where it is normalized to $Z_0[0]$ for determining the vacuum-energy density.

with an additional term $\delta m^2 (\Phi, \Phi)/2$ in the interacting part $S_{\text{int}}[\Phi]$. If we shift the integration variable $\Phi = \Phi' + \varphi$ we obtain

$$G_c^{\text{amp}}(1 \dots n) = \frac{\delta^n}{\delta\varphi_1 \dots \delta\varphi_n} \frac{1}{Z[0]} \exp \left[-\frac{i}{2}(\varphi, \Delta_F^{-1} \varphi) \right] \int \mathcal{D}\Phi' \exp \left(i S_0[\Phi'] + i S_{\text{int}}[\Phi' + \varphi] \right) \Big|_{\varphi=0}, \quad (3.55f)$$

where the normalization is given by

$$Z[0] = \int \mathcal{D}\Phi' \exp \left[i S_0[\Phi'] + i S_{\text{int}}[\Phi'] \right]. \quad (3.55g)$$

The connected, amputated n -point functions are again determined by the logarithm of the generating functionals, i.e.

$$G_c^{\text{amp}}(1 \dots n) = \frac{\delta^n}{\delta\varphi_1 \dots \delta\varphi_n} \left[-\frac{i}{2}(\varphi, \Delta_F^{-1} \varphi) + \ln \left\{ \frac{\int \mathcal{D}\Phi' \exp \left(i S_0[\Phi'] + i S_{\text{int}}[\Phi' + \varphi] \right)}{\int \mathcal{D}\Phi' \exp \left(i S_0[\Phi'] + i S_{\text{int}}[\Phi'] \right)} \right\} \right] \Big|_{\varphi=0}. \quad (3.55h)$$

Let's take as examples the 2- and 4-point functions in lowest order perturbation theory: It is seen immediately that for vanishing interaction only the connected, amputated 2-point function

$$G_c^{\text{amp}(0)}(x_1, x_2) = -i\Delta_F^{-1}(x_1, x_2) = i \left(\square_{x_1} + m_{\text{phys}}^2 \right) \delta^{(4)}(x_1 - x_2) \quad (3.55i)$$

exists. Obviously, a connected 4-point function shows up only with interaction: Since $V(\Phi' + \varphi) = \mathcal{O}(\varphi^0, \varphi^1, \varphi^2, \varphi^3) + \lambda\varphi^4/4!$, one finds in first-order perturbation theory for this amputated Green function

$$\begin{aligned} G_c^{\text{amp}(1)}(x_1, x_2, x_3, x_4) &= \frac{\delta^4}{\delta\varphi(x_1) \dots \delta\varphi(x_4)} \left(\frac{-i\lambda}{4!} \right) \int d^4x \varphi^4(x) = (-i\lambda) \delta^{(4)}(x_1 - x_2) \delta^{(4)}(x_2 - x_3) \delta^{(4)}(x_3 - x_4) \\ \Rightarrow G_c^{\text{amp}(1)}(p_1, p_2, p_3, p_4) &= (2\pi)^4 \delta^{(4)}(p_1 + p_2 + p_3 + p_4) (-i\lambda), \end{aligned} \quad (3.55j)$$

which agrees with the Feynman rules for graph (C1) in Fig. 18 or the amputation of Eq. (3.44).

Since the connected, amputated Green functions directly give the S matrix (see, e.g. Eq. (3.48m)) one can define a **S -matrix functional**

$$\mathcal{F}[\varphi] := \mathcal{N} \int \mathcal{D}\Phi' \exp \left(i S_0[\Phi'] + i S_{\text{int}}[\Phi' + \varphi] \right) \quad (3.55k)$$

(c.f. **Nair**, eq. (8.49)), which after functional differentiation and Fourier transformation gives the S matrix

$$S_{k_1, \dots, k_m \rightarrow k'_1, \dots, k'_n} = \left(\frac{i}{\sqrt{Z_\Phi}} \right)^{m+n} \prod_i^m \left(\int d^4x_i e^{-ik_i \cdot x_i} \right) \prod_j^n \left(\int d^4y_j e^{ik'_j \cdot y_j} \right) \frac{\delta^{n+m}}{\delta\varphi(x_1) \dots \delta\varphi(x_m) \delta\varphi(y_1) \dots \delta\varphi(y_n)} \ln \mathcal{F}[\varphi] \Big|_{\varphi=0} \quad (3.55l)$$

(**Nair**, eq. (5.24)). The non-interacting part $-i(\varphi, \Delta_F^{-1} \varphi)/2$ in Eq. (3.55h), which only contributes to the 2-point function can be omitted in this expression. With the help of the chain rule (our conventions for Fourier transforms are given in Eq. (3.19))

$$\frac{\delta}{\delta\tilde{\varphi}(k)} = \int d^4x \frac{\delta\varphi(x)}{\delta\tilde{\varphi}(k)} \frac{\delta}{\delta\varphi(x)} = \int \frac{d^4x}{(2\pi)^4} e^{ik \cdot x} \frac{\delta}{\delta\varphi(x)} \quad (3.55m)$$

this can written more compactly as

$$S_{k_1, \dots, k_m \rightarrow k'_1, \dots, k'_n} = \left(\frac{(2\pi)^4 i}{\sqrt{Z_\Phi}} \right)^{m+n} \frac{\delta^{n+m}}{\delta\tilde{\varphi}(-k_1) \dots \delta\tilde{\varphi}(-k_m) \delta\tilde{\varphi}(k'_1) \dots \delta\tilde{\varphi}(k'_n)} \ln \mathcal{F}[\varphi] \Big|_{\varphi=0} \quad (3.55n)$$

Though this has been derived only for a scalar theory the formulas (3.55l) or (3.55n) can be generalized (with obvious modifications) to other theories.

For the generating functional of the **proper** or **one-particle-irreducible diagrams** see the next **chapter 3.2**.

Free Propagators of Other Theories:

- (a) Charged scalar particles are described by two fields with the same mass or equivalently by a complex field $\Phi(x)$ with the free Lagrangian

$$\mathcal{L}_0 = (\partial_\mu \Phi^*) (\partial^\mu \Phi) - m^2 \Phi^* \Phi \quad (3.56)$$

(note the missing factor 1/2 compared to the neutral Lagrangian (3.1)). This is the topic in **Problem 20** where one also should show that the 2-point function invokes the same Feynmann propagator as in the neutral case

$$G_2(x - y) \equiv \langle \Phi^*(y) \Phi(x) \rangle = i \Delta_F(x - y). \quad (3.57)$$

(b) A massive spin-1 particle (also called a vector particle) is described by the field $V_\mu(x)$ and the free Lagrangian

$$\mathcal{L}_0^V = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} m_V^2 V_\mu V^\mu, \quad F_{\mu\nu} := \partial_\mu V_\nu - \partial_\nu V_\mu \quad (3.58)$$

(notice the different sign of the mass term compared to the scalar case!). As can be derived in **Problem 26 a)** its propagator is

$$\tilde{D}_V^{\mu\nu}(k) = -\frac{1}{k^2 - m_V^2 + i0^+} \left[g^{\mu\nu} - \frac{k^\mu k^\nu}{m_V^2} \right]. \quad (3.59)$$

(c) In an analogous way one can treat **free spin- $\frac{1}{2}$ particles**, i.e. fermions, with the Lagrange density

$$\mathcal{L}_0 = \bar{\psi} (i\partial - m) \psi, \quad \partial \equiv \gamma^\mu \partial_\mu, \quad [\gamma^\mu, \gamma^\nu]_+ = 2g^{\mu\nu}. \quad (3.60)$$

To derive the equation of motions (the **Dirac equations**) for $\psi, \bar{\psi}$ one should use

$$\mathcal{L}_0 = \frac{i}{2} [\bar{\psi} \gamma^\mu (\partial_\mu \psi) - (\partial_\mu \bar{\psi}) \gamma^\mu \psi] - m \bar{\psi} \psi \quad (3.61)$$

but for the action both forms are equally valid (after an integration by part). To obtain a generating functional for fermionic Green functions, one has to introduce **anticommuting external sources** $\eta(x), \bar{\eta}(x)$ and to integrate functionally over Grassmann-valued fields ⁷³:

$$Z_0[\eta, \bar{\eta}] = \int \mathcal{D}\bar{\psi}(x) \mathcal{D}\psi(x) \exp \left[i \int d^4x (\mathcal{L}_0(\psi, \bar{\psi}) + \bar{\psi}\eta + \bar{\eta}\psi) \right]. \quad (3.62)$$

As in the bosonic case one finds by completing the square

$$Z_0[\eta, \bar{\eta}] = \text{const.} \cdot \exp \left[-i \int d^4x d^4y \bar{\eta}(x) S_F(x, y) \eta(y) \right], \quad (3.63)$$

where

$$S_F(x, y) = (i\partial - m + i0^+)^{-1}(x, y) = \int \frac{d^4k}{(2\pi)^4} e^{ik \cdot (x-y)} \frac{1}{\not{k} - m + i0^+} \quad (3.64)$$

is the Feynman propagator of the fermion.

Interactions can be included – in principle – as in the bosonic case, unless they follow from a gauge principle (see chapter 3.3).

Detail 29: $\sigma - \omega$ (or Walecka) Model

Walecka has proposed a relativistic model for the description of nuclei [44], in which nucleons (represented by the Dirac field Ψ with mass M) interact with each other by the exchange of scalar mesons (σ, m_σ) and vector mesons (ω_μ, m_ω) :

$$\mathcal{L}_W = \bar{\Psi} (i\partial - M) \Psi + \frac{1}{2} [(\partial_\mu \sigma)^2 - m_\sigma^2 \sigma^2] - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - g_\sigma \bar{\Psi} \Psi \sigma - g_\omega \bar{\Psi} \gamma_\mu \Psi \omega^\mu, \quad F_{\mu\nu} \equiv \partial_\mu \omega_\nu - \partial_\nu \omega_\mu. \quad (3.65a)$$

Aiming at a description of the strong interaction inside nuclei, the corresponding dimensionless coupling constants g_σ and g_ω of the mesons to the nucleons are not small: $g^2/(4\pi) = \mathcal{O}(10)$, while, e.g. in quantum electrodynamics the so-called fine-structure constant has the value $e^2/(4\pi) = 1/137$. Hence perturbation theory is not applicable which is, in general, also the case for all **binding problems** (another "weites Feld" **{Fontane}** which is not covered here ...)

⁷³ As one wants to work with commuting numbers in the path integral, the individual terms in the exponent (action, Lagrangian, source terms) have to be **Grassmann-even**, i.e. they should contain an even number of Grassmann-valued factors.

Why is this Lagrangian a possible model for the mutual interaction of nucleons? To answer this question we consider the non-relativistic limit for the generating functional (without external mesons): After integrating out the meson fields (Gaussian integral!) we have

$$Z[\bar{\eta}, \eta] = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi\mathcal{D}\sigma \prod_{\mu} \mathcal{D}\omega_{\mu} e^{i \int d^4x [\mathcal{L} + \bar{\eta}\Psi + \bar{\Psi}\eta]} = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \exp\left\{i \int d^4x \left[\bar{\Psi}(i\hat{\not{p}} - M)\Psi + \bar{\eta}\Psi + \bar{\Psi}\eta \right]\right\} \cdot e^{iS_{\sigma\omega}[\bar{\Psi}, \Psi]} \quad (3.65b)$$

$$S_{\sigma\omega}[\bar{\Psi}, \Psi] = -\frac{1}{2} \int d^4x d^4y \left[g_{\sigma}^2 \rho_S(x) D_{\sigma}(x-y) \rho_S(y) + g_{\omega}^2 J_{\mu}(x) D^{\mu\nu}(x-y) J_{\nu}(y) \right]. \quad (3.65c)$$

Here $\rho_S(x) = \bar{\Psi}(x)\Psi(x)$ is the scalar density of the nucleons and

$$J_{\mu}(x) = \bar{\Psi}(x)\gamma_{\mu}\Psi(x) \quad (3.65d)$$

their current while $\tilde{D}_{\sigma}(k) = 1/(k^2 - m_{\sigma}^2 + i0^+)$ denotes the usual Feynman propagator of the scalar field and $D^{\mu\nu}(x-y)$ the one of the vector meson. As derived in **Problem 27** the nucleon current is conserved: $\partial^{\mu}J_{\mu} = 0$ and thus the terms proportional to $k^{\mu}k^{\nu}$ in Eq. (3.59) do not contribute to the action (3.65c) bei. Because of that the behaviour of the vector-meson propagator at high k is less "dangerous" and the model remains renormalizable.

The non-relativistic limit is most transparent when we allow the "velocity of light $c \rightarrow \infty$ " so that it is recommended to re-introduce the natural constants c, \hbar . If we use $\square = \partial^2/(c^2\partial t^2) - \Delta$ then the scalar propagator in position space, e.g., turns into

$$\begin{aligned} D_{\sigma}(x-y) &= \int \frac{d^4k}{(2\pi\hbar)^4} \frac{\exp[-ik \cdot (x-y)/\hbar]}{k_0^2/(c^2\hbar^2) - \mathbf{k}^2/\hbar^2 - m_{\sigma}^2 c^2/\hbar^2 + i0^+} \xrightarrow{c \rightarrow \infty} -\hbar^2 \delta(x_0 - y_0) \int \frac{d^3k}{(2\pi\hbar)^3} \frac{\exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})/\hbar]}{\mathbf{k}^2 + m_{\sigma}^2 c^2} \\ &= -\delta(x_0 - y_0) \frac{1}{4\pi|\mathbf{x} - \mathbf{y}|} \exp\left(-\frac{m_{\sigma}c}{\hbar}|\mathbf{x} - \mathbf{y}|\right), \end{aligned} \quad (3.65e)$$

i.e. an instantaneous Yukawa term where the Compton wavelength $\hbar/(m_{\sigma}c)$ of the exchanged particle determines the range. The same is valid for the vector-meson propagator (3.59), which, however has an opposite sign compared to that of the scalar exchange.

The behaviour of the Dirac nucleons in the non-relativistic limit is standard in relativistic quantum mechanics (see, e.g. **{Bjorken-Drell}**, ch. 4). While the usual approach is an elimination of the "small" components in the Dirac equation or the systematic Foldy-Wouthuysen transformation, in the path integral one may simply integrate out the small component (see **Problem 28***). Then one obtains a non-relativistic action for the "large" component, the bi-spinor $\phi(\mathbf{x}, t)$ with a dominant central potential and a sub-dominant spin-orbit potential. In addition, the spatial components of the nucleon current (3.65d) are suppressed since in this case the nucleons only move slowly compared to the velocity of light.

If we substitute all this simplifications into Eq. (3.65b) and in leading order replace $\rho_S(x) \simeq J_0(x) \simeq \phi^{\dagger}(\mathbf{x}, t)\phi(\mathbf{x}, t)$, then all c -factors cancel and – returning to our standard system of units $\hbar = c = 1$ – we obtain

$$S_{\sigma\omega}[\phi^{\dagger}, \phi] = -\frac{1}{2} \int dt \int d^3x d^3y \phi^{\dagger}(\mathbf{x}, t)\phi(\mathbf{x}, t) \left[\underbrace{-\frac{g_{\sigma}^2}{4\pi} \frac{e^{-m_{\sigma}r}}{r} + \frac{g_{\omega}^2}{4\pi} \frac{e^{-m_{\omega}r}}{r}}_{=: V_{\sigma\omega}(r=|\mathbf{x}-\mathbf{y}|)} \right] \phi^{\dagger}(\mathbf{y}, t)\phi(\mathbf{y}, t). \quad (3.65f)$$

Comparison with Eqs. (2.131) and (2.107) identifies $V_{\sigma\omega}(r)$ as two-particle potential between nucleons in a fermionic Schrödinger theory. In other words: The **exchange of scalar mesons** leads to an **attractive** Yukawa potential, the **exchange of vector mesons** to a **repulsive** interaction which dominates at small distances if $g_{\omega} > g_{\sigma}$. For $m_{\omega} > m_{\sigma}$ the scalar exchange dominates at larger distances and together this generates a potential as depicted in Fig. 21. This potential reflects the empirical properties of the nucleon-nucleon interaction: Attractive at larger distances to bind the nucleons in the nucleus and strongly repulsive at small distances so that the density of heavy nuclei is practically constant.

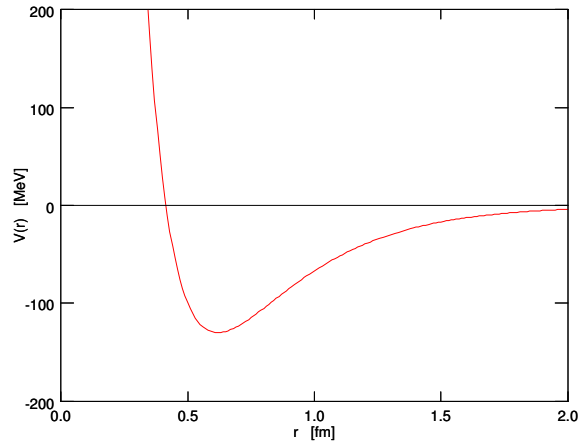


Fig. 21 : The non-relativistic potential (3.65f) between nucleons generated in the Walecka model by the exchange of scalar σ - and vectorial ω -mesons. The meson masses are taken as $m_{\sigma} = 520$ MeV, $m_{\omega} = 783$ MeV and the coupling constants as $g_{\sigma}^2/(4\pi) = 8.72$, $g_{\omega}^2/(4\pi) = 15.15$ [46].

If one also considers the $1/M^2$ -corrections in **Problem 28***, then one sees that also a **strong spin-orbit interaction** is generated by the $\sigma - \omega$ -exchange: Although being suppressed by the large nucleon mass the large scalar and vector potentials add in absolute value in

this term while they nearly cancel in the central potential. This strong spin-orbit interaction has been observed empirically long ago in the excitation spectra of atomic nuclei. Therefore the Walecka model offers a relativistic description of nuclei: By fitting its few parameters to experimental data it gives (in a relativistic mean-field Hartree approximation, see **chapter 2.7**) an equally good account of closed-shell nuclei as sophisticated non-relativistic potential models. In addition, as mentioned before, it is renormalizable which, however, is not very relevant in practice as the exchange of scalar and vector mesons can only be an effective or schematic theory of nucleon-nucleon interactions; for instance, it is well-known that the longest range of this interaction is mediated by the exchange of the lightest hadrons, the pions, which are not contained in this model at all.

However, as mentioned above, the quantization of fermionic theories whose interaction with bosonic fields is governed by a **gauge principle** – as, e.g. **Quantum-Electro-Dynamics (QED)** or **Quantum-Chromo-Dynamics (QCD)** – needs a special treatment. This is due to the fact that the gauge fields are necessarily massless and that in consequence the inversion of the bosonic kernel is not possible if the gauge degrees of freedom have not been separated. We will address that problem in **chapter 3.3**.

3.2 Effective Action

We now consider again a scalar theory (e.g. that of Eq. (3.2)) and denote explicitly the dependence on Planck’s elementary quantum:

$$Z[J] = \exp\left(\frac{i}{\hbar}W[J]\right). \tag{3.66}$$

One can define a **“classical field”** as vacuum expectation value of the field operator in presence of the source

$$\Phi_{\text{cl}}(x) := \frac{\delta W[J]}{\delta J(x)} = \frac{1}{Z} \int \mathcal{D}\Phi \Phi(x) \exp\left\{\frac{i}{\hbar} \int d^4y [\mathcal{L} + J(y)\Phi(y)]\right\}. \tag{3.67}$$

Of course, this field depends on the source J since otherwise the functional integral over an odd integrand would vanish. We assume that this relation can be inverted (which for weak sources is feasible at least perturbatively), i.e.

$$J = J(\Phi_{\text{cl}}). \tag{3.68}$$

Then one defines the quantity

$$\Gamma[\Phi_{\text{cl}}] := \left\{ W[J] - \int d^4x J(x)\Phi_{\text{cl}}(x) \right\}_{J=J(\Phi_{\text{cl}})}. \tag{3.69}$$

as **effective action**. Note that this is a **Legendre transformation** similar as in classical mechanics by which one goes from the Lagrange to the Hamilton function. One can show (for the 2-point function: See **Problem 22**) that the effective action is the generating functional for the **proper** or **one-particle-irreducible diagrams**

$$\Gamma[\Phi_{\text{cl}}] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^4x_1 \dots d^4x_n \Gamma^{(n)}(x_1 \dots x_n) \Phi_{\text{cl}}(x_1) \dots \Phi_{\text{cl}}(x_n). \tag{3.70}$$

These are those diagrams which do not collapse into two disconnected lower-order diagrams when one cuts a single internal line (see Fig. 22).

The effective actions gets an additional meaning from a relation which is obtained by functional differentiation of the definition (3.69) w.r.t. classical field (see **Problem 22**)

$$\frac{\delta \Gamma[\Phi_{\text{cl}}]}{\delta \Phi_{\text{cl}}(x)} = -J(x). \tag{3.71}$$

If the external source vanishes, we then have

$$\left. \frac{\delta \Gamma[\Phi_{\text{cl}}]}{\delta \Phi_{\text{cl}}} \right|_{J=0} = 0, \tag{3.72}$$

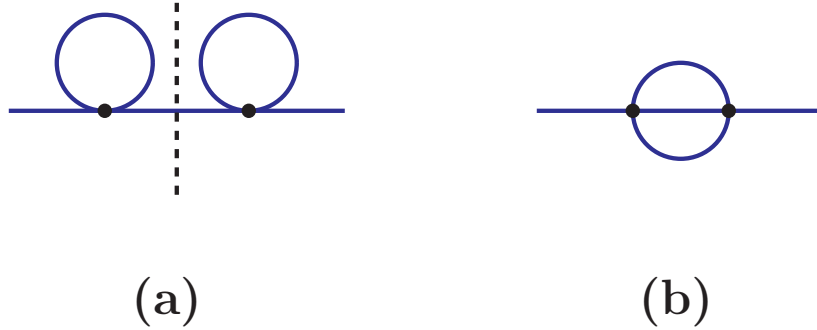


Fig. 22 : (a) An one-particle-reducible graph which can be cut along the dashed line
 (b) An one-particle-irreducible graph (in 2nd order perturbation theory for the Φ^4 -theory).

which is the exact counterpart to the equation of motion for a classical field. The main difference is, however, that $\Gamma[\Phi_{\text{cl}}]$ contains **all quantum corrections** explaining the name “effective action”. Borrowing from thermodynamics one can interpret $-W[J]$ as vacuum energy induced by the external source and understand the effective action $\Gamma[\Phi_{\text{cl}}]$ as analogon to Gibbs’ free energy whose minimum determines the dynamically most stable state of the system ⁷⁴. Studying the effective action, therefore allows us to determine the ground state of the system including all quantum fluctuations. This is particularly simple if the solutions of Eq. (3.72) are constant because then one has only to determine the minimum of a *function* and not of a functional:

$$\Phi_{\text{cl}} = \text{const.} \implies \Gamma[\Phi_{\text{cl}}] = -\mathcal{V} \cdot V_{\text{eff}}(\Phi_{\text{cl}}) . \quad (3.73)$$

Here \mathcal{V} is the space-time volume and V_{eff} the **effective potential**.

How can one calculate the effective action? Apart from perturbation theory we also have to our disposal the **semi-classical expansion** which we already have used several times in the first two main parts of this lecture. Also here it is based on the application of the stationary-phase method to the functional integral

$$Z[J] = \int \mathcal{D}\Phi \exp \left\{ \frac{i}{\hbar} \int d^4x \left[\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 - V(\Phi) + J\Phi \right] \right\} \equiv \int \mathcal{D}\Phi e^{iS[\Phi, J]/\hbar} . \quad (3.74)$$

The field configuration which is stationary fulfills $\delta S[\Phi, J]/\delta \Phi = 0$, i.e.

$$(\square + m^2) \Phi_0(x) + V'(\Phi_0) = J(x) , \quad (3.75)$$

and we assume that for $J = 0$ the solution is $\Phi_0 = 0$. In leading order of an expansion in \hbar the functional integral (3.74) is given by the value of the integrand for the stationary configuration:

$$Z^{(0)}[J] = \exp \left(\frac{i}{\hbar} S[\Phi_0] + \frac{i}{\hbar} \int d^4x J(x) \Phi_0(x) \right) = \exp \left(\frac{i}{\hbar} W^{(0)} \right) . \quad (3.76)$$

According to Eq. (3.67) the “classical field” is given in this order by

$$\Phi_{\text{cl}}^{(0)}(x) = \Phi_0(x) + \int d^4y J(y) \frac{\delta \Phi_0(y)}{\delta J(x)} + \frac{\delta S[\Phi_0]}{\delta J(x)} = \Phi_0(x) + \int d^4y \frac{\delta S[\Phi_0, J]}{\delta \Phi_0(y)} \frac{\delta \Phi_0(y)}{\delta J(x)} = \Phi_0(x) . \quad (3.77)$$

⁷⁴See, e.g. **Peskin & Schroeder**, ch. 11.3.

Here the chain rule has been used and the fact that $S[\Phi, J]$ is stationary at Φ_0 . Consequently, we have the expected result that for $\hbar = 0$ the effective action is identical with the classical action:

$$\boxed{\Gamma^{(0)}[\Phi_{\text{cl}}] = S[\Phi_{\text{cl}}]} \quad (3.78)$$

As usual, the quantum corrections are generated by fluctuations around the stationary configuration. Setting

$$\Phi(x) = \Phi_0(x) + \sqrt{\hbar} \phi(x) \quad (3.79)$$

we obtain

$$Z[J] = Z^{(0)}[J] \cdot \int \mathcal{D}\phi \exp \left\{ i \int d^4x \left[\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} (m^2 + V''(\Phi_0)) \phi^2 - \sum_{m \geq 3} \hbar^{m/2-1} \frac{1}{m!} V^{(m)}(\Phi_0) \phi^m \right] \right\}. \quad (3.80)$$

Obviously the quadratic terms in ϕ are the leading ones in a systematic expansion in powers of \hbar . We will see that the quadratic fluctuations lead to one-loop diagrams and it is not difficult to derive that in general the \hbar -expansion is an **expansion in loops**.

Let us now calculate the one-loop correction to the classical action. From Eq. (3.80) we obtain by means of the usual Gaussian integral

$$\int \mathcal{D}\phi \exp \left\{ -\frac{i}{2} \int d^4x \phi(x) [\square + m^2 + V''(\Phi_0)] \phi(x) \right\} = \frac{\text{const.}}{\text{Det}^{1/2}(\square + m^2 + V''(\Phi_0))}. \quad (3.81)$$

We may write the constant as value of the integral for $V = 0$ as we do not need the normalization of the generating functional. In this way the quantum correction to the effective action also vanishes automatically for vanishing interaction. Employing the trace-representation of the determinant (**Problem 13**) we obtain

$$Z^{(1)}[J] = Z^{(0)}[J] \cdot \exp \left\{ -\frac{1}{2} \text{tr} \ln \left[1 + \frac{1}{\square + m^2 - i0^+} V''(\Phi_0) \right] \right\}, \quad (3.82)$$

or

$$W^{(1)}[J] = S[\Phi_0, J] + \frac{1}{2} i\hbar \text{tr} \ln [1 - \Delta_F V''(\Phi_0)]. \quad (3.83)$$

For evaluating the effective action we use $\Phi_{\text{cl}} = \Phi_0 + \mathcal{O}(\hbar)$. Moreover, since $S[\Phi, J]$ is stationary at Φ_0 we also have $S[\Phi_{\text{cl}}, J] = S[\Phi_0, J] + \mathcal{O}(\hbar^2)$. By this it follows that

$$\boxed{\Gamma[\Phi_{\text{cl}}] = S[\Phi_{\text{cl}}] + \frac{1}{2} i\hbar \text{tr} \ln [1 - \Delta_F V''(\Phi_{\text{cl}})] + \mathcal{O}(\hbar^2)}. \quad (3.84)$$

The perturbative expansion of

$$\begin{aligned} \frac{1}{2} i\hbar \text{tr} \ln [1 - \Delta_F V''(\Phi_0)] &= -i\hbar \sum_{n=1}^{\infty} \frac{1}{2n} \text{tr} [\Delta_F V''(\Phi_0)]^n \\ &= -i\hbar \sum_{n=1}^{\infty} \frac{1}{2n} \int d^4z_1 \dots d^4z_n \Delta_F(z_1 - z_2) V''(\Phi_0(z_2)) \dots V''(\Phi_0(z_n)) \Delta_F(z_n - z_1) V''(\Phi_0(z_1)) \end{aligned} \quad (3.85)$$

shows that the additional term includes the contributions of all one-loop diagrams made up of n propagators $i\Delta_F(z_i - z_{i+1})$ and n vertices $-iV''(\Phi_0(z_{i+1})) = -i\lambda\Phi_0^2(z_{i+1})/2$ (see Fig. 23).

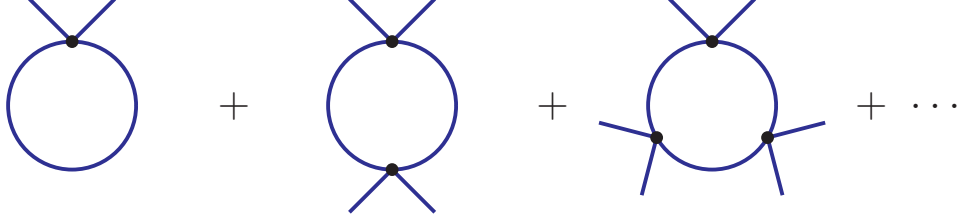


Fig. 23 : One-loop correction for the effective action in the Φ^4 -theory.

In many cases one only is interested in the effective potential which we already have introduced above for constant fields. However, it also can be seen as the first term in an expansion of the effective action in higher and higher derivatives of the field

$$\Gamma[\Phi_{\text{cl}}] = \int d^4x \left[-V_{\text{eff}}(\Phi_{\text{cl}}) + \frac{1}{2} Z_{\text{eff}}(\Phi_{\text{cl}}) \partial_\mu \Phi_{\text{cl}} \partial^\mu \Phi_{\text{cl}} + \dots \right]. \quad (3.86)$$

For the Φ^4 -theory we obtain with $\Phi_{\text{cl}} = \text{const.}$

$$V_{\text{eff}}(\Phi_{\text{cl}}) = \frac{1}{2} m^2 \Phi_{\text{cl}}^2 + \frac{\lambda}{4!} \Phi_{\text{cl}}^4 - \frac{i\hbar}{2} \int \frac{d^4k}{(2\pi)^4} \ln \left[1 - \frac{\lambda}{2} \frac{\Phi_{\text{cl}}^2}{k^2 - m^2 + i0^+} \right] + \mathcal{O}(\hbar^2). \quad (3.87)$$

The loop integral is divergent and must be made finite by a counter term of the form

$$V_{\text{counterterm}}(\Phi_{\text{cl}}) = \frac{A}{2} \Phi_{\text{cl}}^2 + \frac{B}{4!} \Phi_{\text{cl}}^4. \quad (3.88)$$

The constants A, B can be determined by requiring that the physical mass and the physical coupling constant are measured at $\Phi_{\text{cl}} = 0$:

$$\left. \frac{\partial^2 V_{\text{eff}}}{\partial \Phi_{\text{cl}}^2} \right|_{\Phi_{\text{cl}}=0} = m_{\text{phys}}^2, \quad \left. \frac{\partial^4 V_{\text{eff}}}{\partial \Phi_{\text{cl}}^4} \right|_{\Phi_{\text{cl}}=0} = \lambda_{\text{phys}}. \quad (3.89)$$

A particularly interesting case happens if one starts from an originally massless theory: $m^2 = 0$. However, one then has to impose the renormalization condition that the coupling constant has a fixed value at, say $\Phi_{\text{cl}} = M$

$$\lambda_M = \left. \frac{\partial^4 V_{\text{eff}}}{\partial \Phi_{\text{cl}}^4} \right|_{\Phi_{\text{cl}}=M}. \quad (3.90)$$

Then one obtains [47]

$$V_{\text{eff}}(\Phi_{\text{cl}}) = \frac{\lambda_M}{4!} \Phi_{\text{cl}}^4 + \frac{\hbar \lambda_M^2}{(16\pi)^2} \Phi_{\text{cl}}^4 \left(\ln \frac{\Phi_{\text{cl}}^2}{M^2} - \frac{25}{16} \right) + \dots \quad (3.91)$$

As the last term is negative for small Φ_{cl} the minimum is shifted from the origin $\Phi_{\text{cl}} = 0$, i.e. the quantum corrections of the one-loop correction have generated a mass “**spontaneously**”. Due to Eq. (3.71) this means that a vacuum expectation value of the field $\Phi_{\text{cl}}^{\text{min}}$ exists even for vanishing external source $J(x)$. However, as one can verify, this value lies outside the validity of the semi-classical expansion (the correction is as large as the classical contribution) so that this mechanism of **dynamical mass generation** remains unsettled.

3.3 Quantization of Gauge Theories

The free Lagrangian (3.60) for electrons is invariant under the **global gauge transformation**

$$\psi(x) \longrightarrow e^{-ie\Theta} \psi(x), \quad \bar{\psi}(x) \longrightarrow \bar{\psi}(x) e^{ie\Theta}. \quad (3.92)$$

Here Θ is a constant parameter and the electric charge e of the particles has been taken out explicitly for convenience. One can extend the gauge transformation (3.92) to a **local** one

$$\boxed{\psi(x) \longrightarrow e^{-ie\Theta(x)} \psi(x), \quad \bar{\psi}(x) \longrightarrow \bar{\psi}(x) e^{ie\Theta(x)},} \quad (3.93)$$

if one introduces a “**gauge field**” $A_\mu(x)$ which compensates the additional term from the derivative in \mathcal{L}_0 :

$$\mathcal{L}_0 \longrightarrow \mathcal{L} = \bar{\psi}(x) (i\cancel{\partial} - m - e\cancel{A}(x)) \psi(x). \quad (3.94)$$

To achieve that $A_\mu(x)$ obviously has to transform like

$$A_\mu(x) \longrightarrow A_\mu(x) + \partial_\mu\Theta(x). \quad (3.95)$$

If one adds an invariant kinetic energy term for the “photon field” A_μ which at most is quadratic in the derivatives, then the Lagrangian for **QuantumElectro-Dynamics (QED)** is complete:

$$\boxed{\mathcal{L}_{\text{QED}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi} (i\cancel{\partial} - m - e\cancel{A}) \psi, \quad F_{\mu\nu} := \partial_\mu A_\nu - \partial_\nu A_\mu.} \quad (3.96)$$

Note that the photons have to be **massless** – a mass term of the form $A_\mu A^\mu$ would violate the gauge invariance. The interaction between electrons and photons has thus been generated from “**gauging**” the phase transformation (3.92). As mathematically the group of these transformations constitutes an U(1) group one says that QED is an (abelian) U(1) gauge theory.

This remarkable gauge principle can be extended to **non-abelian gauge groups**: Let the Lie algebra of a (compact, semi-simple) Lie group G ⁷⁵ be generated by the (hermitean) generators T^a satisfying

$$\boxed{[T^a, T^b] = if^{abc} T^c, \quad a = 1 \dots n} \quad (3.97)$$

(identical indices are to be summed over). The constants f^{abc} are the structure constants which characterize the Lie algebra of the group G. As known from the treatment of angular momentum in quantum mechanics the generators can be realized in different (matrix) representations: Most important for physical applications are the **fundamental representation** as smallest possible representation (according to which the fermions transform) and the **adjoint representation** which is defined by

$$(T^a)_{bc} = -if^{abc}. \quad (3.98)$$

Both the field tensor $F_{\mu\nu}$ as well as the gauge field must transform under the adjoint representation of the gauge group (see, e.g. **Das**, ch. 12.2). We have

$$\text{tr} (T^a T^b) = C_2 \delta_{ab}, \quad (3.99)$$

⁷⁵For an explanation of these concepts see, e.g., <http://de.wikipedia.org/wiki/Liealgebra> or introductions to group theory for physicists like **{Georgi}**. Here all this mostly is too “heavy artillery” as we only will consider the group $SU(N)$ – the group of unitary transformations U of N -dimensional vectors with $\det U = 1$ (i.e. with traceless generators) – in the following.

where the constant C_2 only depends on the representation (usually $C_2 = 1/2$ is chosen for the fundamental representation).

Examples :

- a) $G = SU(2)$: $f^{abc} \equiv \epsilon^{abc}$, (total antisymmetric tensor, $\epsilon^{123} = 1$). In the fundamental representation the generators are given by the **Pauli matrices**: $T^a = \tau^a/2$ with

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.100)$$

- b) $G = SU(3)$: The gauging of this group leads to **QuantumChromoDynamics (QCD)**, the theory of strong interactions of quarks and gluons. In the fundamental representation the generators are given by the **Gell-Mann matrices** : $T^a = \lambda^a/2$, $a = 1 \dots 8$ with

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \\ \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \end{aligned} \quad (3.101)$$

The structure constants f^{abc} are totally antisymmetric and the non-vanishing elements have the values (as can be seen from the explicit representation (3.101))

$$f^{123} = 1, f^{147} = f^{246} = f^{257} = f^{345} = \frac{1}{2}, f^{156} = f^{367} = -\frac{1}{2}, f^{458} = f^{678} = \sqrt{\frac{3}{2}}. \quad (3.102)$$

In general one has

$$n = N^2 - 1 \quad \text{generators for } SU(N). \quad (3.103)$$

The fermion field now appears in N species, for instance, there exist 2 states of the nucleon – proton and neutron – for isospin $SU(2)$ and 3 colored quarks for color $SU(3)$. It transforms under the fundamental representation

$$\boxed{\psi(x) = \exp(-ig\Theta^a T^a) \psi'(x)}, \quad \psi(x) = \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_N(x) \end{pmatrix}, \quad (3.104)$$

where T^a is a matrix representation of the generators. The free Lagrangian (3.60) (in which m now is a mass matrix) is again invariant under the global transformation (3.104) but no longer under the **local gauge transformation**

$$\psi(x) = \exp[-ig\Theta^a(x)T^a] \psi'(x). \quad (3.105)$$

For compensation we need a gauge field $A_\mu^a(x)$, $a = 1 \dots n$ which transforms like

$$A_\mu^a(x) = A_\mu^{\prime a}(x) + g f^{abc} \Theta^b(x) A_\mu^{\prime c}(x) + \partial_\mu \Theta^a(x) + \mathcal{O}(\Theta^2) \quad (3.106)$$

under an infinitesimal gauge transformation.

Proof: We write the gauge transformation (3.105) as

$$\psi(x) = U(x) \psi'(x) \quad \text{with} \quad U(x) = e^{-ig\Theta^a(x)T^a}, \quad U^\dagger(x)U(x) = U(x)U^\dagger(x) = 1 \quad (3.107a)$$

and introduce again a (matrix-valued) gauge field $\mathcal{A}_\mu(x)$ which should compensate the additional terms which have appeared by the local gauge transformation of the free fermionic Lagrangian

$$\begin{aligned} \mathcal{L}(\bar{\psi}, \psi, \mathcal{A}) &= \bar{\psi} [\gamma^\mu (i\partial_\mu - g\mathcal{A}_\mu) - m] \psi = \bar{\psi}' U^\dagger(x) \left\{ \gamma^\mu [iU(x)\partial_\mu + i(\partial_\mu U(x)) - g\mathcal{A}_\mu U(x)] - mU(x) \right\} \psi' \\ &= \mathcal{L}(\bar{\psi}', \psi', \mathcal{A}') + \bar{\psi}' \gamma^\mu \left[i \left(U^\dagger \partial_\mu U(x) \right) + g\mathcal{A}'_\mu - gU^\dagger(x)\mathcal{A}_\mu U(x) \right] \psi'. \end{aligned} \quad (3.107b)$$

To cancel the unwanted terms the vector potential \mathcal{A}_μ must thus transform as

$$\mathcal{A}_\mu = U(x)\mathcal{A}'_\mu U^\dagger(x) + \frac{i}{g} (\partial_\mu U(x)) U^\dagger(x). \quad (3.107c)$$

For the abelian theory this agrees with Eq. (3.95) (there the coupling constant has been denoted by e). In a non-abelian theory we write

$$\mathcal{A}_\mu(x) =: A_\mu^a(x) T^a \quad (3.107d)$$

and restrict ourselves to infinitesimal transformations (which is always possible in Lie algebras) $U(x) = 1 - ig\Theta^a(x)T^a + \mathcal{O}(\Theta^2)$. Then we obtain from Eq. (3.107c)

$$\begin{aligned} A_\mu^a T^a &= A_\mu^{a'} T^a - ig\Theta^b(x) T^b A_\mu^{a'} T^a + igA_\mu^{a'} T^a \Theta^b(x) T^b + \partial_\mu \Theta^a(x) T^a \\ &= A_\mu^{a'} T^a + \partial_\mu \Theta^a(x) T^a - ig\Theta^b(x) \underbrace{[T^b, T^a]}_{=ifbacT^c} A_\mu^{a'} = A_\mu^{a'} T^a + \partial_\mu \Theta^a(x) T^a + gf^{bac}\Theta^b(x) A_\mu^{a'} T^c. \end{aligned} \quad (3.107e)$$

If we exchange $a \leftrightarrow c$ in the last term and use $f^{bca} = f^{abc}$, we get Eq. (3.106).

Hence, if we add an invariant, kinetic term for the gauge fields then the Lagrange density of a non-abelian gauge theory is given by

$$\mathcal{L}_{\text{non-abelian}} = -\frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu} + \bar{\psi} (i\not{D} - m) \psi \quad (3.108)$$

where

$$D_\mu(x) = \partial_\mu + igT^a A_\mu^a(x) \quad (3.109)$$

is the **covariant derivative**. In components it reads

$$(D_\mu(x))_{jk} = \partial_\mu \delta_{jk} + ig(T^a)_{jk} A_\mu^a(x), \quad (3.110)$$

where $(T^a)_{ij}$ is the matrix representation of the generator T^a in the fundamental representation. Note that e.g. in $SU(N)$: $j, k = 1, \dots, N$ while a, b run from 1 to $n = N^2 - 1$. In the adjoint representation we have

$$(D_\mu(x))^{ab} = \partial_\mu \delta^{ab} + gf^{acb} A_\mu^c(x) \quad (3.111)$$

and therefore we can write the behaviour of the potential (3.106) under a gauge transformation simply as

$$A_\mu^a(x) \longrightarrow A_\mu^a(x) + \delta A_\mu^a(x), \quad \delta A_\mu^a(x) = (D_\mu(x))^{ab} \Theta^b \equiv (D_\mu(x)\Theta)^a. \quad (3.112)$$

The field tensor can be determined from the relation

$$[D_\mu, D_\nu] = ig\mathcal{F}_{\mu\nu} = igF_{\mu\nu}^a T^a \quad (3.113)$$

with the result

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - gf^{abc} A_\mu^b A_\nu^c . \quad (3.114)$$

It is now **non-linear** in the vector potentials – therefore the gauge bosons carry "charges" (e.g. color) and interact with each other, in contrast to the abelian case.

That the kinetic term for the gauge bosons is gauge invariant can be seen from the behaviour of the covariant derivative under gauge transformations: This quantity is constructed in such a way that $\bar{\psi}(i\not{D} - m)\psi$ is invariant under the gauge transformation (3.107a), i.e.

$$D_\mu(x) \longrightarrow U(x) D_\mu(x) U^\dagger(x) . \quad (3.115a)$$

Then Eq. (3.113) transforms as

$$\mathcal{F}_{\mu\nu}(x) \longrightarrow -\frac{i}{g} \left[U(x) D_\mu(x) U^\dagger(x), U(x) D_\nu(x) U^\dagger(x) \right] = -\frac{i}{g} U(x) \left[D_\mu(x), D_\nu(x) \right] U^\dagger(x) \equiv U(x) \mathcal{F}_{\mu\nu}(x) U^\dagger(x) \quad (3.115b)$$

and, indeed, the kinetic term for the gauge bosons

$$-\frac{1}{2} \text{tr} (\mathcal{F}_{\mu\nu} \mathcal{F}^{\mu\nu}) \longrightarrow -\frac{1}{2} \text{tr} \left(U(x) \mathcal{F}_{\mu\nu} \mathcal{F}^{\mu\nu} U^\dagger(x) \right) = -\frac{1}{2} \text{tr} (\mathcal{F}_{\mu\nu} \mathcal{F}^{\mu\nu}) = -\frac{1}{4} F_{\mu\nu}^a F^{\mu\nu a} \quad (3.115c)$$

does not change (in the final step it was used that in a trace one can move factors cyclically).

As already mentioned we encounter difficulties when trying to quantize gauge theories because gauge fields are physically equivalent if they are connected by a gauge transformation (3.106). As this is not tied to the existence of fermions we will first consider the pure "Yang-Mills theory" without fermions. Naively the generating functional would be

$$Z^{\text{YM}}[J] = \int \mathcal{D}A_\mu^a(x) \exp \left[i \int d^4x (\mathcal{L} + J_\mu^a A^{a\mu}) \right] . \quad (3.116)$$

In particular, for the free case ($g = 0$) the field tensor equals the abelian one and after an integration by parts we have

$$Z_0^{\text{YM}}[J] = \int \mathcal{D}A_\mu^a(x) \exp \left\{ i \int d^4x \left[\frac{1}{2} A_\mu^a (g^{\mu\nu} \square - \partial^\mu \partial^\nu) A_\nu^a + J_\mu^a A^{a\mu} \right] \right\} . \quad (3.117)$$

Following the usual scheme of completing the square we would obtain

$$Z_0^{\text{YM}}[J] = \frac{\text{const.}}{\text{Det}^{1/2} K} \exp \left\{ -\frac{i}{2} \int d^4x d^4y J^{a\mu}(x) (K^{-1})_{\mu\nu}^{ab}(x, y) J^{b\nu}(y) \right\} \quad (3.118)$$

where

$$K_{\mu\nu}^{ab}(x, y) = \delta^{ab} \delta^4(x - y) (g_{\mu\nu} \square - \partial_\mu \partial_\nu) \quad (3.119)$$

has to be inverted. However, K does **not** have an inverse: There exist eigenfunctions $k_\nu \exp(ik \cdot x)$ with eigenvalue 0! (Equivalent aspects of this fact are that K is a projection operator which projects out the transverse degrees of freedom of the gauge field or that the spin-1 propagator (3.59) diverges for $m = 0$). Therefore $\text{Det} K$ vanishes and the previous approach to derive the Feynman rules is not applicable.

This difficulty arises from the fact that we have summed over all gauge-field configurations in the path integral, also over those which are connected by gauge transformations. These are redundant, i.e. unphysical. We have to take out the (infinite) contribution of such configurations from the path integral, i.e. in order to quantize a gauge theory one has to **fix the gauge**. This can be done by a condition

$$\mathcal{H}^a(A_\mu^\Theta) = h^a(x) \quad (3.120)$$

where the index Θ shall indicate the chosen gauge with gauge parameter Θ . The decisive step now is to multiply the path integral for the generating functional with a “1” in the form

$$1 = \Delta_{FP}(A) \int \mathcal{D}\Theta(x) \delta [\mathcal{H}(A_\mu^\Theta(x)) - h(x)] \tag{3.121}$$

where

$$\mathcal{D}\Theta(x) = \prod_{a=1}^n \prod_j d\Theta^a(x_j) \tag{3.122}$$

is the invariant functional measure in the group space (for $SU(2)$ e.g. this means functional integration over the 3 Euler angles by which the group can be parametrized) and

$$\delta [\mathcal{H}(x) - h(x)] = \prod_{a=1}^n \prod_j \delta (\mathcal{H}^a(x_j) - h^a(x_j)) \tag{3.123}$$

is the functional δ -function. The **Faddeev-Popov** factor Δ_{FP} is given by

$$\Delta_{FP}(A) = \text{Det} \left[\frac{\delta \mathcal{H}(A_\mu^\Theta)}{\delta \Theta} \right], \tag{3.124}$$

where the determinant also has to be taken in group space.

Detail 30: A Two-dimensional Example ⁷⁶

Let us assume that in the integral

$$Z = \int d^2r \exp[iS(\mathbf{r})] \tag{3.125a}$$

the “action” S only depends on the radius r of the vector $\mathbf{r} = (r, \varphi)$. Then the integrand is invariant under a rotation $\mathbf{r} \rightarrow \mathbf{r}^\Theta = (r, \varphi + \Theta)$ by the fixed angle Θ . Of course, normally one would use this invariance immediately to perform the φ -integration which gives a factor 2π . But let’s assume that we are unable to identify the “relevant degree of freedom” (here the radius r) – nevertheless it is possible to factor out the contribution of the irrelevant degree of freedom (φ) in the integral: We fix the rotation angle Θ by the constraint

$$\mathcal{H}(\mathbf{r}^\Theta) = h = \text{const.} \tag{3.125b}$$

and integrate over all rotation angles. Due to the relation $\delta(F(x) - h) = \sum_i \delta(x - x_i) / |F'(x_i)|$ where $F(x_i) = h$, we thus have

$$1 = \Delta(\mathbf{r}) \int d\Theta \delta (\mathcal{H}(\mathbf{r}^\Theta) - h), \text{ with } \Delta(\mathbf{r}) = \left. \frac{\partial \mathcal{H}(\mathbf{r}^\Theta)}{\partial \Theta} \right|_{\Theta=\Theta_0}, \tag{3.125c}$$

provided that the equation $\mathcal{H}(\mathbf{r}^\Theta) = h$ has just **one** solution Θ_0 . Hence we obtain for the integral in Eq. (3.125a)

$$Z = \int d\Theta \underbrace{\int d^2r e^{iS(r)} \Delta(\mathbf{r}) \delta (\mathcal{H}(\mathbf{r}^\Theta) - h)}_{:= Z^\Theta}, \tag{3.125d}$$

where Z^Θ now is independent of Θ . This is shown by rotation with another angle Θ' :

$$Z^{\Theta'} = \int d^2r e^{iS(r)} \Delta(\mathbf{r}) \delta (\mathcal{H}(\mathbf{r}^{\Theta'}) - h). \tag{3.125e}$$

By construction the Faddeev-Popov factor is independent of the rotation angle as is the “action” S . Thus, if we choose $\mathbf{r}^{\Theta'} = (r, \varphi + \Theta') =: (r, \varphi') = \mathbf{r}'$ as new integration variable, we get

$$Z^{\Theta'} = \int d^2r' e^{iS(r')} \Delta(\mathbf{r}') \delta (\mathcal{H}(\mathbf{r}') - g) \equiv Z^{\Theta=0} \tag{3.125f}$$

⁷⁶Cheng & Li, p. 250 - 252

and we can do the angle integration, i.e. we can factorize the contribution of the irrelevant degrees of freedom

$$Z = 2\pi \cdot Z^{\Theta=0}. \quad (3.125g)$$

The choice of the constraint \mathcal{H} is as arbitrary as is the choice of the constant h ; we only have to make sure that the rotation angle Θ is fixed unambiguously. A (trivial) example is $\mathcal{H}(\mathbf{r}^\Theta) = \varphi + \Theta \stackrel{!}{=} h$, which fixes the polar angle for all r and leads to $\Delta(\mathbf{r}) = 1$.

One therefore has assumed additionally that for each Θ^a there exists precisely one gauge field A^a which fulfills the gauge condition (3.120)⁷⁷. If we now perform a gauge transformation in the path-integral representation of the generating functionals

$$Z_0^{\text{YM}}[J] = \int D\Theta \int \mathcal{D}A^\Theta \Delta_{FP}(A^\Theta) \exp [iS_0[A^\Theta] + i(J, A^\Theta)] \delta [\mathcal{H}(A^\Theta) - h(x)] \quad (3.126)$$

then the action $S_0[A]$ is invariant as well as the Faddeev-Popov factor Δ_{FP} and the integration measure. If we only consider gauge-invariant quantities then also in the source term

$$(J, A^\Theta) \equiv \int d^4x J^{\mu a}(x) A_\mu^{\Theta a}(x) \quad (3.127)$$

we can replace A^Θ by $A^{\Theta'}$ ⁷⁸. By re-gauging we thus obtain

$$\begin{aligned} Z_0^{\text{YM}}[J] &= \int D\Theta \int \mathcal{D}A^{\Theta'} \Delta_{FP}(A^{\Theta'}) \exp (iS_0[A^{\Theta'}] + i(J, A^{\Theta'})) \delta [\mathcal{H}(A^{\Theta'}) - h(x)] \\ &= \text{const.} \int \mathcal{D}A^{\Theta'} \Delta_{FP}(A^{\Theta'}) \exp (iS_0[A^{\Theta'}] + i(J, A^{\Theta'})) \delta [\mathcal{H}(A^{\Theta'}) - h(x)], \end{aligned} \quad (3.128)$$

as now the integration over the gauge parameters can be performed. This only produces an (infinite) factor which cancels when calculating Green functions. In this way we have integrated over all configurations which only are produced by a gauge transformation.

As the functions $h^a(x)$ in the gauge fixing (3.120) are arbitrary, one may functionally integrate over them with the weight

$$\exp \left(-\frac{i}{2\lambda} \int d^4x h^a(x) h^a(x) \right) \quad (3.129)$$

where λ is an arbitrary parameter. In this way the gauge fixing becomes a part of the Lagrangian and one obtains

$$Z_0^{\text{YM}}[J] = \text{const.} \int \mathcal{D}A \text{Det} \left[\frac{\delta \mathcal{H}_a(A)}{\delta \Theta} \right] \exp \left[i \int d^4x \left(\mathcal{L}_0 - \frac{1}{2\lambda} \mathcal{H}^2(A) + J^{\mu a} A_\mu^a \right) \right]. \quad (3.130)$$

Exactly the same purpose serves the representation of the determinant (of the Faddeev-Popov factor) as an integral over **fictitious, anticommuting** fields $\chi^a(x), \bar{\chi}^a(x)$:

$$\text{Det} \left[\frac{\delta \mathcal{H}_a(A)}{\delta \Theta} \right] = \int \mathcal{D}\bar{\chi}(x) \mathcal{D}\chi(x) \exp \left[i \int d^4x d^4y \bar{\chi}^a(x) K_{ab}(x, y) \chi^b(y) \right], \quad (3.131)$$

where

$$K_{ab}(x, y) = \frac{\delta \mathcal{H}_a(A(x))}{\delta \Theta_b(y)}. \quad (3.132)$$

These are the “**Faddeev-Popov ghosts**” – scalar fields anticommuting like fermionic fields.

⁷⁷Non-perturbatively this is not the case in general, a phenomenon called **Gribov ambiguity**.

⁷⁸ (J, A) is not gauge-invariant. Consequently, also Green functions are not gauge-independent but only S -matrix elements.

How does one determine the kernel K in Eq. (3.132) ? We know how the gauge field transforms under an infinitesimal gauge transformation (see Eq. (3.106)). If, for simplicity, we only consider **linear gauge fixings**

$$\mathcal{H}^a(A) = \mathcal{H}^\mu A_\mu^a(x) \quad (3.133)$$

(where \mathcal{H}^μ could also be an operator), we obtain

$$K_{ab}(x, y) = \mathcal{H}^\mu \left(f^{abc} A_\mu^c(x) + \delta_{ab} \frac{1}{g} \partial_\mu \right) \delta^{(4)}(x - y) = \frac{1}{g} \mathcal{H}^\mu (D_\mu(x))^{ab} \delta^{(4)}(x - y), \quad (3.134)$$

where $D_\mu(x)$ is the covariant derivative – now in the adjoint representation (3.111). We can take out the factor g^{-1} from K_{ab} by a re-definition of the ghost fields and thus find

$$Z_0^{\text{YM}}[J] = \text{const.} \int \mathcal{D}A \mathcal{D}\bar{\chi} \mathcal{D}\chi \exp \left\{ i \int d^4x \left[\mathcal{L}_0 - \frac{1}{2\lambda} (\mathcal{H}_a^\mu A_\mu^a)^2 \right] \right\} \cdot \exp \left\{ i \int d^4x \left[J^{a\mu} A_\mu^a + \bar{\chi}^a \mathcal{H}^\mu (D_\mu(x))^{ab} \chi^b \right] \right\}. \quad (3.135)$$

The covariant derivative in the last exponential function also contains a term of order g which rather is a part of the interaction and therefore (for getting the free propagators) can be replaced by $\partial_\mu \delta_{ab}$.

Notes :

- a) In **abelian theories** (like **QED**), in which the structure constants are $f^{abc} = 0$ the ghosts do not couple to the gauge field and therefore are not relevant.
- b) In a **non-abelian theory** (like **QCD**) they couple in general to the gauge bosons (the gluons) but only in $\mathcal{O}(g)$.
- c) In a covariant gauge

$$\mathcal{H}_\mu = \partial_\mu \quad (3.136)$$

we now obtain after an integration by part for the **free generating functional** (the ghosts can be integrated out immediately and only contribute to the irrelevant constant in front of the path integral)

$$\begin{aligned} Z_0[J] &= \text{const.} \int \mathcal{D}A \exp \left\{ i \int d^4x \left[\frac{1}{2} A_\mu \left(g^{\mu\nu} \square - \partial^\mu \partial^\nu + \frac{1}{\lambda} \partial^\mu \partial^\nu \right) A_\nu + J^\mu A_\mu \right] \right\} \\ &= \text{const.}' \exp \left\{ -\frac{i}{2} \int d^4x d^4y J^\mu(x) \Delta_{\mu\nu}(x, y) J^\nu(y) \right\}, \end{aligned} \quad (3.137)$$

where the kernel fulfills

$$\left[g^{\mu\nu} \square_x - \left(1 - \frac{1}{\lambda} \right) \partial_x^\mu \partial_x^\nu \right] \Delta_{\nu\rho}(x, y) = g_\rho^\mu \delta^4(x - y). \quad (3.138)$$

This can now be inverted in Fourier space and one obtains the following propagator for the gauge bosons (**Problem 26 b**)

$$\Delta_{\mu\nu}(k) = -\frac{1}{k^2 + i0^+} \left[g_{\mu\nu} - (1 - \lambda) \frac{k_\mu k_\nu}{k^2 + i0^+} \right]. \quad (3.139)$$

If one chooses the gauge parameter $\lambda = 1$, then one works in **Feynman gauge**, for $\lambda = 0$ in **Landau gauge**. In non-abelian gauge theories the gauge-boson propagator (3.139) gets an additional factor δ_{ab} . Physical observables, as cross sections, masses, decay rates must be independent of the gauge parameter λ which gives a necessary criterion for a correct calculation. On the other hand Green functions are gauge dependent (see, e.g. Eqs. (3.142a) and (3.142b)).

- d) One can obtain the ghost propagator in a covariant gauge directly from the corresponding part of the free generating functional if $\partial_\mu (D_\mu)^{ab} = \delta_{ab} \square + \mathcal{O}(g)$ is used. From

$$Z_0 = \dots \int \mathcal{D}\bar{\chi} \mathcal{D}\chi \exp \left[\int d^4x \bar{\chi}^a(x) \delta_{ab} \square \chi^B(x) \right] \quad (3.140)$$

one can read off

$$\Delta_{FP}^{ab}(k) = -\delta_{ab} \frac{1}{k^2 + i0^+}. \quad (3.141)$$

- e) There exist gauges in which the Faddeev-Popov factor is independent of the gauge field and in which therefore no ghosts appear, e.g. the **axial gauge** $n^\mu A_\mu^a = 0$, (n^μ is a spacelike vector) or temporal gauge $A_0^a = 0$. However, these gauges result in a complicated gluon propagator and are not explicitly covariant.

Detail 31: Infrared Problem

Quantized gauge theories not only have a divergence problem at high energies when one is calculating loops (“**ultraviolet problem**”) which is treated (maybe one even can say “solved”) by renormalization but also at very small energies (“**infrared problem**”) because the gauge bosons are massless. Among other things this shows up in the full fermionic Green functions which in reality do not exhibit a simple pole but a branch point at $p^2 = m^2$. One can study that in **QED** by invoking the **Bloch-Nordsieck approximation** which simplifies drastically the fermion spin degrees of freedom but correctly describes the effect of low-energy (“soft”) photons⁷⁹ and one obtains (**Problem 30***)

$$G_2(p) = \frac{i m^{1+2\kappa} Z_2}{(p^2 - m^2 + i0)^{1+\kappa}}, \quad (3.142a)$$

with the gauge-dependent exponent

$$\kappa = \frac{e^2}{8\pi^2} (3 - \lambda). \quad (3.142b)$$

A physical electron, thus, is always surrounded by a cloud of (very soft) photons (similar as in the polaron problem the bare electron is surrounded by a cloud of phonons, which, however, have a fixed frequency = mass) and the LSZ formulas are strictly not applicable. As a remedy one is giving the photons a small mass μ and is including processes with ultra-soft photons (summed incoherently) which cannot be distinguished from the actual final state due to the finite energy resolution of the detector. The Bloch-Nordsieck theorem then guarantees that the limit $\mu \rightarrow 0$ can be performed in the final result and that essentially the photon mass is replaced by the energy resolution. One can do that also in non-abelian theories like **QCD** but that doesn't circumvent the main problem, viz. the “**confinement**” of quarks and gluons which do neither appear in the initial nor the final state as free particles. For the treatment of infrared divergencies in this case see **{Muta}**, ch. 6.

The full generating functional – including the fermions – and with interactions reads

$$Z[J, \eta, \bar{\eta}] = \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{D}\bar{\chi} \mathcal{D}\chi \exp \left\{ i \int d^4x [\mathcal{L}_0 + \mathcal{L}' + J_\mu^a A^{a\mu} + \bar{\psi}\eta + \bar{\eta}\psi] \right\}, \quad (3.143)$$

where

$$\mathcal{L}_0 = \frac{1}{2} A_\mu^a \left[g^{\mu\nu} \square - \left(1 - \frac{1}{\lambda} \right) \partial^\mu \partial^\nu \right] A_\nu^a + \bar{\psi} (i\partial - m) \psi + \bar{\chi}^a \square \chi^a \quad (3.144)$$

⁷⁹In this approximation the Dirac matrices for the electron are replaced by a constant four-vector, essentially the velocity, since it doesn't change practically in processes with low-energy emitted and absorbed photons.

is the free Lagrangian density (i.e. everything quadratic in the fields) while \mathcal{L}' contains the couplings

$$\mathcal{L}' = -g\bar{\psi}T^a A^a \psi + g f^{abc} \bar{\chi}^a \chi^b \partial \cdot A^c + \frac{g}{2} f^{abc} (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a) A^{\mu b} A^{\nu c} - \frac{g^2}{4} f^{abc} f^{ade} A_\mu^b A_\nu^c A^{\mu d} A^{\nu e} \quad (3.145)$$

(a)
(b)
(c)
(d)

These determine the vertices of the theory displayed in Fig. 24. Note that the different vertices are all fixed by **one coupling constant** g .

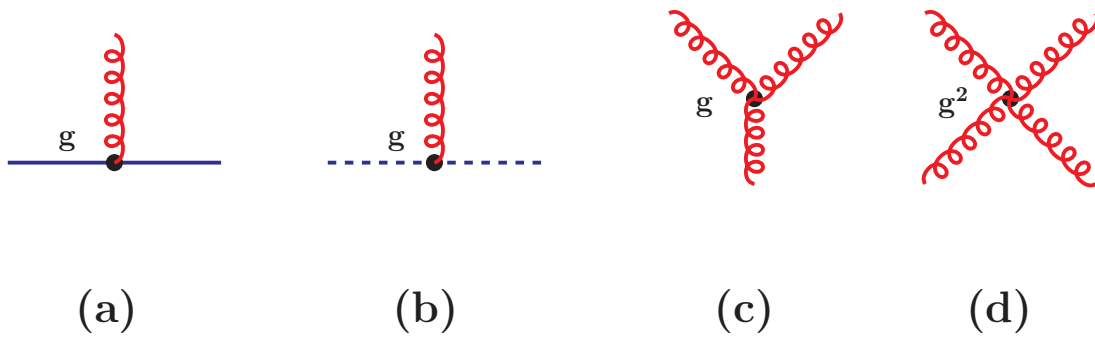


Fig. 24 : Vertices of a non-abelian gauge theory (like **QCD**) according to Eq. (3.145). The full blue line represents the fermions (quarks), the dashed blue line the Faddeev-Popov ghosts and the curly red lines the gauge bosons (gluons).

With that (and the propagators following from the quadratic terms) it is easy to derive the Feynman rules, say for **QCD**,⁸⁰

Detail 32: BRST symmetry

That this gives a consistent, renormalizable theory in all orders is due to a symmetry which the gauge-fixed, non-abelian Lagrangian with ghost fields possesses: Instead of the classical local gauge invariance the full Lagrangian in a covariant gauge

$$\begin{aligned} \mathcal{L} &= \mathcal{L}_f + \mathcal{L}_g + \mathcal{L}_{gauge} + \mathcal{L}_{FP} \\ \mathcal{L}_f &= \bar{\psi}(x) (i\not{D}(x) - m) \psi(x), \quad D_\mu(x) = \partial_\mu + ig T^a A_\mu^a(x) \\ \mathcal{L}_g &= -\frac{1}{4} F_{\mu\nu}^a F^{\mu\nu a}, \quad F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g f^{abc} A_\mu^b A_\nu^c \\ \mathcal{L}_{gauge} &= -\frac{1}{2\lambda} (\partial^\mu A_\mu^a)^2, \quad \mathcal{L}_{FP} = \bar{\chi}^a \partial^\mu (D_\mu(x))^{ab} \chi^b, \quad D_\mu^{ab} = \partial_\mu \delta^{ab} + g f^{acb} A_\mu^c(x) \end{aligned} \quad (3.146a)$$

is invariant under the **Becchi-Rouet-Stora-Tyutin (BRST) transformation**:

$$\begin{aligned} \delta A_\mu^a &= \omega (D^\mu \chi)^a, \quad \delta \psi = ig \omega \chi^a T^a \psi \\ \delta \bar{\chi}^a &= -\frac{1}{\lambda} \omega \partial^\mu A_\mu^a, \quad \delta \chi^a = -\frac{g}{2} \omega f^{abc} \chi^b \chi^c, \end{aligned} \quad (3.146b)$$

where ω is a Grassmann valued constant parameter. One finds (**Problem 31***)

$$\delta (D_\mu \chi)^a = 0, \quad \delta (f^{abc} \chi^b \chi^c) = 0 \quad (3.146c)$$

⁸⁰See, e.g. **Cheng & Li**, ch. 9.2 .

and

$$\delta (\partial_\mu A^{\mu a}) = 0, \quad (3.146d)$$

if the equation of motion for the ghost field χ^a is used. This means that applying the BRST transformation twice on gauge and ghost fields yields zero

$$\delta_2 \delta_1 \Phi^a = 0, \quad (3.146e)$$

where $\Phi^a = A_\mu^a$ or χ^a or $\bar{\chi}^a$ and the two transformations could have different parameters $\omega_{1/2}$. These transformations induce the following change of the Lagrangian

$$\delta \mathcal{L} = -\partial^\mu \left[\frac{\omega}{\lambda} (\partial^\nu A_\nu^a) D_\mu \chi^a \right], \quad (3.146f)$$

i.e. a total derivative and therefore demonstrate the invariance of the action.

It is advantageous to represent the gauge-fixing term in the Lagrangian by an auxiliary field

$$B^a(x) = \frac{1}{\lambda} \partial^\mu A_\mu^a(x) \quad (3.146g)$$

(again an application of the “undoing the square”-trick or the Hubbard-Stratonovich transformation!)

$$\exp \left\{ -\frac{i}{2\lambda} \int d^4x \left[\partial_\mu A_\mu^a(x) \right]^2 \right\} = \text{const.} \int \mathcal{D}B(x) \exp \left\{ i \int d^4x \left[\frac{\lambda}{2} B^a(x) B^a(x) + A_\mu(x) \partial^\mu B^a(x) \right] \right\}. \quad (3.146h)$$

This allows to choose directly the Landau gauge ($\lambda = 0$) and simplifies the BRST transformation (3.146b):

$$\begin{aligned} \delta A_\mu^a &= \omega (D^\mu \chi)^a, & \delta \psi &= ig \chi^a T^a \psi \omega \\ \delta \bar{\chi}^a &= -B^a \omega, & \delta \chi^a &= -\frac{g}{2} f^{abc} \chi^b \chi^c \omega, & \delta B^a &= 0. \end{aligned} \quad (3.146i)$$

allowing an easier proof of the invariance (see **Problem 31**).

According to Noether's theorem (see **chapter 1.8**) a conserved current

$$J_\mu^{\text{BRST}} = F_{\mu\nu}^a D^\nu \chi^a + B^a D_\mu \chi^a - \frac{1}{2} f^{abc} (\partial_\mu \bar{\chi}^a) \chi^b \chi^c \quad (3.146j)$$

is associated with the BRST invariance and the spatial integral over the 0th component defines a conserved “charge” Q^{BRST} which in the quantized theory is the generator of the BRST transformations. We assume that the BRST symmetry is not “broken”, i.e. that not only the Lagrangian (or the Hamiltonian) remain unchanged under the transformation but also the physical states:

$$\begin{aligned} e^{-i\omega \hat{Q}^{\text{BRST}}} |\text{phys}\rangle &= (1 - i\omega \hat{Q}^{\text{BRST}}) |\text{phys}\rangle = |\text{phys}\rangle \\ \implies Q^{\text{BRST}} |\text{phys}\rangle &= 0. \end{aligned} \quad (3.146k)$$

(This is a necessary constraint for the states in the Hilbert space of the gauge theory and obviously requires the language and formalism of canonical quantization – the path integral doesn't know anything about states!)

This can be used to show that the gauge-fixing and ghost terms, which have been added to the Lagrangian, do not give a contribution to physical matrix elements of the theory (**Nair**, ch. 12.4). To achieve that we define the Grassmann-valued quantity

$$\Xi := -\partial^\mu \bar{\chi}^a - \frac{\lambda}{2} \bar{\chi}^a B^a \quad (3.146l)$$

and by applying the BRST- transformationen (3.146i) find that

$$\begin{aligned} \delta \Xi &:= \delta \left[-\partial^\mu \bar{\chi}^a - \frac{\lambda}{2} \bar{\chi}^a B^a \right] = \omega \partial^\mu B^a A_\mu^a - \partial^\mu \omega (D_\mu \chi)^a - \frac{\lambda}{2} (-\omega B^a) B^a = \omega (\mathcal{L}_{\text{gauge}} + \mathcal{L}_{FP}) \\ &\hat{=} i\omega \left[\hat{Q}^{\text{BRST}}, \hat{\Xi} \right]_+, \end{aligned} \quad (3.146m)$$

i.e. that the additional terms added to the original Lagrangian may be written as a BRST variation. The equivalence displayed in the last term of Eq. (3.146m) is due to the fact that in the quantized theory the variation of a Grassmann-valued operator is given by the anti-commutator with the generator

$$e^{i\omega \hat{Q}^{\text{BRST}}} \hat{\Xi} e^{-i\omega \hat{Q}^{\text{BRST}}} = \hat{\Xi} + i\omega \hat{Q}^{\text{BRST}} \hat{\Xi} - i\hat{\Xi} \omega \hat{Q}^{\text{BRST}} = \hat{\Xi} + i\omega \hat{Q}^{\text{BRST}} \hat{\Xi} + i\omega \hat{\Xi} \hat{Q}^{\text{BRST}} \hat{\Xi} \equiv \hat{\Xi} + i\omega \left[\hat{Q}^{\text{BRST}}, \hat{\Xi} \right]_+ =: \hat{\Xi} + \delta \Xi. \quad (3.146n)$$

By this it follows that

$$\langle \text{phys} | \mathcal{L}_{\text{gauge}} + \mathcal{L}_{FP} | \text{phys}' \rangle = i \left\langle \text{phys} \left| \left[\hat{Q}^{\text{BRST}}, \hat{\Xi} \right]_+ \right| \text{phys}' \right\rangle = 0 \quad (3.146o)$$

between arbitrary physical states which implies that the added terms do not contribute to physical processes,

The BRST invariance also gives relations for Green functions which are essential for the renormalizability of the theory. These relations are known as **Ward** or **Slavnov-Taylor identities** and sketched in **Das**, ch. 12.5.

3.4 Worldline Formalism and Spin in the Path Integral

In this chapter we will study the **effective action** in one-loop approximation by means of a quantum-mechanical formalism which has (re)gained significance in recent years. Surprisingly the motivation for this development came from "String Theory" where new methods for perturbative expansions had been found which – in special cases – could be transferred to quantum field theory ⁸¹.

We start again with a scalar theory and recall that the one-loop correction to the effective action is given by

$$\Gamma^{(1)}[\Phi_{cl}] = \frac{i\hbar}{2} \ln \frac{\mathcal{D}\text{et}(\square + m^2 + V''(\Phi_{cl}))}{\mathcal{D}\text{et}(\square + m^2)} = \frac{i\hbar}{2} \text{tr} \ln \left[\frac{\square + m^2 + V''(\Phi_{cl}) - i0^+}{\square + m^2 - i0^+} \right] \quad (3.147)$$

(see Eq. (3.84)). Using the integral representation of the logarithm

$$\ln \frac{a}{b} = \int_0^\infty dT \frac{1}{T} (e^{-bT} - e^{-aT}), \quad \text{Re } a, \text{Re } b > 0, \quad (3.148)$$

we write that as

$$\Gamma^{(1)}[\Phi_{cl}] = \text{const.} - \frac{i\hbar}{2} \int_0^\infty dT \frac{1}{T} \text{tr} \exp \left\{ -iT \left[-(i\partial_\mu)(i\partial^\mu) + m^2 + V''(\Phi_{cl}) - i0^+ \right] \right\}. \quad (3.149)$$

Here we have put the interaction-independent part in an (infinite) constant which will be omitted in the following (a constant term in the action is irrelevant). However, the trace to be taken in Eq. (3.149) over all degrees of freedom cannot be evaluated simply in momentum space (as was done for the effective potential) as $V''(\Phi_{cl})$ now depends on the space-time point x . By writing it as

$$\text{tr} \exp \{ \dots \} = \int d^4x \langle x | \exp \left\{ -iT \left[-\hat{p}_\mu \hat{p}^\mu + m^2 + V''(\Phi_{cl}(\hat{x})) \right] \right\} | x \rangle \quad (3.150)$$

we see that formally this is a matrix element of the time-evolution operator for a quantum-mechanical particle with "mass" $-1/2$ which moves under the influence of the "potential" $V''(\Phi_{cl}(x))$ in four-dimensional Minkowski space. The particle starts at "time" 0 at the space-time point x and returns to that point at "time" T . Based on this quantum-mechanical analogy we therefore can give immediately a path-integral representation for Eq. (3.150) (see **Problem 23**) and we obtain the following expression for the one-loop correction to the effective action

$$\Gamma^{(1)}[\Phi_{cl}] = -\frac{i\hbar}{2} \int_0^\infty dT \frac{e^{-im^2T}}{T} \oint_{x(0)=x(T)} \mathcal{D}x(t) \exp \left\{ i \int_0^T dt \left[-\frac{1}{4} \dot{x}^2 + V''(\Phi_{cl}(x(t))) \right] \right\}. \quad (3.151)$$

This is referred to as **worldline** or particle representation as the system is no longer described by quantized fields but by particles with trajectories $x_\mu(t)$ parametrized by the **proper time** t . Note that this also holds for the usual time x_0 and that one has to integrate over the final proper time T at the very end of the calculation. Eq. (3.151) offers the possibility to perform one-loop calculations with arbitrary many external lines in a fast and efficient way. This is because the expression (3.151) contains many Feynman diagrams which only arise by a permutation of the external lines. To see that one may expand the interacting part of the exponent, say for the Φ^4 -theory

$$\exp \left\{ i \int_0^T dt V''(\Phi_{cl}(x(t))) \right\} = \sum_{n=0} \frac{(i\lambda)^n}{2^n n!} \int_0^T dt_1 dt_2 \dots dt_n \Phi_{cl}^2(x(t_1)) \Phi_{cl}^2(x(t_2)) \dots \Phi_{cl}^2(x(t_n)), \quad (3.152)$$

and realize that **all** time orderings of the respective interactions are included. In addition, one does not have to perform four-dimensional momentum integrations but only one-dimensional time integrations.

⁸¹See, e.g., Ref. [48]. Further examples for the application of the worldline technique can be found in Ref. [49].

Can this formalism also be applied to **fermions**? The answer is “**Yes**”, but it requires an explicit description of the spin degrees of freedom in the quantum-mechanical path integral. This is an old problem with many suggestions for a solution. Here we will present a description by Grassmann-valued trajectories for the case of quantum electrodynamics with the Lagrangian (3.96). We only consider processes without external fermions, i.e. the generating functional

$$Z[J] = \int \mathcal{D}A_\mu(x) \mathcal{D}\bar{\psi}(x) \mathcal{D}\psi(x) \exp \left\{ \frac{i}{\hbar} \int d^4x [\mathcal{L}_{\text{QED}}(\psi, \bar{\psi}, A) + J_\mu A^\mu] \right\}. \quad (3.153)$$

Since the Lagrangian is bilinear in the fermion fields we may integrate them out immediately with the result

$$\begin{aligned} Z[J] &= \int \mathcal{D}A_\mu(x) \mathcal{D}\text{et} (i\cancel{D} - m - e\cancel{A}) \exp \left\{ \frac{i}{\hbar} \int d^4x [\mathcal{L}_0(A) + J_\mu A^\mu] \right\} \\ &= \int \mathcal{D}A_\mu(x) \exp \left\{ \frac{i}{\hbar} \left[-i\hbar \text{tr} \ln (i\cancel{D} - m - e\cancel{A}) + \int d^4x (\mathcal{L}_0(A) + J_\mu A^\mu) \right] \right\}. \end{aligned} \quad (3.154)$$

Here $\mathcal{L}_0(A)$ is the free Lagrangian of the photons (we do not display the gauge-fixing term explicitly). As this part does not contain any interaction we immediately can write down the effective action in zeroth and first order semi-classical approximation:

$$\Gamma^{(0)}[A_{\text{cl}}] = \int d^4x \mathcal{L}_0(A_{\text{cl}}) = \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right] = \int d^4x \frac{1}{2} (\mathbf{E}^2 - \mathbf{B}^2) \quad (3.155)$$

$$\Gamma^{(1)}[A_{\text{cl}}] = -i\hbar \text{tr} \ln \frac{i\cancel{D} - m + i0^+}{i\cancel{D} - m + i0^+} = -i\hbar \text{tr} \ln [1 - eS_F \cancel{A}_{\text{cl}}]. \quad (3.156)$$

In the following we will set again $\hbar = 1$ and omit the index “cl” for the photon field A_μ to simplify the notation. \mathbf{E}, \mathbf{B} are the corresponding electric and magnetic field strengths. In addition we have normalized $\Gamma^{(1)}$ such that it vanishes for $e = 0$. As can be seen, the effective action in first semi-classical (or one-loop) approximation is given by the fermionic determinant, i.e. by the pair production of charged electrons and positrons. When expanding the logarithm in powers of the coupling constant (or in powers of the photon field)

$$\Gamma^{(1)}[A] = i \sum_{n=1} \frac{e^{2n}}{2n} \text{tr} [S_F \cancel{A}]^{2n} \quad (3.157)$$

only even powers appear which can be proved by using the charge conjugation properties of Feynman propagator and vertex (**Furry-Theorem**)⁸². This is depicted in Fig. 25.

Note that the fermionic effective action has a different sign compared to the scalar theory in Eq. (3.147) which has its origin in the integration over the anticommuting fields $\psi, \bar{\psi}$. Moreover, there is a factor of 2 as two charged particles run in the loop here.

We now want to derive a worldline representation of the fermionic effective action in one-loop approximation. To achieve that we first iterate the Dirac operator $i\cancel{D} - m$ in Eq. (3.156)

$$\Gamma^{(1)}[A] = -\frac{i}{2} \ln [\text{Det} (i\cancel{D} - m) (-i\cancel{D} - m)] = -\frac{i}{2} \ln [\text{Det} (\cancel{D}^2 + m^2)], \quad (3.158)$$

which is possible due to the relation⁸³ $\text{Det}(\cancel{D} - m) = \text{Det}(\gamma_5 \cancel{D} \gamma_5 - m) = \text{Det}(-\cancel{D} - m)$. Now we have

$$\begin{aligned} \cancel{D}^2 &= \gamma^\mu \gamma^\nu D_\mu D_\nu = \left(g^{\mu\nu} + \frac{1}{2} [\gamma^\mu, \gamma^\nu] \right) D_\mu D_\nu = D^2 + \frac{1}{4} [\gamma^\mu, \gamma^\nu] [D_\mu, D_\nu] \\ &= (\partial + ieA)^2 + \frac{1}{4} [\gamma^\mu, \gamma^\nu] ie (\partial_\mu A_\nu - \partial_\nu A_\mu) = (\partial + ieA)^2 + \frac{ie}{2} \gamma^\mu \gamma^\nu F_{\mu\nu}. \end{aligned} \quad (3.159)$$

⁸²See, e.g., **Itzykson & Zuber**, p. 276.

⁸³ $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$ anticommutes with all Dirac matrices and fulfills $\gamma_5^2 = 1$.

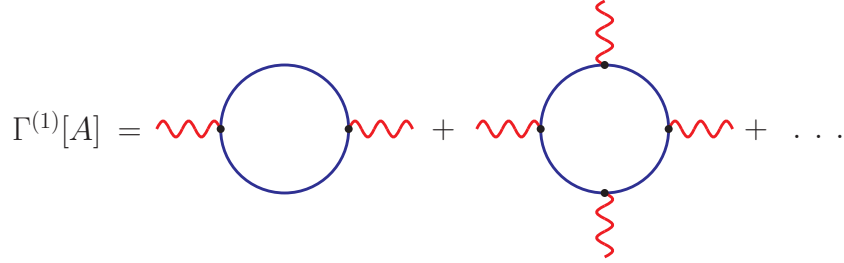


Fig. 25 : One-loop approximation for the effective action of Quantum Electrodynamics. The wavy lines represent the photons.

If we use the integral representation (3.148) and define

$$H(\hat{x}, \hat{p}, \gamma) := -(\hat{p} + eA(\hat{x}))^2 + \frac{ie}{2}\gamma^\mu\gamma^\nu F_{\mu\nu}(\hat{x}) \quad (3.160)$$

as “Hamiltonian” of the system, then we may again express

$$\Gamma^{(1)}[A] = \frac{i}{2} \int_0^\infty dT \frac{e^{-im^2T}}{T} \text{tr} \int d^4x \langle x | e^{-iT H(\hat{x}, \hat{p}, \gamma)} | x \rangle \quad (3.161)$$

formally as matrix element of a quantum-mechanical operator $\hat{U}(T, 0)$. The symbol “tr” indicates the trace over the Dirac matrices. As usual we split the proper-time evolution into N steps and obtain

$$\begin{aligned} \text{tr} \hat{U}(T, 0) &\equiv \text{tr} \int d^4x \langle x | e^{-iT H(\hat{x}, \hat{p}, \gamma)} | x \rangle \\ &= \text{tr} \lim_{N \rightarrow \infty} \int d^4x_1 \dots d^4x_N \frac{d^4p_1}{(2\pi)^4} \dots \frac{d^4p_N}{(2\pi)^4} \exp \left[-i \sum_{i=1}^N p_i \cdot (x_i - x_{i-1}) \right] \\ &\quad \cdot \exp[-iH_W(x_N, p_N, \gamma_N)\Delta t] \dots \exp[-iH_W(x_1, p_1, \gamma_1)\Delta t], \end{aligned} \quad (3.162)$$

where $x_0 = x_N$ has to be taken. Here

$$H_W(x, p, \gamma) = \int d^4y \left\langle x - \frac{y}{2} \left| \hat{H} \right| x + \frac{y}{2} \right\rangle e^{-ip \cdot y} \quad (3.163)$$

is the **Wigner transform (or the Weyl symbol) of the Hamiltonian**, which – as we know – is the appropriate classical analogon for the (Weyl-ordered) quantum operator. In the following we will omit the index “W”.

We need two essential steps to derive a path integral with spin from Eq. (3.162) [50], [51]:

1. As the Dirac matrices do not commute, the ordering of the factors is all-important and it is not possible to combine the individual exponents. By giving the Dirac matrices an artificial time dependence we can write the (proper) time evolution operator as a time-ordered path integral

$$\begin{aligned} \text{tr} \hat{U}(T, 0) &= \text{tr} \oint_{x(0)=x(T)} \frac{\mathcal{D}'x \mathcal{D}p}{(2\pi)^4} \mathcal{T} \exp \left\{ -i \int_0^T dt [p \cdot \dot{x} + H(x(t), p(t), \gamma(t))] \right\} \\ &= \text{tr} \oint \frac{\mathcal{D}'x \mathcal{D}p}{(2\pi)^4} \exp \left\{ -i \int_0^T dt \left[p \cdot \dot{x} + H \left(x(t), p(t), \frac{\delta}{\delta \rho(t)} \right) \right] \right\} \\ &\quad \cdot \mathcal{T} \exp \left[\int_0^T dt \rho^\mu(t) \gamma_\mu(t) \right]_{\rho^\mu=0}. \end{aligned} \quad (3.164)$$

Here $\rho^\mu(t)$ are Grassmann sources which we assume to anticommute with the Dirac matrices⁸⁴. The time-ordering symbol \mathcal{T} would be devastating for all subsequent manipulations in the path integral since we want it to be based on numbers and not on operators. Fortunately, in this special case the time ordering can be eliminated by the relation

$$\begin{aligned} Y(T) &\equiv \mathcal{T} \exp \left\{ \int_0^T dt \rho^\mu(t) \gamma_\mu(t) \right\} \\ &= \exp \left\{ - \int_0^T dt_1 \int_0^{t_1} dt_2 \rho^\mu(t_1) \rho_\mu(t_2) \right\} \cdot \exp \left\{ \int_0^T dt \rho^\mu(t) \gamma_\mu \right\}. \end{aligned} \quad (3.165)$$

This can be proved by solving the evolution equation

$$\frac{\partial Y(T)}{\partial T} = \rho^\mu(T) \gamma_\mu Y(T), \quad Y(0) = 1 \quad (3.166)$$

by means of the Magnus expansion⁸⁵

$$Y(T) = \exp \left\{ \int_0^T dt \rho^\mu(t) \gamma_\mu + \frac{1}{2} \int_0^T dt_1 \int_0^{t_1} dt_2 [\rho_\mu(t_1) \gamma^\mu, \rho_\nu(t_2) \gamma^\nu] + \dots \right\}. \quad (3.167)$$

The commutator gives $-2\rho_\mu(t_1)\rho^\mu(t_2)$ which is a commuting number. Therefore all higher terms in the expansion, expressed by multiple commutators, vanish. Due to that result we now may omit the artificial time-dependence of the Dirac matrices.

2. The differentiations w.r.t. $\rho^\mu(t)$ required in Eq. (3.164), can only be performed analytically in all orders if the variables appear *linearly* in the exponent. This can be achieved by using the trick of "undoing the square" which we already have employed in **chapter 1.6**. Since $\rho^\mu(t)$ are anticommuting and we want to have a Grassmann-even object in the exponent of the time-evolution operator we have to undo the square by a Grassmann path integral. We therefore use the identity

$$\begin{aligned} \exp \left\{ - \int_0^T dt_1 \int_0^{t_1} dt_2 \rho^\mu(t_1) \rho_\mu(t_2) \right\} &= \int \mathcal{D}\xi \exp \left\{ \int_0^T dt \left[-\frac{1}{4} \xi_\mu(t) \dot{\xi}^\mu(t) + \rho^\mu(t) \xi_\mu(t) \right] \right\} \\ &\cdot \left[\int \mathcal{D}\xi \exp \left(-\frac{1}{4} \int_0^T dt \xi_\mu(t) \dot{\xi}^\mu(t) \right) \right]^{-1}. \end{aligned} \quad (3.168)$$

The boundary conditions for the Grassmann path integral are

$$\xi_\mu(0) + \xi_\mu(T) = 0. \quad (3.169)$$

Eq. (3.168) can be verified by the stationary phase method which is exact for quadratic actions.

Finally we use the representation

$$\exp \left\{ \int_0^T dt \rho^\mu(t) \gamma_\mu \right\} = \exp \left\{ \gamma_\mu \frac{\partial}{\partial \Gamma_\mu} \right\} \exp \left\{ \int_0^T dt \rho^\mu(t) \Gamma_\mu \right\} \Big|_{\Gamma_\mu=0} \quad (3.170)$$

and obtain

$$\begin{aligned} \text{tr } \hat{U}(T, 0) &= \text{tr} \exp \left(\gamma \cdot \frac{\partial}{\partial \Gamma} \right) \oint \frac{D'x Dp}{(2\pi)^4} \mathcal{D}\xi \mathcal{N}_0^{\text{spin}} \\ &\cdot \exp \left\{ -i \int_0^T dt \left[p \cdot \dot{x} - \frac{i}{4} \xi \cdot \dot{\xi} + H(x, p, \xi + \Gamma) \right] \right\} \Big|_{\Gamma=0}. \end{aligned} \quad (3.171)$$

⁸⁴This is the reason why we write γ_μ , see footnote 73.

⁸⁵This is the continuous analogon to the better-known Baker-Campbell-Hausdorff formula, see, e.g. Ref. [52].

Here

$$\mathcal{N}_0^{\text{spin}} = \left[\int \mathcal{D}\xi \exp \left(-\frac{1}{4} \int_0^T dt \xi_\mu \dot{\xi}^\mu \right) \right]^{-1} \quad (3.172)$$

is a normalization factor for the spin integral. Note that, in general, the procedure required in Eq. (3.170) is **not** only a replacement of the variable Γ by the corresponding Dirac matrix γ but also involves an antisymmetrization. For example, we have

$$\exp \left\{ \gamma \cdot \frac{\partial}{\partial \Gamma} \right\} \Gamma_\mu \Big|_{\Gamma=0} = \gamma_\mu, \quad (3.173)$$

but

$$\begin{aligned} \exp \left\{ \gamma \cdot \frac{\partial}{\partial \Gamma} \right\} \Gamma_\mu \Gamma_\nu \Big|_{\Gamma=0} &= \frac{1}{2} \left(\gamma \cdot \frac{\partial}{\partial \Gamma} \right)^2 \Gamma_\mu \Gamma_\nu \Big|_{\Gamma=0} = \frac{1}{2} \left(\gamma \cdot \frac{\partial}{\partial \Gamma} \right) (\gamma_\mu \Gamma_\nu + \Gamma_\mu \gamma_\nu) \Big|_{\Gamma=0} \\ &= \frac{1}{2} (-\gamma_\nu \gamma_\mu + \gamma_\mu \gamma_\nu). \end{aligned} \quad (3.174)$$

Taking the trace over the Dirac matrices entails the simplification that only the "1" in the series expansion of $\exp(i\gamma \cdot \partial/\partial \Gamma)$ remains: At most terms with up to four Γ 's can show up, the trace over an odd number of γ -matrices vanishes as well as the trace over Eq. (3.174); finally we have $\text{tr} \gamma_0 \gamma_1 \gamma_2 \gamma_3 = -i \text{tr} \gamma_5 = 0$. By that Eq. (3.171) simply becomes

$$\text{tr} \hat{U}(T, 0) = 4 \oint_p \frac{\mathcal{D}'x \mathcal{D}p}{(2\pi)^4} \oint_{ap} \mathcal{D}\xi \mathcal{N}_0^{\text{spin}} \exp \left\{ -i \int_0^T dt \left[p \cdot \dot{x} - \frac{i}{4} \xi \cdot \dot{\xi} + H(p, x, \xi) \right] \right\}, \quad (3.175)$$

where we indicate by the subscripts "p" or "ap" that periodic or antiperiodic boundary conditions have to be taken for the x or ξ integral. From Eq. (3.160) we see that the Hamilton function

$$H(p, x, \xi) = -\Pi^2 + \frac{ie}{2} \xi_\mu \xi_\nu F^{\mu\nu} \quad (3.176)$$

is a quadratic function of the kinematic momentum

$$\Pi_\mu = p_\mu - eA_\mu. \quad (3.177)$$

By shifting the integration variable in the phase-space path integral (3.175) we may perform the (functional) momentum integration and obtain

$$\text{tr} \hat{U}(T, 0) = \oint_p \mathcal{D}'x \oint_{ap} \mathcal{D}\xi \mathcal{N}_0(T) \exp \left\{ i \int_0^T dt L(x, \dot{x}, \xi, \dot{\xi}) \right\} \quad (3.178)$$

with the normalization

$$\mathcal{N}_0(T) = \left[\int \mathcal{D}\xi \exp \left(-\frac{1}{4} \int_0^T dt \xi \cdot \dot{\xi} \right) \right]^{-1} \cdot \int \frac{\mathcal{D}\Pi}{(2\pi)^4} \exp \left(i \int_0^T dt \Pi^2 \right) \quad (3.179)$$

and the Lagrange function

$$L(x, \dot{x}, \xi, \dot{\xi}) = -\frac{1}{4} \dot{x}^2 + \frac{i}{4} \xi \cdot \dot{\xi} - e \dot{x} \cdot A(x) - \frac{ie}{2} F_{\mu\nu}(x) \xi^\mu \xi^\nu. \quad (3.180)$$

As can be seen, the spin of the relativistic particle is described by a Grassmann trajectory $\xi_\mu(t)$ over which one has to integrate functionally with antiperiodic boundary conditions. The Lagrange function (3.180) has a simple

interpretation: It contains kinetic terms for the orbital and spin motion of a relativistic particle and a coupling of the spin current $\xi^\mu \xi^\nu$ to the electromagnetic field strength (non-relativistically this is the well-known $\boldsymbol{\sigma} \cdot \mathbf{B}$ term). In addition, $\dot{x} \cdot A(x)$ describes the usual interaction of the convection current with the vector potential. The effective action of **QED** therefore is given in one-loop approximation by

$$\Gamma^{(1)}[A] = 2i \int_0^\infty dT \frac{e^{-im^2 T}}{T} \oint_{x(0)=x(T)} \mathcal{D}'x \oint_{\xi(0)=-\xi(T)} \mathcal{D}\xi \mathcal{N}_0(T) \exp \left\{ i \int_0^T dt L(x, \dot{x}, \xi, \dot{\xi}) \right\}. \quad (3.181)$$

It is advantageous to split the trajectory into

$$x(t) = x_0 + y(t), \quad \text{with} \quad \int_0^T dt y(t) = 0. \quad (3.182)$$

and to integrate separately over the "zero mode" x_0 . Then we obtain

$$\begin{aligned} \Gamma^{(1)}[A] &= 2i \int_0^\infty dT \frac{e^{-im^2 T}}{T} \int d^4 x_0 \underbrace{\frac{\int \mathcal{D}y \mathcal{D}\xi \exp(iS[y, \xi])}{\int \mathcal{D}y \mathcal{D}\xi \exp(iS_0[y, \xi])}}_{:= \langle \exp(i(S-S_0)) \rangle} \\ &\cdot \int_{y(0)=y(T)} \mathcal{D}'y \oint_{\xi(0)=-\xi(T)} \mathcal{D}\xi \mathcal{N}_0(T) \exp \left\{ i \int_0^T dt L_0(x, \dot{x}, \xi, \dot{\xi}) \right\}, \end{aligned} \quad (3.183)$$

where L_0 is the free Lagrange density ($e = 0$). The free path integral can be performed immediately: Due to the normalization factor (3.179) the spin integral is one and the functional y -integral is that of a free particle with mass $-1/2$ ($1/2$) for the temporal (spatial) component. From Eq. (1.51) one therefore obtains

$$\int_{y(0)=y(T)} \mathcal{D}'y \oint_{\xi(0)=-\xi(T)} \mathcal{D}\xi \mathcal{N}_0(T) \exp \left\{ i \int_0^T dt L_0(x, \dot{x}, \xi, \dot{\xi}) \right\} = \sqrt{\frac{-1/2}{2\pi iT}} \sqrt{\frac{1/2}{2\pi iT}}^3 = \frac{i}{(4\pi iT)^2}. \quad (3.184)$$

If we write the effective action as

$$\Gamma^{(1)}[A] = \int d^4 x_0 \delta \mathcal{L}[A] \quad (3.185)$$

then the first quantum correction to the classical Lagrangian is given by

$$\delta \mathcal{L}[A] = \frac{1}{8\pi^2} \int_0^\infty dT \frac{e^{-im^2 T}}{T^3} \left\langle \exp \left\{ -ie \int_0^T dt \left[\dot{y} \cdot A + \frac{i}{2} F_{\mu\nu} \xi^\mu \xi^\nu \right] \right\} \right\rangle. \quad (3.186)$$

Here the averaging is defined as in Eq. (3.183) as ratio of the path integral with interaction to the free path integral.

Example: The Euler-Heisenberg Effective Lagrangian

Let us consider the case of a **constant** electromagnetic field $F_{\mu\nu}$, for which the **Fock-Schwinger gauge**

$$A_\mu(y) = \frac{1}{2} y^\nu F_{\nu\mu} \quad (3.187)$$

is most convenient. Then the action is quadratic in the bosonic (b) as well as in the fermionic (f) components and can be written as

$$S[y, \xi] = \left(x_\mu, \mathcal{O}_b^{\mu\nu} x_\nu \right) + \left(\xi_\mu, \mathcal{O}_f^{\mu\nu} \xi_\nu \right) \quad (3.188)$$

with

$$\mathcal{O}_b^{\mu\nu}(t-t') = \left[\frac{1}{4}g^{\mu\nu} \frac{\partial^2}{\partial t^2} - \frac{e}{2}F^{\mu\nu} \frac{\partial}{\partial t} \right] \delta(t-t') \quad (3.189)$$

$$\mathcal{O}_f^{\mu\nu}(t-t') = \left[\frac{i}{4}g^{\mu\nu} \frac{\partial}{\partial t} - \frac{ie}{2}F^{\mu\nu} \right] \delta(t-t') . \quad (3.190)$$

Note that $\mathcal{O}_b = -i\partial\mathcal{O}_f/\partial t$ which is an expression of a **super-symmetry** between bosonic and fermionic components [53].

As the path integral (3.186) is now a Gaussian we can perform all functional integrations immediately and obtain

$$\begin{aligned} \delta\mathcal{L}[A] &= \frac{1}{8\pi^2} \int_0^\infty dT \frac{e^{-im^2T}}{T^3} \left(\frac{\mathcal{D}\text{et}_{ap}\mathcal{O}_f}{\mathcal{D}\text{et}'_p\mathcal{O}_b} \right)^{1/2} \cdot \left(\frac{\mathcal{D}\text{et}'_p\mathcal{O}_b^{(0)}}{\mathcal{D}\text{et}_{ap}\mathcal{O}_f^{(0)}} \right)^{1/2} \\ &= \frac{1}{8\pi^2} \int_0^\infty dT \frac{e^{-im^2T}}{T^3} \mathcal{D}\text{et}'_p{}^{-1/2} \left[1 - 2e\frac{1}{\partial_t^2} F \partial_t \right] \mathcal{D}\text{et}_{ap}^{1/2} \left[1 - 2e\frac{1}{\partial_t} F \right] . \end{aligned} \quad (3.191)$$

Due to the super-symmetry the bosonic and the fermionic determinant would cancel (up to a constant) but the boundary conditions are different. Another difference is that the zero mode x_0 has been eliminated in the bosonic determinant which is indicated by a prime: $\mathcal{D}\text{et}'$. “Det” here means a determinant both in functional space as in the Lorentz indices; hence only a power 1/2 (and not $d/2 = 2$) of the determinants appear. The inverse operators (or worldline Green functions) $1/\partial_t^2$ and $1/\partial_t$ can be calculated by expanding their eigenfunctions in Fourier modes

$$\sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} b_k e^{2\pi ikt/T} , \quad \text{or} \quad \sum_{k=-\infty}^{+\infty} f_k e^{2\pi i(k+1/2)t/T} \quad \text{respectively} \quad (3.192)$$

in the bosonic and fermionic case, respectively. These expansions obey the boundary conditions, eliminate the zero mode and diagonalize the corresponding operator. Applying the $(\ln \det = \text{tr} \ln)$ -rule then gives for the bosonic determinant

$$\begin{aligned} \mathcal{D}\text{et}'_p &= \exp \left\{ \text{tr} \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \ln \left[1 - \frac{2e}{2\pi ik/T} F \right] \right\} = \exp \left\{ \text{tr} \sum_{k=1}^{\infty} \ln \left[1 + \frac{e^2 T^2}{k^2 \pi^2} F^2 \right] \right\} \\ &= \exp \left\{ - \sum_{n=1}^{\infty} \left(\frac{-e^2 T^2}{\pi^2} \right)^n \frac{1}{n} \zeta(2n) \text{tr} F^{2n} \right\} . \end{aligned} \quad (3.193)$$

In the last line we have expanded the logarithm: $\ln(1+x) = x - x^2/2 + x^3/3 + \dots$ and used the Riemann Zeta-function ⁸⁶

$$\zeta(2n) = \sum_{k=1}^{\infty} \frac{1}{k^{2n}} = \frac{2^{2n-1} \pi^{2n}}{(2n)!} |B_{2n}| . \quad (3.194)$$

$B_0 = 1, B_2 = 1/6, B_4 = -1/30$ etc. are the Bernoulli numbers and “tr” denotes the trace over Lorentz indices. The fermionic determinant is calculated in a similar way:

$$\begin{aligned} \mathcal{D}\text{et}_{ap} &= \exp \left\{ \text{tr} \sum_{k=-\infty}^{+\infty} \ln \left[1 - \frac{2e}{2\pi i(k+1/2)/T} F \right] \right\} \\ &= \exp \left\{ - \sum_{n=1}^{\infty} \left(\frac{eT}{i\pi} \right)^n \frac{1}{n} \text{tr} F^n \sum_{k=-\infty}^{+\infty} \left(k + \frac{1}{2} \right)^{-n} \right\} . \end{aligned} \quad (3.195)$$

⁸⁶See, e.g. , {Gradshteyn-Ryzhik}, eq. 0.233.3 .

The trace over odd powers of the antisymmetric field strength tensor $F_{\mu\nu}$ vanishes and if we use the formula ⁸⁷

$$\sum_{k=-\infty}^{+\infty} \frac{1}{(k+1/2)^{2n}} = 2^{2n+1} \sum_{k=1}^{\infty} \frac{1}{(2k-1)^{2n}} = 2^{2n} \frac{2^{2n}-1}{(2n)!} \pi^{2n} |B_{2n}| \quad (3.196)$$

we obtain for the fermionic determinant

$$\text{Det}_{ap} = \exp \left\{ - \sum_{n=1}^{\infty} (-4e^2 T^2)^n \frac{2^{2n}-1}{2n(2n)!} |B_{2n}| \text{tr} F^{2n} \right\}. \quad (3.197)$$

Inserted into Eq. (3.191) this gives

$$\delta\mathcal{L}[A] = \frac{1}{8\pi^2} \int_0^{\infty} \frac{dT}{T^3} e^{-im^2 T} \exp \left\{ - \sum_{n=1}^{\infty} \frac{(-4e^2 T^2)^n}{2n(2n)!} (2^{2n-1}-1) |B_{2n}| \text{tr} F^{2n} \right\}. \quad (3.198)$$

Although one can do the summation analytically ⁸⁸, it is more instructive to expand the individual terms and to integrate term-by-term over T : The F -independent term gives a (divergent) constant, the quadratic one renormalizes the classical Lagrangian (3.155) while the term quartic in F gives an additional piece

$$\delta\mathcal{L}^{(4)} = \frac{1}{8\pi^2} \int_0^{\infty} \frac{dT}{T^3} e^{-im^2 T} \left\{ -\frac{7}{180} e^4 T^4 \text{tr} F^4 + \frac{1}{72} e^4 T^4 (\text{tr} F^2)^2 \right\}. \quad (3.199)$$

Because of

$$\text{tr} F^2 = 2(\mathbf{E}^2 - \mathbf{B}^2) \quad (3.200)$$

$$\text{tr} F^4 = 2(\mathbf{E}^2 - \mathbf{B}^2)^2 + 4(\mathbf{E} \cdot \mathbf{B})^2 \quad (3.201)$$

we finally obtain

$$\delta\mathcal{L}^{(4)} = \frac{2\alpha^2}{45m^4} [(\mathbf{E}^2 - \mathbf{B}^2)^2 + 7(\mathbf{E} \cdot \mathbf{B})^2], \quad (3.202)$$

where $\alpha = e^2/(4\pi) \simeq 1/137.036$ denotes the fine-structure constant. This is the effective Lagrangian of [H. Euler](#) ⁸⁹ and [Heisenberg](#) describing non-linear effects in electrodynamics due to quantum corrections.

Detail 33: Color in the Path Integral

For the treatment of spin in the world-line path integral we have used special properties of the Dirac matrices. How can that be taken over to other inner degrees of freedom of fermions, for example the color of quarks? One possible method using fermionic auxiliary variables has been developed by D'Hoker and Gagné [54] which we will follow here. We consider that part in Eq. (3.164) which describes the dynamics of the inner degrees of freedom and leave out the orbital motion which is treated as usual. This means: We want to find a path-integral representation for

$$Z[M] := \text{tr} \left(\mathcal{T} e^{i \int_0^T d\tau M(\tau)} \right) =: \text{tr} U(T, 0) \quad (3.203a)$$

where $M(\tau)$ is a traceless, hermitean $N \times N$ matrix which describes the inner degrees of freedom – e.g., a combination of Gell-Mann matrices. Again the task is to replace the time-ordering symbol (which is necessary because $M(\tau)$ doesn't commute at different times) by a suitable functional integral over a (Grassmann even) action made up by auxiliary fields.

⁸⁷{Gradshteyn-Ryzhik}, eq. 0.233.5 .

⁸⁸Schwinger's classical result can be found , for example, in [Itzykson & Zuber](#), p. 196.

⁸⁹Ann. Phys. **26** (1936) 398. Of course, the great L. Euler whose name is attached to the Γ -function and many other results, lived much earlier. Also at that time ‘‘Ann. Phys.’’ was the abbreviation for ‘‘Annalen der Physik’’...

Assertion: Eq. (3.203a) can be represented by the worldline path integral

$$Z[M] = \mathcal{N} \int_0^{2\pi} d\phi \int_{\text{ap}} \mathcal{D}\bar{\lambda} \mathcal{D}\lambda \exp \left\{ i\phi \left(\bar{\lambda}\lambda + \frac{N}{2} - 1 \right) \right\} \exp \left\{ - \int_0^T d\tau \left[\bar{\lambda}\dot{\lambda} - i\bar{\lambda}M(\tau)\lambda \right] \right\}. \quad (3.203b)$$

Here $\bar{\lambda}, \lambda$ are N -component Grassmann variables over which one has to integrate functionally with anti-periodic ("ap") boundary conditions $\bar{\lambda}(T) = -\bar{\lambda}(0), \lambda(T) = -\lambda(0)$. In the first exponential factor they can be taken at an arbitrary time between 0 and T , i.e. one is allowed to write there $\frac{1}{T} \int_0^T d\tau \bar{\lambda}\lambda$. \mathcal{N} is a normalization factor to be determined.

Proof: Grassmann integration over $\bar{\lambda}, \lambda$ (with the help of Eq. (2.147)) gives

$$Z[M] = \mathcal{N} \int_0^{2\pi} d\phi \mathcal{D}\text{et} \left[\frac{d}{d\tau} - iM - \frac{i\phi}{T} \right] e^{i\phi(N/2-1)}. \quad (3.203c)$$

As usual the functional determinant is calculated as infinite product of the eigenvalues of the corresponding operator. The eigenfunctions $f(\tau)$ are solutions of the equation $df/d\tau = (iM + i\phi/T + \kappa) f$, i.e.

$$f(\tau) = \exp \left(\kappa\tau + i\frac{\phi\tau}{T} \right) U(\tau, 0) f(0). \quad (3.203d)$$

Since M is hermitean, $U(\tau, 0)$ in Eq. (3.203a) is unitary at every time and we can write

$$U(\tau, 0) \equiv \mathcal{T} \exp \left[i \int_0^\tau d\tau' M(\tau') \right] = \exp \left[i \text{diag}(m_1(\tau), \dots, m_N(\tau)) \right], \quad (3.203e)$$

where

$$\sum_{n=1}^N m_n(\tau) = 0 \quad (3.203f)$$

since M is assumed to be traceless. The eigenvalues κ are determined by the boundary condition $f(T) = -f(0)$ as

$$\kappa_n^{(k)} = \frac{i}{T} [(2k+1)\pi - \phi - m_n(T)], \quad k = 0, \pm 1, \pm 2 \dots \quad (3.203g)$$

With that the functional determinant is found to be

$$\mathcal{D}\text{et} \left[\frac{d}{d\tau} - iM - \frac{i\phi}{T} \right] = \prod_{n=1}^N \prod_{k=0}^{\infty} \left[\frac{\pi^2(2k+1)^2}{T^2} \right] \prod_{l=0}^{\infty} \left[1 - \frac{(\phi + m_n(T))^2}{(2l+1)^2\pi^2} \right] = \mathcal{D}\text{et} \left[\frac{d}{d\tau} \right] \cdot \prod_{n=1}^N \cos \left(\frac{\phi + m_n(T)}{2} \right). \quad (3.203h)$$

In the last step the product representation of the cosine function (see, e.g. eq. 1.431.3 in **{Gradshteyn-Ryzhik}**) has been used. After inserting that and splitting the cosine into exponential functions we have

$$\begin{aligned} Z[M] &= \frac{\mathcal{N}}{2^N} \mathcal{D}\text{et} \left[\frac{d}{d\tau} \right] \cdot \int_0^{2\pi} d\phi e^{i(N/2-1)\phi} \exp \left(-i\phi N/2 - \frac{i}{2} \sum_{n=1}^N m_n(T) \right) \prod_{n=1}^N \left[1 + e^{i(\phi+m_n(T))} \right] \\ &= \frac{\mathcal{N}}{2^N} \mathcal{D}\text{et} \left[\frac{d}{d\tau} \right] \cdot \int_0^{2\pi} d\phi e^{-i\phi} \left\{ 1 + \sum_n e^{i(\phi+m_n(T))} + \sum_{n,m < n} e^{i(\phi+m_n(T))} e^{i(\phi+m_m(T))} + \dots \right\} \end{aligned} \quad (3.203i)$$

where Eq. (3.203f) has been used. Due to the orthogonality relation $\int_0^{2\pi} d\phi \exp(ik\phi) = 2\pi \delta_{k0}$, obviously only the term which contains just one factor $e^{i\phi}$ contributes in the expansion of the product. Hence the desired result

$$Z[M] = \frac{2\pi\mathcal{N}}{2^N} \mathcal{D}\text{et} \left[\frac{d}{d\tau} \right] \cdot \sum_{n=1}^N e^{im_n(T)} = \text{tr} \left(\mathcal{T} e^{i \int_0^T d\tau M(\tau)} \right), \quad (3.203j)$$

follows if the normalization factor is chosen as $\mathcal{N}^{-1} = 2\pi \mathcal{D}\text{et} \left[\frac{d}{d\tau} \right] / 2^N$.

A method which employs bosonic auxiliary variables can be found in Ref. [55].

3.5 Anomalies

Due to the global symmetry of the **QCD** Lagrangian under the transformation

$$\psi(x) \longrightarrow e^{i\alpha} \psi(x), \quad \bar{\psi}(x) \longrightarrow \bar{\psi}(x) e^{-i\alpha} \quad (3.204)$$

the **vector current**

$$V_\mu(x) = \bar{\psi}(x) \gamma_\mu \psi(x) \quad (3.205)$$

is conserved in **QCD**. As the masses of u -, d - and s -quarks in nature are small compared to a typical hadronic scale (estimates are $m_{u/d} < 10$ MeV, $m_s \simeq 130$ MeV), they can be neglected in many cases. Then the resulting Lagrangian

$$\mathcal{L}_{m=0} = -\frac{1}{4}F^{a\mu\nu}F_{\mu\nu}^a + \bar{\psi}(x)(i\cancel{\partial} - gA^aT^a)\psi \quad (3.206)$$

is also invariant under an **axial** transformation

$$\psi(x) \longrightarrow e^{i\alpha\gamma_5}\psi(x), \quad \bar{\psi}(x) \longrightarrow \bar{\psi}(x)e^{i\alpha\gamma_5}, \quad (3.207)$$

where $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$ anticommutes with all Dirac matrices. According to the classical Noether theorem the **axial current**

$$A_\mu(x) = \bar{\psi}(x)\gamma_\mu\gamma_5\psi(x) \quad (3.208)$$

should also be conserved in this limit:

$$\partial^\mu A_\mu(x) \stackrel{?}{=} 0. \quad (3.209)$$

The fact that this does **not** hold for the quantized theory is called an "**anomaly**". Besides the theoretical interest for this phenomenon there are also practical reasons to study anomalies: For example, the decay $\pi^0 \rightarrow 2\gamma$ can only be obtained in the strength observed experimentally when the axial anomaly is taken into account!

How does the axial (or Adler-Bell-Jackiw (ABJ)) anomaly show up in the path-integral representation? To answer this question we recall **chapter 1.8** where we derived Noether's theorem in quantum mechanics. As seen in **Problem 27** this applies to field theory in a completely analogous way: We consider the full generating functional (gauge fixing and ghosts are irrelevant and are omitted to simplify the notation)

$$Z[\eta, \bar{\eta}] = \int \mathcal{D}\bar{\psi}(x)\mathcal{D}\psi(x)\mathcal{D}A(x) \exp\left[i\int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi)\right]. \quad (3.210)$$

and perform, for instance the vector transformation (3.204) as a **local** substitution of integration variables, i.e we set

$$\psi(x) = e^{-i\alpha(x)}\psi'(x), \quad \bar{\psi}(x) = \bar{\psi}'(x)e^{i\alpha(x)}. \quad (3.211)$$

As the numerical value of the integral does not change we have

$$\begin{aligned} & \int \mathcal{D}\bar{\psi}(x)\mathcal{D}\psi(x)\mathcal{D}A(x) \exp\left[i\int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi)\right] \\ &= \int \mathcal{D}\bar{\psi}'(x)\mathcal{D}\psi'(x)\mathcal{J}^{-1}\mathcal{D}A(x) \exp\left[i\int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi)\right] \Big|_{\substack{\psi=\exp(-i\alpha(x))\psi' \\ \bar{\psi}=\bar{\psi}'\exp(i\alpha(x))}}. \end{aligned} \quad (3.212)$$

Here

$$\mathcal{J} = \text{Det}_{xx'}\left(\frac{\partial\psi(x)}{\partial\psi'(x')}\right) \cdot \text{Det}_{xx'}\left(\frac{\partial\bar{\psi}(x)}{\partial\bar{\psi}'(x')}\right) \quad (3.213)$$

is the **Jacobi determinant** of the transformation (3.211) which – as we know from **chapter 2.5** – appears inversely when integrating over Grassmann variables. Calculating the Jacobi determinant of the vector transformation (3.211) we obtain

$$\mathcal{J}_V = \text{Det}_{xx'}\left(e^{-i\alpha(x)}\delta(x-x')\right) \text{Det}_{xx'}\left(e^{i\alpha(x)}\delta(x-x')\right) = 1, \quad (3.214)$$

since this is an unitary (phase) transformation. Restricting ourselves to **infinitesimal** transformations we expand Eq. (3.212) up to first order in $\alpha(x)$ to get

$$\begin{aligned} 0 &= i\int \mathcal{D}\bar{\psi}(x)\mathcal{D}\psi(x)\mathcal{D}A(x) \left\{ i\delta\mathcal{J} + \int d^4x [\delta\mathcal{L}_V - i\alpha(x)\bar{\psi}\eta + i\alpha(x)\bar{\eta}\psi] \right\} \\ &\quad \cdot \exp\left[i\int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi)\right]. \end{aligned} \quad (3.215)$$

Here $\delta\mathcal{J}_V = 0$ is the contribution of the Jacobian and

$$\delta\mathcal{L}_V = \bar{\psi}\gamma^\mu\psi\partial_\mu\alpha(x) \quad (3.216)$$

the infinitesimal change of the Lagrangian caused by the vector transformation (3.211). As we only have made a local transformation of the fermion fields it doesn't vanish⁹⁰. With an integration by parts we can get rid of the derivative acting on $\alpha(x)$ and obtain

$$0 = i \int \mathcal{D}\bar{\psi}(x) \mathcal{D}\psi(x) \mathcal{D}A(x) \int d^4x \alpha(x) \{ -\partial_\mu V^\mu(x) - i\bar{\psi}\eta + i\bar{\eta}\psi \} \cdot \exp \left[i \int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi) \right]. \quad (3.217)$$

Here $V^\mu(x)$ exactly is the vector current (3.205). Since $\alpha(x)$ is arbitrary the whole functional integral over the curly bracket must vanish and this for arbitrary values of the external source $\eta(x)$, $\bar{\eta}(x)$. Using again the notation

$$\langle \mathcal{O} \rangle \equiv \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{D}A \mathcal{O}(\psi, \bar{\psi}, A) e^{i \int d^4x \mathcal{L}_{m=0}(\psi, \bar{\psi}, A)} \quad (3.218)$$

we therefore see that for $\bar{\eta} = \eta = 0$ Noether's theorem for the vector transformation in the path-integral formulation simply reads

$$\boxed{\langle \partial_\mu V^\mu \rangle = 0.} \quad (3.219)$$

By differentiation w.r.t. the external sources $\bar{\eta}, \eta$ additional **Ward identities** can be obtained which are exact relations between n -point functions into which the conserved Noether current has been inserted.

If we would carry out this derivation as well for the axial vector transformations (3.207) we would obtain Ward identities for the axial current, in particular also $\langle \partial_\mu A^\mu \rangle = 0$. However, this **not correct** because in this case the Jacobian gives a contribution as first recognized by **Fujikawa** [56]. The Jacobi determinant of the axial transformation namely is

$$\mathcal{J}_A = \text{Det}(e^{-i\alpha\gamma_5}) \cdot \text{Det}(e^{-i\alpha\gamma_5}) = e^{-2i \text{tr} \alpha \gamma_5}, \quad (3.220)$$

where we have used again the formal relation between determinant and the trace of the logarithm of a matrix (see **Problem 13**). For infinite matrices this expression (in general) is divergent and Fujikawa has proposed to use a **gauge invariant** regularization which suppresses the high-energy modes of the Dirac field:

$$\mathcal{J}_A = \lim_{M \rightarrow \infty} \exp \left[-2i \text{tr} \left(\alpha \gamma_5 e^{-\not{D}^2/M^2} \right) \right], \quad (3.221)$$

where D_μ is the covariant derivative. Other regularizations yield the same result provided they conserve the vector current. Recall the relation

$$\not{D}^2 = D^2 + \frac{1}{4} [\gamma^\mu, \gamma^\nu] [D_\mu, D_\nu] = D^2 + \frac{gT^a}{2} \sigma^{\mu\nu} F_{\mu\nu}^a \quad (3.222)$$

which we already have encountered in the abelian case in **chapter 3.4**⁹¹. We now have to calculate

$$\lim_{M \rightarrow \infty} \text{tr} \left(\gamma_5 e^{-\not{D}^2/M^2} \right) = \lim_{M \rightarrow \infty} \text{tr} \int d^4x \left\langle x \left| \gamma_5 \exp \left[-\frac{1}{M^2} \left(D^2 + \frac{gT^a}{2} \sigma^{\mu\nu} F_{\mu\nu}^a \right) \right] \right| x \right\rangle. \quad (3.223)$$

As the regulator mass M should go to infinity we can focus our attention to the asymptotic part of the spectrum in which the momentum of the Dirac field is large while the gauge field remains bounded. If we expand in

⁹⁰Recall that in a local **gauge** transformation the gauge field has to transform in a very specific way to compensate that change. Here, however, the gauge field remains unchanged.

⁹¹ $\sigma_{\mu\nu} = i[\gamma_\mu, \gamma_\nu]/2$, T^a are the generators of the $SU(N)$ Lie algebra.

powers of $F_{\mu\nu}^a$, we have to "bring down" four Dirac matrices from the exponential function in order to obtain a non-vanishing trace with γ_5 . This is because $\text{tr } \gamma_5 = \text{tr } \gamma_5 \gamma_\mu \gamma_\nu = 0$. Then the leading term of this "heat kernel" expansion is the one in which we expand the exponential function up to order $(\sigma \cdot F)^2$ and neglect the gauge field in all other terms. This gives

$$\lim_{M \rightarrow \infty} \text{tr} \left(\gamma_5 e^{-\not{D}^2/M^2} \right) = \lim_{M \rightarrow \infty} \int d^4x \text{tr} \left[\gamma_5 \frac{1}{2} \left(\frac{gT^a}{2M^2} \sigma_{\mu\nu} F_{\mu\nu}^a \right)^2 \right] \langle x | e^{-\partial^2/M^2} | x \rangle. \quad (3.224)$$

The matrix element in Eq. (3.224) has the value

$$\langle x | e^{-\partial^2/M^2} | x \rangle = \int \frac{d^4k}{(2\pi)^4} e^{k^2/M^2} = \frac{1}{(2\pi)^4} (-\pi M^2)^{1/2} (\pi M^2)^{3/2} = \frac{iM^4}{16\pi^2}. \quad (3.225)$$

The trace over the Dirac indices can also be calculated easily

$$\text{tr} \left(\gamma_5 \sigma^{\mu\nu} \sigma^{\alpha\beta} \right) = -4i \epsilon^{\alpha\beta\mu\nu}, \quad (3.226)$$

where $\epsilon^{\alpha\beta\mu\nu}$ is the total antisymmetric tensor in four dimensions. Hence

$$\lim_{M \rightarrow \infty} \text{tr} \left(\gamma_5 e^{-\not{D}^2/M^2} \right) = -\frac{g^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} \text{tr} (T^a T^b) \int d^4x F_{\alpha\beta}^a(x) F_{\mu\nu}^b(x). \quad (3.227)$$

Using $\text{tr } T^a T^b = \delta_{ab}/2$ we thereby have for the Jacobian of the axial transformation

$$\mathcal{J}_A = \exp \left[-i \int d^4x \alpha(x) N_f \frac{g^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} F_{\mu\nu}^a(x) F_{\alpha\beta}^a(x) \right]. \quad (3.228)$$

The factor $N_f = 3$ originates from the trace over those individual quarks which can be considered massless, i.e. over their "flavor".

By this somewhat lengthy calculation we have found how the integrand of the generating functional changes under an axial transformation. For infinitesimal $\alpha(x)$ we then obtain with the help of Eq. (3.215)

$$0 = i \int \mathcal{D}\bar{\psi}(x) \mathcal{D}\psi(x) \mathcal{D}A(x) \int d^4x \alpha(x) \left\{ -\partial_\mu A^\mu(x) + N_f \frac{g^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} F_{\mu\nu}^a(x) F_{\alpha\beta}^a(x) - i\alpha(x) \bar{\psi}\eta + i\alpha(x) \bar{\eta}\psi \right\} \cdot \exp \left[i \int d^4x (\mathcal{L}_{m=0}(\psi, \bar{\psi}, A) + \bar{\psi}\eta + \bar{\eta}\psi) \right]. \quad (3.229)$$

In particular, for vanishing sources we have

$$\langle \partial_\mu A^\mu \rangle = N_f \frac{g^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} \langle F_{\mu\nu}^a F_{\alpha\beta}^a \rangle. \quad (3.230)$$

This is in direct correspondence with the ABJ relation in operator notation which was first found by a perturbative analysis of diagrams like the one shown in Fig. 26. The path-integral derivation has the advantage that it holds in all orders and thereby is in agreement with the so-called Bardeen theorem which says that the anomaly is not changed in higher orders. The regularization of the divergent trace used above may look somehow *ad hoc* but it can be justified by a more careful treatment (for instance, by a zetafunction regularization [57]).

Finally we want to sketch how the anomaly determines the decay $\pi^0 \rightarrow 2\gamma$: Consider the S matrix element

$$\langle \gamma(k_1, \epsilon_1) \gamma(k_2, \epsilon_2) | S | \pi^0(q) \rangle = i(2\pi)^4 \delta(q - k_1 - k_2) \epsilon^\mu(k_1) \epsilon^\nu(k_2) \Gamma_{\mu\nu}(k_1, k_2, q), \quad (3.231)$$

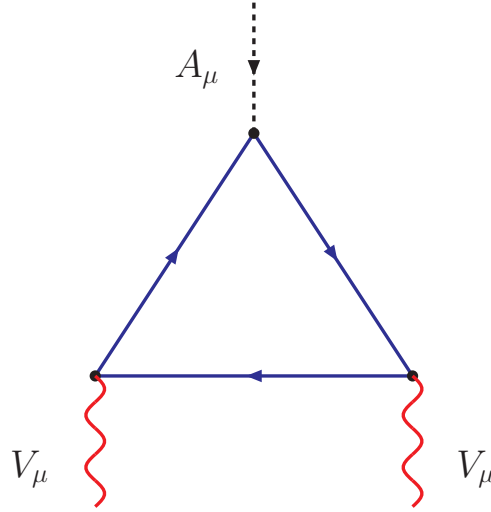


Fig. 26 : Triangle diagram for the axial current A_μ and two vector currents V_μ which gives an anomalous contribution for the divergence of the axial current.

where $k_i, \epsilon_i, i = 1, 2$ denote the momenta and polarisations of the photons. In the "soft pion limit" (i.e. $q_\mu \rightarrow 0$) the amplitude

$$\Gamma_{\mu\nu}(k_1, k_2, q) = e^2 (q^2 - m_\pi^2) \int d^4x_1 d^4x_2 e^{ik_1 \cdot x_1 + ik_2 \cdot x_2} \langle 0 | \mathcal{T} J_\mu^{\text{em}}(x_1) J_\nu^{\text{em}}(x_2) \Phi_\pi(0) | \rangle \quad (3.232)$$

can be related to the anomalous divergence of the axial current from the coupling of the quarks (here not to the gluons but) to the electromagnetic current J_μ^{em} . This can be done by means of the PCAC relation ⁹²

$$\partial_\mu A_\mu^a = f_\pi m_\pi^2 \Phi_\pi^a. \quad a = 1, 2, 3. \quad (3.233)$$

In Eq. (3.230) we therefore have to replace g^2 by the electromagnetic coupling constant $e^2 \simeq 4\pi/137$ and to modify the trace terms:

$$\partial^\mu A_\mu^a = \frac{e^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} F_{\mu\nu} F_{\alpha\beta} \underbrace{\text{tr}(\tau^a Q^2)}_{=: S^a}. \quad (3.234)$$

Here τ^a is the isospin matrix of the pion and Q the matrix of quark charges. The trace factor only contributes for $a = 3$ (i.e. for neutral pions) and has the value ⁹³

$$S^{(a=3)} = N_c (Q_d^2 - Q_u^2) = 3 \cdot \left(\frac{4}{9} - \frac{1}{9} \right) = 1. \quad (3.235)$$

The further calculation for the decay rate ⁹⁴ then gives

$$\Gamma(\pi^0 \rightarrow 2\gamma) = \frac{\alpha^2}{64\pi^3} \frac{m_\pi^3}{f_\pi^2}, \quad (3.236)$$

⁹² "Partially conserved axial current". $f_\pi \simeq 93$ MeV is the pion decay constant.

⁹³ It is amusing that already in 1949 Steinberger has evaluated the triangle diagram with *nucleons* in the loop [58] for which one also obtains the value 1 .

⁹⁴ See, e.g., **Peskin & Schroeder**, p. 674 - 676 .

in good agreement with the experimental result $\Gamma = 7.8 \pm 0.6$ eV. Without the color of the quarks running in the loop ⁹⁵ it would be smaller by a factor $N_c^2 = 9$.

(Much) more about anomalies in quantum field theory can be found in **{Bertlmann}**.

3.6 Lattice Field Theories

Up to now in this field-theoretical part we have used mostly methods of perturbation theory to evaluate path integrals. This is may be sufficient for theories with small coupling constants (like **QED** for which $\alpha \simeq 1/137$) but clearly is not sufficient in the region of strong coupling which occur in **QCD** at low energies ⁹⁶. This is exactly the region in which quarks and gluons do not show up as asymptotically observable particles but combine to form the observed hadrons. Moreover, perturbation theory is not complete: Phenomena like tunneling through a barrier or non-linear soliton solutions of classical field equations and probably also the "confinement" of quarks and gluons in **QCD** depend non-analytically on the coupling constant, i.e. are non-perturbative effects.

The exact treatment of non-perturbative effects in the path integral requires a (numerical) calculation of the functional integral as we already have done in **chapter 1.9** for quantum-mechanical problems. We recall that we have discretized the path integral there, in accordance with its original, heuristic introduction, and evaluated in Euclidean time. Similarly, the numerical treatment now will be performed on a finite **Euclidean space-time lattice** with lattice constant a . In field theory this has the additional advantage that all momentum integrals are cut off at $\sim 1/a$ and thus the ultraviolet divergences are regularized automatically. There is an obvious disadvantage that translation and rotation invariance are violated and will only be restored if the lattice is made larger and finer.

We start our introduction in this vast theoretical field by first treating a scalar theory. Consider the partition function

$$Z = \oint \mathcal{D}\Phi(x) e^{-S_E[\Phi]}, \quad (3.237)$$

where

$$S_E[\Phi] = \int d^4x \left[\frac{1}{2} (\partial\Phi)^2 + \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 \right] = \int d^4x \left[\frac{1}{2} \Phi(x) (-\square + m^2) \Phi(x) + \frac{\lambda}{4!} \Phi^4(x) \right] \quad (3.238)$$

is the Euclidean action (for instance of the Φ^4 -theory). In the following we will omit the index "E" as we will work exclusively in Euclidean space:

$$x_0 = -ix_4, \quad (3.239)$$

so that, for example, $\square\Phi = \sum_{\mu=1}^4 \partial_\mu^2 \Phi$.

Let's apply a naive discretization: We introduce a 4-dimensional space-time lattice with N lattice points and lattice distance a in such a way that each lattice point is determined by a 4-dimensional vector n :

$$x \equiv a(n_1, n_2, n_3, n_4) = a \sum_{\mu=1}^4 n_\mu e_\mu, \quad (3.240)$$

where e_μ is a unit vector in direction μ .

The integers n_μ are between $-N/2$ and $N/2$ and it is advisable to extend them outside that range: $n \hat{=} n + N$ (periodic lattice). In the discrete case the 4-dimensional integration is replaced by

$$\int d^4x \dots \longrightarrow a^4 \sum_n \dots \quad (3.241)$$

⁹⁵A different interpretation is advocated in Ref. [59].

⁹⁶The property of **asymptotic freedom** of **QCD** allows application of perturbation theory also at high energies.

and the scalar field exists at each lattice point

$$\Phi(x) \longrightarrow \Phi(n) = \Phi(n_1, n_2, n_3, n_4) \equiv \Phi_n . \quad (3.242)$$

Finally we replace the Laplace operator by the simplest, symmetric form

$$\square \Phi(x) \longrightarrow \frac{1}{a^2} \sum_{\mu=1}^4 [\Phi(n + e_\mu) + \Phi(n - e_\mu) - 2\Phi(n)] \equiv \frac{1}{a^2} \sum_{\mu=1}^4 (\Phi_{n+\mu} + \Phi_{n-\mu} - 2\Phi_n) , \quad (3.243)$$

which tends to the l.h.s. in the continuum limit $a \rightarrow 0$. With that the lattice action (which is now a *function* of the fields Φ_n) reads

$$\begin{aligned} S\{\Phi_n\} &= \sum_n \left\{ \frac{a^2}{2} \sum_{\mu=1}^4 [-\Phi_n \Phi_{n+\mu} - \Phi_n \Phi_{n-\mu} + 2\Phi_n^2] + a^4 \left(\frac{m^2}{2} \Phi_n^2 + \frac{\lambda}{4!} \Phi_n^4 \right) \right\} \\ &= \sum_n \left\{ -a^2 \sum_{\mu=1}^4 \Phi_n \Phi_{n+\mu} + \frac{a^2}{2} (8 + m^2 a^2) \Phi_n^2 + a^4 \frac{\lambda}{4!} \Phi_n^4 \right\} \end{aligned} \quad (3.244)$$

and the partition function becomes

$$Z = \int \left(\prod_n d\Phi_n \right) e^{-S\{\Phi_n\}} . \quad (3.245)$$

It is obvious that the lattice action is not unique: It is possible to add arbitrary terms which vanish for $a \rightarrow 0$. In particular, one may try to improve the discretization such that the errors are of higher order than the ones from the given "naive" form. This is the basic philosophy behind the "improved actions" which are used more and more frequently⁹⁷. Similarly we calculate correlation functions

$$\langle \Phi_{n_1} \Phi_{n_2} \dots \Phi_{n_k} \rangle = \frac{1}{Z} \int \left(\prod_n d\Phi_n \right) \Phi_{n_1} \Phi_{n_2} \dots \Phi_{n_k} e^{-S\{\Phi_n\}} . \quad (3.246)$$

As an example let's consider the 2-point function in the free discretized theory. We obtain (**Problem 32 a**)

$$\langle \Phi_n \Phi_{n'} \rangle = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} \frac{1}{2 \sum_{\mu} [1 - \cos(ap_{\mu})] / a^2 + m^2} e^{ip \cdot x} , \quad (3.247)$$

where $x_{\mu} = a(n_{\mu} - n'_{\mu})$ is the distance on the lattice. From this result we can see the following points:

- (1) The momentum integration is cut off: $|p_{\mu}| \leq \pi/a$ and only extends over the first "Brillouin zone".
- (2) For $a \rightarrow 0$ we obtain from the expansion $1 - a \cos(ap_{\mu}) \rightarrow a^2 p_{\mu}^2 / 2 + \dots$ the usual (Euclidean) Feynman propagator

$$\langle \Phi_n \Phi_{n'} \rangle \longrightarrow \int_{-\pi/a \rightarrow -\infty}^{\pi/a \rightarrow +\infty} \frac{d^4 p}{(2\pi)^4} \frac{1}{m^2 + p^2 + \mathcal{O}(a^2)} e^{ip \cdot x} . \quad (3.248)$$

- (3) For $a \neq 0$ the dispersion law in the continuum is changed

$$m^2 + p^2 \longrightarrow m^2 + \frac{4}{a^2} \sum_{\mu} \sin^2 \left(\frac{ap_{\mu}}{2} \right) . \quad (3.249)$$

⁹⁷See, e.g. Ref. [60].

However, there are no additional zeros which would indicate (additional) asymptotically propagating particles. This is not the case if **fermions** are put on the lattice: As can be derived in **Problem 32 b)** in a naive discretization one obtains

$$\langle \psi_\alpha(n) \bar{\psi}_\beta(n') \rangle = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} \left[-i \sum_\mu \gamma_\mu^E \tilde{p}_\mu + m \right]_{\alpha\beta} \frac{\exp(ip \cdot x)}{m^2 + \sum_\mu \tilde{p}_\mu^2}, \quad \tilde{p}_\mu := \frac{\sin(ap_\mu)}{a}, \quad (3.250)$$

where the Euclidean Dirac matrices fulfill $[\gamma_\mu^E, \gamma_\nu^E]_+ = 2\delta_{\mu\nu}$. Although $\tilde{p}_\mu \rightarrow p_\mu$ for $a \rightarrow 0$, the propagator (3.250) "repeats" itself at the end of the Brillouin zone since $\tilde{p}_\mu = \sin(\pi - p_\mu a)/a \rightarrow \pi/a - p_\mu$ for $p_\mu \rightarrow \pi/a$. This means that one doesn't have propagation of a single species of particles but $2^4 - 1 = 15$ additional copies ... Euphemistically one calls that "**fermion doubling**".

It is possible to remove the coupling constant λ from the action by rescaling of the field:

$$\Phi'_n = \sqrt{\lambda} \Phi_n. \quad (3.251)$$

Then we obtain

$$S\{\Phi_n\} = \frac{1}{\lambda} S'\{\Phi'_n\} \quad (3.252)$$

with

$$S'\{\Phi'_n\} = \sum_n \left\{ \frac{a^2}{2} \sum_{\mu=1}^4 [-\Phi'_n \Phi'_{n+\mu} - \Phi'_n \Phi'_{n-\mu} + 2\Phi_n'^2] + a^4 \left(\frac{m^2}{2} \Phi_n'^2 + \frac{1}{4!} \Phi_n'^4 \right) \right\} \quad (3.253)$$

and for the partition function (constant factors are irrelevant)

$$Z = \int \left(\prod_n d\Phi'_n \right) e^{-\frac{1}{\lambda} S'\{\Phi'_n\}}. \quad (3.254)$$

If we compare that with the partition function in statistical mechanics we see the correspondence

$$\frac{1}{\lambda} \longleftrightarrow \frac{1}{k_B T}, \quad (3.255)$$

i.e. an **expansion for strong couplings** corresponds to a **high-temperature expansion** of statistical systems.

3.6.1 Gauge Theories on the Lattice

Gauge theories on a space-time lattice require a particular treatment in order to maintain gauge invariance in each step. In 1974 **K. Wilson** has proposed a formulation where the gauge fields are not defined on the lattice points but on "**links**":

$$U(n, \mu) = \exp[iga\mathcal{A}_\mu(n)], \quad \mathcal{A}_\mu = A_\mu^a T^a \in SU(N), \quad \left(T^a = \frac{\lambda_a}{2} \text{ for } SU(3) \right) \quad (3.256)$$

is the link which points from the point n in positive direction μ . Wilson has also proposed an action which reduces to the Euclidean Yang-Mills action

$$S_{YM} = \frac{1}{2} \int d^4x \operatorname{tr} \mathcal{F}_{\mu\nu} \mathcal{F}_{\mu\nu} = \frac{1}{4} \int d^4x \mathcal{F}_{\mu\nu}^a \mathcal{F}_{\mu\nu}^a, \quad \mathcal{F}_{\mu\nu} \equiv F_{\mu\nu}^a T^a \quad (3.257)$$

in the continuum limit:

$$S_{\text{Wilson}} = \beta \sum_{n, \mu, \nu} \left\{ 1 - \frac{1}{N} \operatorname{Re} \operatorname{tr} \left[U(n, \mu) U(n + \mu, \nu) U(n + \mu + \nu, -\mu) U(n + \nu, -\nu) \right] \right\}. \quad (3.258)$$

Here β is a yet undetermined factor and the summation has to be performed over all elementary squares (“plaquettes”) of the lattice:

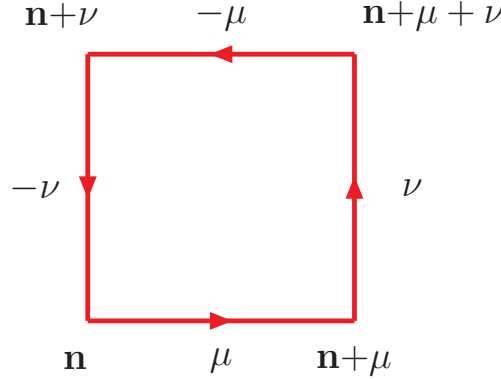


Fig. 27 : The elementary plaquette in lattice gauge theory.

Detail 34: Wilson’s Action at Small Lattice Distances

It is relatively easy to show that the Wilson action goes over into the continuum action for $a \rightarrow 0$. For that we use $U(n, \mu) U(n + \mu, -\mu) = 1$, i.e.

$$U(n, \mu) = U^{-1}(n + \mu, -\mu) . \tag{3.259a}$$

Then we obtain

$$S_{\text{Wilson}} = \beta \sum_{\text{plaquettes}} \left\{ 1 - \frac{1}{N} \text{Re tr} \left[e^{iga\mathcal{A}_\mu(x)} e^{iga\mathcal{A}_\nu(x+a\epsilon_\mu)} e^{-iga\mathcal{A}_\mu(x+a\epsilon_\nu)} e^{-iga\mathcal{A}_\nu(x)} \right] \right\} . \tag{3.259b}$$

To combine the exponential functions we utilize the Baker-Campbell-Hausdorff formula

$$e^{a\hat{A}} e^{a\hat{B}} = \exp \left(a\hat{A} + a\hat{B} + \frac{a^2}{2} [\hat{A}, \hat{B}] + \mathcal{O}(a^3) \right) . \tag{3.259c}$$

Then the result is

$$S_{\text{Wilson}} = \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \exp \left\{ iga (\mathcal{A}_\mu(x) + \mathcal{A}_\nu(x+a\epsilon_\mu) - \mathcal{A}_\mu(x+a\epsilon_\nu) - \mathcal{A}_\nu(x)) \right. \right. \\ \left. \left. + \frac{(iga)^2}{2} \left([\mathcal{A}_\mu(x), \mathcal{A}_\nu(x+a\epsilon_\mu)] - [\mathcal{A}_\mu(x) + \mathcal{A}_\nu(x+a\epsilon_\mu), \mathcal{A}_\mu(x+a\epsilon_\nu)] \right. \right. \right. \\ \left. \left. \left. - [\mathcal{A}_\mu(x) + \mathcal{A}_\nu(x+a\epsilon_\mu) - \mathcal{A}_\mu(x+a\epsilon_\nu), \mathcal{A}_\nu(x)] \right) \right\} \right\} . \tag{3.259d}$$

By a Taylor expansion of the vector fields we obtain

$$S_{\text{Wilson}} = \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \exp \left\{ iga (a\partial_\mu \mathcal{A}_\nu(x) - a\partial_\nu \mathcal{A}_\mu(x)) + (iga)^2 [\mathcal{A}_\mu(x), \mathcal{A}_\nu(x)] \right\} \right\} \\ \xrightarrow{a \rightarrow 0} \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \left(1 + iga^2 \mathcal{F}_{\mu\nu} + \frac{1}{2} (iga^2)^2 \mathcal{F}_{\mu\nu} \mathcal{F}_{\mu\nu} + \dots \right) \right\} . \tag{3.259e}$$

In the limit $a \rightarrow 0$ only the 2nd order term contributes since $\text{tr} \mathcal{F}_{\mu\nu} = 0$ (the $SU(N)$ generators are traceless) and we have

$$S_{\text{Wilson}} \xrightarrow{a \rightarrow 0} \beta \frac{1}{2} \sum_{n, \mu\nu} \frac{1}{N} \frac{1}{2} (ga^2)^2 \text{tr} \mathcal{F}_{\mu\nu} \mathcal{F}_{\mu\nu} = \frac{\beta g^2}{2N} \int d^4x \text{tr} \sum_{\mu\nu} \mathcal{F}_{\mu\nu}(x) \mathcal{F}_{\mu\nu}(x) . \tag{3.259f}$$

The factor $\frac{1}{2}$ has its origin in the relation $\sum_P = \frac{1}{2} \sum_{\mu\nu}$.

Thus we have to choose

$$\boxed{\beta = \frac{2N}{g^2}} \quad (3.260)$$

to obtain the action (3.257) of the continuum theory; for $N = 1$ one has to take $\beta = 1/g^2$. The Wilson action is distinguished by the property that it is **invariant under a local gauge transformation**

$$U(n, \mu) \longrightarrow V(n) U(n, \mu) V^{-1}(n + \mu) \quad (3.261)$$

with an arbitrary matrix $V \in SU(N)$.

$$\begin{aligned} \text{Proof :} \quad S_{\text{Wilson}} &\longrightarrow \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \left[V(n) U(n, \mu) \underbrace{V^{-1}(n + \mu) V(n + \mu)}_{=1} U(n + \mu, \nu) \right. \right. \\ &\quad \cdot \underbrace{V^{-1}(n + \mu + \nu) V(n + \mu + \nu)}_{=1} U(n + \mu + \nu, -\mu) \\ &\quad \left. \left. \cdot \underbrace{V^{-1}(n + \mu + \nu - \mu) V(n + \nu)}_{=1} U(n + \nu, -\nu) V^{-1}(n + \nu - \nu) \right] \right\} \\ &= \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \left[V(n) U U U U V^{-1}(n) \right] \right\} = \beta \sum_P \left\{ 1 - \frac{1}{N} \text{Re tr} \left[U U U U \right] \right\} \\ &= S_{\text{Wilson}} , \end{aligned}$$

as $\text{tr}(\hat{A}\hat{B}) = \text{tr}(\hat{B}\hat{A})$ **q.e.d.**

In this formulation the lattice gauge theory therefore respects the gauge invariance at the expense of translation and thus Lorentz invariance. The latter ones should be restored in the continuum limit. Note that unlike the continuum theory no gauge fixing is necessary since the gauge fields are represented by a finite unitary matrix U (“compact” action). One does not sum over infinite degrees of freedom which are connected by gauge transformations.

3.6.2 Wilson loops and Confinement

To obtain a criterion for the postulated “**confinement**” of the quarks we will study now the energy of a system made up of a quark at $x' = (t, \mathbf{0})$ and an antiquark at $x = (t, \mathbf{R})$. Here the quarks are assumed to be so **heavy** that they do not move and only constitute a source for the gluon fields. If the quarks are not confined we expect that

$$E(R) \longrightarrow 2m \quad \text{for } R \rightarrow \infty , \quad (3.263)$$

where m is the quark mass. **Confinement** means that the potential energy of the quarks grows without bound:

$$E(R) \longrightarrow \infty \quad \text{for } R \rightarrow \infty . \quad (3.264)$$

The quark-antiquark system cannot be represented simply by the state

$$\bar{q}(x') q(x) |0\rangle , \quad (3.265)$$

since this is not gauge invariant. The correct expression

$$\Gamma(x', x, C) = \bar{q}(x') \mathcal{P} \exp \left(ig \int_x^{x'} \mathcal{A}_\mu(y) dy^\mu \right) q(x) |0\rangle = \bar{q}(x') U(x', x, C) q(x) |0\rangle \quad (3.266)$$

contains a phase factor between the field operators creating a quark/antiquark at different space-time points. It is obvious that this factor also depends on the path C which connects x and x' . \mathcal{P} denotes the [path ordering](#) which is necessary because the gauge field does not commute at different points ⁹⁸.

We now want to calculate the overlap between the $q\bar{q}$ -Zustand at $t = 0$ and the same state at $t = T$:

$$\Omega(T, R) = \langle 0 | \Gamma^\dagger [(0, \mathbf{0}), (0, \mathbf{R}), C] \Gamma [(T, \mathbf{0}), (T, \mathbf{R}), C] | 0 \rangle . \quad (3.267)$$

As usual we insert a complete set of intermediate states and investigate the behaviour for large T . Then we see that the intermediate state dominates which has the smallest potential energy of the $q\bar{q}$ system at distance R :

$$\Omega(T, R) \stackrel{T \rightarrow \infty}{\simeq} \text{const. } e^{-E(R)T} . \quad (3.268)$$

On the other hand we may express the overlap by means of the quark field operators:

$$\Omega(T, R) = \langle 0 | \bar{q}(0, \mathbf{R}) U [(0, \mathbf{R}), (0, \mathbf{0}); C] q(0, \mathbf{0}) \bar{q}(T, \mathbf{0}) U [(T, \mathbf{0}), (T, \mathbf{R}); C] q(T, \mathbf{R}) | 0 \rangle . \quad (3.269)$$

For a heavy, non-moving quark the Euclidean Dirac equation reads

$$\gamma_4 (\partial_4 - ig\mathcal{A}_4) q(x) = -mq(x) . \quad (3.270)$$

In this extreme non-relativistic limit it is also allowed to set $\gamma_4 = 1$ and there is no quark pair production by the gauge field which acts like an external field. The solution then simply is

$$q(x_4 = t, \mathbf{x}) = \text{const. } e^{-mt} \mathcal{P} \exp \left(ig \int_0^t dt' \mathcal{A}_4(t') \right) , \quad (3.271)$$

and hence the quark propagator is

$$\langle 0 | q_\beta(t', \mathbf{x}) \bar{q}_\alpha(t, \mathbf{x}) | 0 \rangle = U [(t', \mathbf{x}), (t, \mathbf{x}); C] \delta_{\alpha\beta} e^{-m|t-t'|} . \quad (3.272)$$

If we contract the quark field operators in Eq. (3.269) and use Eq. (3.272) we obtain

$$\begin{aligned} \Omega(T, R) &\simeq \text{const. } e^{-2mT} \langle 0 | U [(T, \mathbf{R}), (0, \mathbf{R})] U [(0, \mathbf{R}), (0, \mathbf{0})] \\ &\quad \cdot U [(0, \mathbf{0}), (T, \mathbf{0})] U [(T, \mathbf{0}), (T, \mathbf{R})] | 0 \rangle \\ &= \text{const. } e^{-2mT} \underbrace{\langle 0 | \text{tr } U [(0, \mathbf{0}), (0, \mathbf{0}); C] | 0 \rangle}_{=: W(C)} . \end{aligned} \quad (3.273)$$

Here C is the rectangular path shown in Fig. 28 (a) . From the [Wilson loop](#) $W(C)$ one can determine the potential energy between a heavy quark and a heavy antiquark:

$$\lim_{T \rightarrow \infty} W(C) = \text{const. } e^{-[E(R)-2m]T} . \quad (3.274)$$

As will be shown the Wilson loop obeys an [area law](#) in the strong-coupling limit

$$W(C) \stackrel{g^2 \rightarrow \infty}{\simeq} e^{-KA(C)} , \quad (3.275)$$

where K is a constant and $A(C)$ is the area enclosed by the path C . For the rectangular path we have $A(C) = TR$ and therefore a [linearly increasing potential](#) between heavy quark and antiquark.

$$E(R) - 2m = KR . \quad (3.276)$$

The graphic picture one can associate with such an increasing potential is that of a [“string”](#) of gluon fields which is generated between the static color sources. Therefore the constant K is also called [“string tension”](#) .

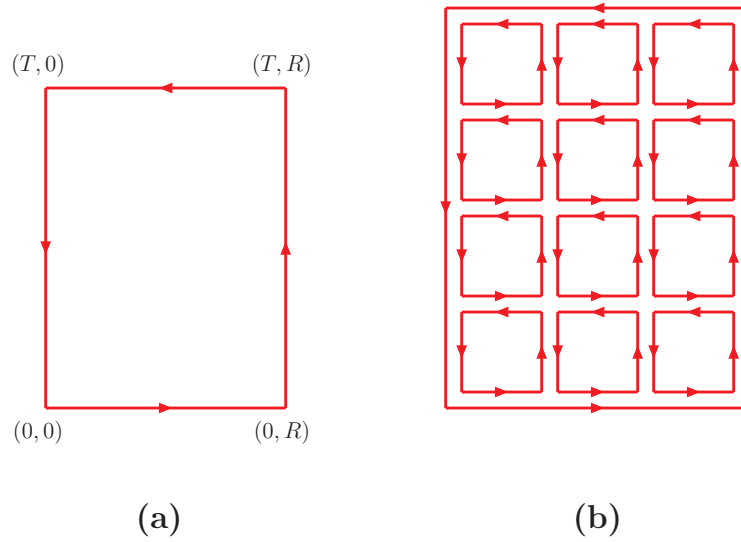


Fig. 28 : (a) Wilson loop with rectangular path. (b) A Wilson loop completely covered by plaquettes.

The Wilson loop can be calculated directly on the lattice:

$$\begin{aligned}
 W(C) &= \langle 0 | \text{tr } U(x, x; C) | 0 \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{A}_\mu(x) \text{tr } U(x, x; C) e^{-S_E[\mathcal{A}]} \\
 &\xrightarrow{\text{lattice}} \frac{1}{Z} \int \prod_{n, \mu} dU(n, n + \mu) \text{tr } U(n, n; C) e^{-S_{\text{Wilson}}(U)}, \quad (3.277)
 \end{aligned}$$

where

$$Z = \int \prod_{n, \mu} dU(n, n + \mu) e^{-S_{\text{Wilson}}(U)} \quad (3.278)$$

is the partition function. Here we do not integrate directly over the gauge fields but over the links U which are proportional to them for small lattice distances.

We now try to calculate the Wilson loop **for large coupling constants analytically**. For that purpose we write the Wilson action (3.258) as

$$S_{\text{Wilson}} = \beta \sum_P \left(1 - \frac{1}{N} \text{Re tr } U_P \right), \quad (3.279)$$

omit the irrelevant constant in the action and expand in powers of $\beta = N/(2g^2)$. This gives

$$W(C) = \frac{1}{Z} \int dU \text{tr } U(x, x; C) \left\{ 1 + \frac{1}{2g^2} \sum_P \text{sp } U_P + \frac{1}{2!} \left(\frac{1}{2g^2} \right)^2 \sum_{P, P'} \text{tr } U_P \text{tr } U_{P'} + \dots \right\}. \quad (3.280)$$

To evaluate that result we should know how to integrate over the group elements of $SU(N)$. This is easy in the $U(1)$ case since there the group elements are phase factors parametrized by $e^{i\Theta}$, $-\pi < \Theta \leq \pi$:

$$\frac{1}{2\pi} \int_{-\pi}^{+\pi} d\Theta = 1, \quad \frac{1}{2\pi} \int_{-\pi}^{+\pi} d\Theta e^{i\Theta} = 0. \quad (3.281)$$

⁹⁸Analogously to the time ordering the path ordering is defined by the following procedure: Parametrize the path from x to x' by a continuously increasing parameter $s \in [0, 1]$ and expand the exponential function $\exp\left(ig \int_0^1 ds \frac{dx_\mu}{ds} \mathcal{A}_\mu(s) ds\right)$ into a power series. Then the matrices $\mathcal{A}_\mu(s)$ have to be ordered such that the largest value of s is on the l.h.s.

In the general case the integration over group elements is done with the help of the **Haar measure**⁹⁹. However, for the present purposes it is sufficient to list the integrals

$$\int dU = 1 \tag{3.282}$$

$$\int dU U_{ij} = 0 \tag{3.283}$$

$$\int dU U_{ij} U_{kl}^\dagger = \frac{1}{N} \delta_{il} \delta_{jk} . \tag{3.284}$$

The second rule says that no “links” should remain after integration while the third rule means that a non-vanishing result is only obtained if one integrates over two “links” in opposite direction. This has the consequence that a Wilson loop has to be covered completely with plaquettes whose adjacent “links” have opposite direction in order to yield a contribution (Fig. 28 (b)). The lowest (non-vanishing in $1/g^2$) contribution to $W(C)$ therefore gives the term with

$$W(C) \sim \left(\frac{1}{2g^2} \right)^{N_P} , \tag{3.285}$$

where N_P is the minimal number of plaquettes required to cover the area enclosed by the path C . Since $A(C) = a^2 N_P$, this is equivalent to the area law

$$W(C) \sim (g^2)^{-A(C)/a^2} = \exp \left(-\frac{TR}{a^2} \ln g^2 \right) . \tag{3.286}$$

Thus in the limit of strong coupling we indeed find

$$E(R) - 2m \sim \frac{\ln g^2}{a^2} R \equiv K R , \quad g \gg 1 \tag{3.287}$$

a **linearly increasing (confining) potential** between heavy quark and antiquark.

However, this result is obviously independent of N , i.e. also an abelian $U(1)$ theory like **QED** leads to confinement in the strong-coupling limit! This seems unreasonable but can be brought into agreement with reality by the following argument: In the continuum limit $a \rightarrow 0$ one has to change the (bare) coupling constant $g = g(a)$ in such a way that the physical observables (e.g. the string tension) do not change. As can be seen from Eq. (3.287) this implies that the (bare) coupling constant has to decrease in the continuum limit. It is generally believed and supported by numerical data – as we will see in the next chapter – that **QCD** and **QED** behave totally different in the limit of weak coupling. While in **QCD** the area law still holds and the quarks remain confined there is a **phase transition** in **QED**. Instead of an area law one finds a **perimeter law** at weak (bare) coupling: The potential between e^+ and e^- approaches a constant at large distances which means that the constituents may appear as free particles at sufficient energy in agreement with the experimental observation.

3.6.3 Numerical Calculation of Observables on the Lattice

Perturbation theory and the strong-coupling expansion are insufficient to describe non-perturbative phenomena in the continuum. This is evident for non-abelian theories like **QCD** but should also hold for the postulated transition of confinement to Coulomb phase in **QED**. In such cases (and with the present state of theoretical tools) there only remains to perform a numerical evaluation of the path integral.

⁹⁹See, e.g., {Creutz}, ch. 8.

We already have covered that extensively in the **chapter 1.9** for the anharmonic oscillator in quantum mechanics. Our aim is to extend that to a 4-dimensional field theory. To simplify the programming effort we illustrate the numerical simulation not for the (much more interesting) $SU(3)$ theory of **QCD** but “only” for the abelian $U(1)$ theory. In this case the “links” are simply given by the phase factors

$$U(n, \mu) = e^{igaA_\mu(n)} = e^{i\Theta_\mu(n)}, \quad 0 < \Theta_\mu(n) \leq 2\pi \quad (3.288)$$

with

$$U(n + \mu, -\mu) = U^{-1}(n, \mu) = U^\dagger(n, \mu) = U^*(n, \mu). \quad (3.289)$$

By means of the Metropolis algorithm we again generate “configurations” (i.e. all possible U ’s on the lattice) distributed according to

$$w(U) = \frac{e^{-S_{\text{Wilson}}(U)}}{\int dU e^{-S_{\text{Wilson}}(U)}}. \quad (3.290)$$

We recall that we have to generate trial configurations (U_t) and then – depending on the value of

$$r = e^{-[S(U_t) - S(U)]} \equiv e^{-\Delta S} \quad (3.291)$$

– have to decide whether we accept these or not. It is reasonable to change the configuration only at one “link” $U(n, \mu)$ because then one only has to calculate the change of the action

$$\begin{aligned} \Delta S = & -\beta \sum_{\nu \neq \mu} \Delta U(n, \mu) \left\{ U(n + \mu, \nu) U^*(n + \nu, \mu) U^*(n, \nu) \right. \\ & \left. + U(n + \mu, -\nu) U^*(n - \nu, \mu) U^*(n, -\nu) \right\} \end{aligned} \quad (3.292)$$

which in 4 dimensions precisely affects 6 “links”. We take

$$\Delta U(n, \mu) = U(n, \mu) \cdot \left[1 - \frac{\exp(2\pi i z_1) + \delta}{|\exp(2\pi i z_1) + \delta|} \right], \quad (3.293)$$

as change where δ is a given parameter and z_1 a random number (uniformly distributed between 0 and 1) After sufficient “sweeps” through the lattice (so that thermalization has occurred) one measures the expectation value of an arbitrary variable $\mathcal{O}(U)$ by

$$\langle \mathcal{O} \rangle = \frac{\int dU \mathcal{O}(U) e^{-S(U)}}{\int dU e^{-S(U)}} \simeq \frac{1}{M} \sum_{i=1}^M \mathcal{O}(U_i). \quad (3.294)$$

A popular observable is the **mean plaquette**

$$\langle P \rangle = \left\langle \left(1 - \frac{1}{N} \sum_P \text{tr} U_P \right) \right\rangle_{N=1}, \quad (3.295)$$

since it is easy to calculate and as an **order parameter** signals the transition to another phase. With a small lattice this easily can be done also on a PC.

Detail 35: FORTRAN Program for the Calculation of the Mean Plaquette¹⁰⁰

```

C
C Calculates mean plaquette in 4-dimensional U(1) theory on a 8^4 lattice
C as function of beta = 1/g^2
C
C Parameter:
C NTH = number of thermalization sweeps
C NHIT = number of additional Monte Carlo calls at each lattice point
C NSWEEP = number of sweeps (<500)
C DELTA = parameter for a new configuration
C BETA0 = initial value of beta
C DBETA = beta step size
C NBETA = number of beta values
C
      PARAMETER(LS=8,LT=8,NN=LS**3*LT)
      COMPLEX U(NN,4),V,ZPI
      DOUBLE PRECISION DSEED
      DIMENSION NNF(NN,4),NNB(NN,4),ACT(500)
      COMMON/ZUF/ DSEED,ZPI,DELTA
      COMMON /PAR/ NAKZ
      DATA PI /3.1415926/
      WRITE(*,*) 'Input: ntherm,nhit,nsweep,delta'
      READ (*,*) N THERM,NHIT,NSWEEP,DELTA
      WRITE(*,*) 'Input: beta0,dbeta,nbeta'
      READ (*,*) BETA0,DBETA,NBETA
C
C auxiliary calculations
C
      LS2 = LS*LS
      LS3 = LS2*LS
      DSEED = 12365.DO
      ZPI = 2.*PI*CMPLX(0.,1.)
      NAKZ = 0
      WRITE (6,100) LS,LT
100  FORMAT(// ' U(1) theory on a (' ,I2,'**3)*',I2,' lattice'//)
      WRITE(6,102) N THERM,NHIT,NSWEEP,DELTA
102  FORMAT(' N THERM =',I3,' NHIT =',I2,' NSWEEP =',I3,
& ' DELTA = ',F6.3//)
C
c calculate next-neighbor addresses
C
      DO 10 IX = 1,LS
        DO 10 IY = 1,LS
          DO 10 IZ = 1,LS
            DO 10 IT = 1,LT
              I = IX + LS*(IY-1+LS*(IZ-1+LS*(IT-1)))
              NNF(I,1) = I - IX + 1 + MOD(IX,LS)
              NNF(I,2) = I - (IY-1-MOD(IY,LS))*LS
              NNF(I,3) = I - (IZ-1-MOD(IZ,LS))*LS2
              NNF(I,4) = I - (IT-1-MOD(IT,LT))*LS3
              NNB(I,1) = I - IX + 1 + MOD(IX+LS-2,LS)
              NNB(I,2) = I - (IY-1-MOD(IY+LS-2,LS))*LS
              NNB(I,3) = I - (IZ-1-MOD(IZ+LS-2,LS))*LS2
              NNB(I,4) = I - (IT-1-MOD(IT+LT-2,LT))*LS3
10    CONTINUE
C
C initialization and thermalization
C
      WRITE(6,*) (' cold start'//)
      DO 12 I = 1,NN
        DO 12 I1 = 1,4
12    U(I,I1) = 1.
        DO 15 I = 1,N THERM
15    CALL UPDATE(U,NN,NHIT,BETA,NNF,NNB)
C
C beta loop
C
      DO 90 IBETA = 1,NBETA
        BETA = BETA0 + (IBETA - 1)*DBETA
C sweeps
        NAKZ = 0
        DO 20 L = 1,NSWEEP
          CALL UPDATE(U,NN,NHIT,BETA,NNF,NNB)
C
C measurement
C
        ACT(L) = 0.
        DO 30 I = 1,NN
          DO 30 K = 1,3
            KP1 = K + 1
            V = 0.
            DO 40 K1 = KP1,4
              I1 = NNF(I,K)
              I2 = NNF(I,K1)
              V = V + U(I1,K1)*CONJG(U(I2,K))*CONJG(U(I,K1))

```

¹⁰⁰Thanks to Manfred Kremer (Mainz/Jülich) who provided the first version of this program.

```

40      CONTINUE
      ACT(L) = ACT(L) + U(I,K)*V
30      CONTINUE
      ACT(L) = (1. - ACT(L)/(6.*NN))
20      CONTINUE
      SACT1 = 0.
      SACT2 = 0.
      DO 50 L = 1,NSWEEP
          SACT1 = SACT1 + ACT(L)
50      SACT2 = SACT2 + ACT(L)**2
      SACT = SACT1/NSWEEP
      SACT2 = SACT2/NSWEEP
      SACT2 = SACT2 - SACT*SACT
      SACT2 = SQRT(SACT2)
      XAKZ = NAKZ/(4.*NHIT*NSWEEP*NN)
C
C print out
C
      WRITE(6,104) BETA,SACT,SACT2,XAKZ
104     FORMAT(' beta =',F7.3,5X,'mean plaquette =',F9.3,
&        ' +/-',F6.3,5X,'acceptance =',F7.3/)
90      CONTINUE
      STOP
      END

C+++++ SUBPROGRAM UPDATE +++++
      SUBROUTINE UPDATE (U,NN,NHIT,BETA,NNF,NNB)
C
C New trial configuration (update)
C
      COMPLEX U(NN,4),V,W,W1,ZPI
      DIMENSION NNF(NN,4),NNB(NN,4)
      DOUBLE PRECISION DSEED
      COMMON /ZUF/ DSEED,ZPI,DELTA
      COMMON /PAR/ NAKZ
      DO 10 I = 1,NN
          DO 10 K = 1,4
              V = 0.
              DO 20 K1 = 1,4
                  IF (K1.EQ. K) GO TO 20
                  I1 = NNF(I,K)
                  I2 = NNF(I,K1)
                  I4 = NNB(I,K1)
                  I5 = NNF(I4,K)
                  V = V + U(I1,K1)*CONJG(U(I2,K))*CONJG(U(I,K1))
&                + U(I4,K1)*CONJG(U(I5,K))*CONJG(U(I4,K1)) ! Birbaumer-
! correction
20      CONTINUE
C
C Metropolis algorithm
C
          DO 30 KIND = 1,NHIT
              CALL CREATE(W1)
              W = W1*U(I,K)
              SNEU = V*W
              SALT = V*U(I,K)
              DACT = (SNEU - SALT)*BETA
              IF (DACT.LT. 0.) THEN
                  P = EXP(DACT)
                  XR = ZUFALL(DSEED)
              END IF
              IF (DACT.GE. 0.) GO TO 7
              IF(XR.GT. P) GO TO 30
              U(I,K) = W
              NAKZ = NAKZ + 1
30      CONTINUE
10      CONTINUE
      RETURN
      END

C+++++ SUBPROGRAMM CREATE +++++
      SUBROUTINE CREATE(U)
C
C creates new exp(i theta)
C
      DOUBLE PRECISION DSEED
      COMPLEX U,ZPI,AO
      COMMON /ZUF/ DSEED,ZPI,DELTA
      AO = ZUFALL(DSEED)*ZPI
      U = CEXP(AO) + DELTA
      U = U/CABS(U)
      RETURN
      END

C+++++ SUBPROGRAMM ZUFALL +++++
      FUNCTION ZUFALL(DSEED)

```

```

C
C generates uniformly distributed random numbers in the interval [0,1]
C
  DOUBLE PRECISION A,C
  DATA A,C /16807.DO,2147483647.DO/
  DSEED = DMOD(A*DSEED,C)
  ZUFALL = DSEED/C
  RETURN
  END

```

If we make a "cold" start with this program on a 8^4 -Gitter and let it run with 100 "sweeps", throwing the Monte-Carlo dice 5 times at each lattice point and demanding 20 different β values¹⁰¹ we obtain the following printout:

```

U(1) theory on a ( 8**3)*8 lattice

N THERM = 20      N HIT = 5      N SWEEP = 100      DELTA = 1.5

cold start
beta = 0.100      mean plaquette = 0.950 +- 0.004      acceptance = 0.969
beta = 0.200      mean plaquette = 0.901 +- 0.004      acceptance = 0.938
beta = 0.300      mean plaquette = 0.852 +- 0.004      acceptance = 0.908
beta = 0.400      mean plaquette = 0.804 +- 0.004      acceptance = 0.878
beta = 0.500      mean plaquette = 0.754 +- 0.004      acceptance = 0.848
beta = 0.600      mean plaquette = 0.706 +- 0.005      acceptance = 0.819
beta = 0.700      mean plaquette = 0.654 +- 0.004      acceptance = 0.788
beta = 0.800      mean plaquette = 0.599 +- 0.006      acceptance = 0.758
beta = 0.900      mean plaquette = 0.536 +- 0.007      acceptance = 0.725
beta = 1.000      mean plaquette = 0.432 +- 0.022      acceptance = 0.682
beta = 1.100      mean plaquette = 0.311 +- 0.024      acceptance = 0.636
beta = 1.200      mean plaquette = 0.251 +- 0.004      acceptance = 0.608
beta = 1.300      mean plaquette = 0.224 +- 0.003      acceptance = 0.589
beta = 1.400      mean plaquette = 0.203 +- 0.003      acceptance = 0.572
beta = 1.500      mean plaquette = 0.188 +- 0.003      acceptance = 0.556
beta = 1.600      mean plaquette = 0.174 +- 0.002      acceptance = 0.542
beta = 1.700      mean plaquette = 0.162 +- 0.002      acceptance = 0.529
beta = 1.800      mean plaquette = 0.152 +- 0.002      acceptance = 0.516
beta = 1.900      mean plaquette = 0.143 +- 0.002      acceptance = 0.504
beta = 2.000      mean plaquette = 0.135 +- 0.002      acceptance = 0.493

```

If one plots the results for different lattice sizes (as in Fig. 29; sorry, the legend is in German...) then one sees that a rather rapid change of the mean plaquette values occurs at $\beta \simeq 0.9 - 1.2$, i.e. the suspected phase transition from the confining phase (large $g^2 \Rightarrow$ small β) to the Coulomb phase (small $g^2 \Rightarrow$ large β) seems to take place.

Since we are working on a very small, finite lattice this transition is not so abrupt as in the infinite system where the order parameter vanishes in the phase where electrons and positrons are free. Nevertheless our result agrees reasonably well with the best calculations which localize the phase transition at $\beta = 1.011131(6)$ [61].

¹⁰¹That takes about 1.5 min on a 2 GHz PC, for the 12^4 lattice about 7.5 min.

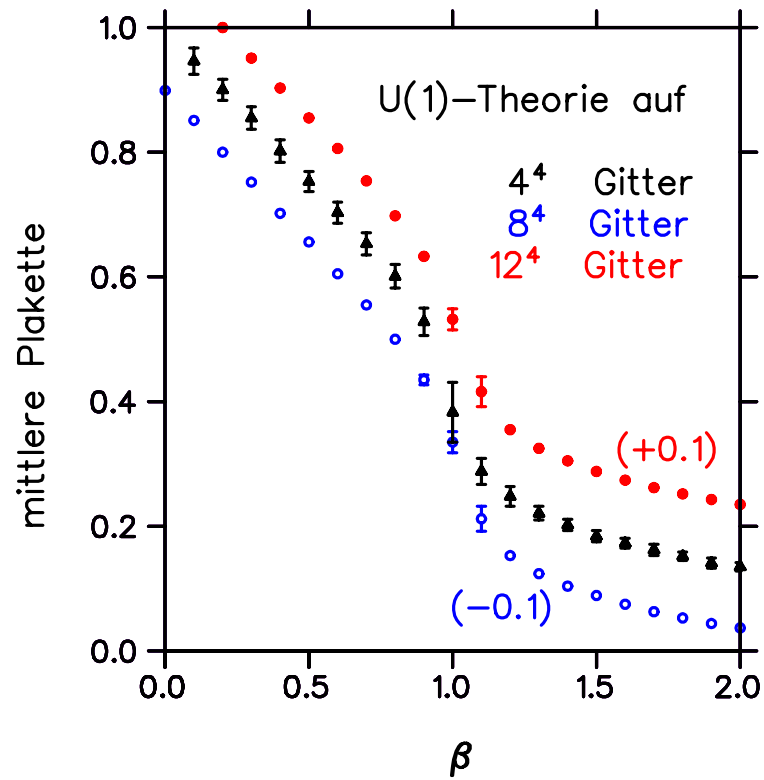


Fig. 29 : Mean plaquette $\langle P \rangle$ as a function of $\beta = 1/g^2$ for different lattice sizes. To make the results better visible, the results for the 8^4 lattice have been shifted downwards by the constant value 0.1 while the ones for the 12^4 lattice by 0.1 upwards.

Additional Literature (in alphabetic order)

- {**Bateman Proj. 2**} A. Erdely (ed.), *Higher Transcendental Functions, based, in part, on notes left by Harry Bateman*, vol. 2 , McGraw-Hill, New York (1953).
- {**Berezin**} F. A. Berezin, *The Method of Second Quantization*, Academic Press, New York (1965).
- {**Bertlmann**} R. A. Bertlmann, *Anomalies in Quantum Field Theory*, Oxford University Press, Oxford (2000).
- {**Bjorken-Drell**} J. D. Bjorken, S. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill, New York (1964)
- {**Bronstein-Semendjajew**} I. N. Bronstein and K. A. Semendjajew, *Taschenbuch der Mathematik*, Harri Deutsch, Zürich and Frankfurt (1965).
- {**Collins**} J. C. Collins, *Renormalization. An introduction to renormalization, the renormalization group, and the operator-product expansion*, Cambridge University Press, Cambridge (1984).
- {**Creutz**} M. Creutz, *Quarks, Gluons and Lattices*, Cambridge University Press, Cambridge (1983).
- {**Dennery-Krzywicki**} Ph. Dennery and A. Krzywicki, *Mathematics for Physicists*, Harper & Row, New York (1967).
- {**Eisenberg-Koltun**} J. M. Eisenberg and D. S. Koltun, *Theory of Meson Interactions with Nuclei*, John Wiley, New York (1980).
- {**Euler**} L. Euler, *Introductio in Analysin Infinitorum*, Lausanne (1748).
- {**Farmelo**} G. Farmelo, *The Strangest Man: The Hidden Life of Paul Dirac, Quantum Genius*, Faber and Faber, London (2009).
- {**Fetter-Walecka**} A. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems*, McGraw-Hill, New York (1971).
- {**Fontane**} Theodor Fontane, *Effi Briest* (1894), last sentence; insel taschenbuch 2131, Inselverlag (1997).
- {**Georgi**} H. Georgi, *Lie Algebras in Particle Physics: From Isospin to Unified Theories*, Frontiers in Physics, vol. 54, Benjamin/Cummings, Reading (1982).
- {**Gradshteyn-Ryzhik**} I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products*, 4th edition, Academic Press, New York (1980).
- {**Handbook**} M. Abramowitz and I. Stegun (eds.), *Handbook of Mathematical Functions*, Dover, New York (1965).
- {**Horn-Johnson**} R. A. Horn and C. R. Johnson, *Matrix Analysis*, Cambridge University Press, Cambridge (1985).
- {**Landau-Lifschitz 1**} L. D. Landau and E. M. Lifschitz, *Course of theoretical physics*, vol. 1, Pergamon Press, Oxford (1978).
- {**Le Bellac**} M. Le Bellac, *Quantum and Statistical Field Theory*, Oxford University Press, Oxford (1991).

- {Lenin}** W. I. Lenin, *What Is to Be Done? Burning Questions of Our Movement* (Russian tr. *Chto delat'?*) (1901). <https://www.marxists.org/archive/lenin/works/1901/witbd/index.htm>
- {Lighthill}** M. J. Lighthill, *Introduction to Fourier Analysis and Generalized Functions* (Cambridge Monographs on Mechanics and Applied Mathematics), Cambridge University Press, Cambridge (1958).
- {Messiah}** Albert Messiah, *Mécanique Quantique*, Dunod, Paris (1959).
- {Messiah 1/2}** A. Messiah, *Quantum Mechanics*, vol. I/II, North Holland, Amsterdam (1965).
- {Muta}** T. Muta, *Foundations of Quantum Chromodynamics – An Introduction to Perturbative Methods in Gauge Theories*, World Scientific, Singapore (1988).
- {Num. Recipes}** W. H. Press, S. A. Teukolsky, W.T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran 77*, 2nd ed., vol. 1, *The Art of Scientific Computing*, Cambridge University Press, Cambridge (1992). **Free**, in Empanel format (<http://www.nr.com/oldverswitcher.html>).
- {Oz}** Amos Oz, *A Tale of Love and Darkness*, translator: Nicolas de Lange, Harcourt (2004)
- {Scheck}** F. Scheck, *Leptons, Hadrons and Nuclei*, North-Holland, Amsterdam (1983).
- {Schiller}** Friedrich Schiller, *Die Verschwörung des Fiesco zu Genua. Ein republikanisches Trauerspiel* (1783).
- {Weiss}** U. Weiss, *Quantum Dissipative Systems*, World Scientific (1999).

Original Publications

References

- [1] D. F. Styer, M. S. Balkin, K. M. Becker, M. R. Burns, C. E. Dudley, S. T. Forth, J. S. Gaumer, M. A. Kramer, D. C. Oertel, L. H. Park, M. T. Rinkoski, C. T. Smith, and T. D. Wotherspoon: “Nine formulations of Quantum Mechanics”, *Am. J. Phys.* **70** (2002), 288.
- [2] R. P. Feynman: “Space-time approach to non-relativistic Quantum Mechanics”, *Rev. Mod. Phys.* **20** (1948), 26.
- [3] P. A. M. Dirac: “The Lagrangian in Quantum Mechanics”, *Phys. Zeit. d. Sowjetunion*, Band 3, Heft 1 (1933).
- [4] J. Schwinger (ed.): “Selected papers on Quantum Electrodynamics”, Dover (1958).
- [5] T. L. Gill and W. W. Zachary: “Constructive representation theory for the Feynman operator calculus”, arXiv: math-ph/0701039.
- [6] I. Daubechies and J. R. Klauder: “Quantum mechanical path integrals with Wiener measures for all polynomial Hamiltonians”, *J. Math. Phys.* **26** (1985), 2239.

- [7] P. A. Horvathy: “The Maslov correction in the semiclassical Feynman integral,” Central Eur. J. Phys. **9** (2011), 1 [arXiv:quant-ph/0702236].
- [8] K. Yeon, K. K. Lee, C. I. Um, T. F. George and L. N. Pandey: “Exact quantum theory of a time-dependent bound quadratic Hamiltonian system”, Phys. Rev. A **48** (1993), 2716.
- [9] I. M. Gel’fand and A. M. Yaglom: “Integration in functional spaces and its applications in Quantum Physics”, J. Math. Phys. **1** (1960), 48 .
- [10] G. V. Dunne and K. Kirsten: “Functional determinants for radial operators”, J. Phys. A **39** (2006), 11915 [arXiv: hep-th/0607066].
- [11] I. H. Duru and H. Kleinert: “Solution of path integral for H atom”, Phys. Lett. B **84** (1979), 30.
- [12] R. Rosenfelder: “Path integrals for potential scattering”, Phys. Rev. A **79** (2009), 012701 [arXiv:0806.3217 [nucl-th]].
- [13] J. Carron and R. Rosenfelder: “A new path-integral representation of the T -matrix in potential scattering”, Phys. Lett. A **375** (2011), 3781 [arXiv:1107.3034 [nucl-th]].
- [14] R. Rosenfelder: ”Scattering Theory with Path Integrals”, J. Math. Phys. **55** (2014), 032106 [arXiv:1302.3419[nucl-th]].
- [15] H. D. I. Abarbanel and C. Itzykson: “Relativistic eikonal expansion”, Phys. Rev. Lett. **23** (1969), 53.
- [16] S. J. Wallace: “ Eikonal expansion”, Ann. Phys. **78** (1973), 190.
- [17] S. Sarkar: “Higher-order terms in the eikonal expansion of the T matrix for potential scattering”, Phys. Rev. D **21** (1980), 3437.
- [18] W. Glöckle, J. Golak, R. Skibiński and H. Witalla: “Exact three-dimensional wave function and the on-shell t matrix for the sharply cut-off Coulomb potential: Failure of the standard renormalization factor”, Phys. Rev. C **79** (2009), 044003 [arXiv:0903.0343 [nucl-th]].
- [19] R. MacKenzie: ”Path integral methods and applications”, arXiv: quant-ph/0004090.
- [20] R. Rosenfelder: ”Quasielastic electron scattering from nuclei”, Ann. Phys. (N.Y.) **128** (1980), 188; erratum: *ibid.* **140** (1982), 203.
- [21] G. Scher, M. Smith and M. Baranger: “Numerical calculations in elementary quantum mechanics using Feynman path integrals”, Ann. Phys. **130** (1980), 290.
- [22] Ch.-Sh. Hsue and J. L. Chern: “Two-step approach to one-dimensional anharmonic oscillators”, Phys. Rev. D **29** (1984), 643.
- [23] M. A. Escobar-Ruiz, E. Shuryak and A. V. Turbiner: ”Three-loop correction to the instanton density. I. The quartic double well potential”, Phys. Rev. D **92** (2015), 025046 [arXiv:1501.03993]
- [24] R. P. Feynman: “Slow electrons in a polar crystal”, Phys. Rev. **97** (1955), 660.
- [25] G. Höhler and A. Müllensiefen: “Störungstheoretische Berechnung der Selbstenergie and der Masse des Polarons”, Z. Phys. **157** (1959), 159.
- [26] M. A. Smondyrev: “Diagrams in the polaron model”, Theor. Math. Phys. **68** (1986), 653.

- [27] R. Rosenfelder: “Perturbation theory without diagrams: The polaron case”, Phys. Rev. E **79** (2009), 016705 [arXiv:0805.4525 [hep-th]].
- [28] R. Rosenfelder and A. W. Schreiber: “Polaron variational methods in the particle representation of field theory: I. General formalism”, Phys. Rev. D **53** (1996), 3337 [arXiv:nucl-th/9504002].
- [29] C. Alexandrou and R. Rosenfelder : “Stochastic solution to highly nonlocal actions: The polaron problem”, Phys. Rep. **215** (1992), 1.
- [30] J. T. Titantah, C. Pierleoni and S. Ciuchi: “Free energy of the Fröhlich polaron in two and three dimensions”, Phys. Rev. Lett. **87** (2001), 206406 [arXiv:cond-math/0010386].
- [31] G.-L. Ingold: “Path integrals and their application to dissipative systems”, in: *Coherent Evolution in Noisy Environments*, Lecture Notes in Physics, vol. 611, pp. 1-53, Springer (2002) [arXiv:quant-ph/0208026].
- [32] A. O. Caldeira and A. J. Leggett: “Quantum tunnelling in a dissipative system”, Ann. Phys. **149** (1983), 374.
- [33] A. Hanke and W. Zwerger: “Density of states of a damped quantum oscillator”, Phys. Rev. E **52** (1995), 6875.
- [34] R. Rosenfelder: “Structure function of a damped harmonic oscillator”, Phys. Rev. C **68** (2003), 034602 [arXiv:nucl-th/0303003].
- [35] Jun-Chen Su and Fu-Hou Zheng: “Correct path-integral formulation of the quantum thermal field theory in the coherent state representation”, Commun. Theor. Phys. **43** (2005), 641 [arXiv: hep-th/0510131].
- [36] J. M. Luttinger: “The asymptotic evaluation of a class of path integrals”, J. Math. Phys. **24** (1983), 2070; **23** (1982), 1011.
- [37] J. Adamowski, B. Gerlach and H. Leschke: “Strong-coupling limit of polaron energy, revisited”, Phys. Lett. **79 A** (1980), 249.
- [38] S. I. Pekar: “Untersuchungen über die Elektronentheorie der Kristalle”, Akademie-Verlag, Berlin (1954).
- [39] E. H. Lieb and L. E. Thomas: “Exact ground state energy of the strong-coupling polaron”, Comm. Math. Phys. **183** (1997), 511.
- [40] T. Tomoda and A. Sevgen: “Path integral approach to nuclear pairing field”, Z. Phys. A **304** (1982) 221.
- [41] H. Kleinert, A. Pelster, B. Kastening and M. Bachmann: “Recursive graphical construction of Feynman diagrams and their multiplicities in ϕ^4 - and in $\phi^2 A$ -theory”, Phys. Rev. E **62** (2000), 1537 [arXiv:hep-th/9907168].
- [42] L. T. Hue, H. T. Hung and H. N. Long: “General formula for symmetry factors of Feynman diagrams”, arXiv:1011.4142 [hep-th].
- [43] P. Kopietz: “Two-loop β -function from the exact renormalization group”, arXiv: hep-th/0007128; (in the published version Nucl. Phys. B **595** (2001), 493 the appendix has been removed!)
- [44] J. D. Walecka: ” A theory of highly condensed matter”, Ann. Phys. **83** (1974), 491.
- [45] B. D. Serot and J. D. Walecka: “The relativistic nuclear many-body problem”, Adv. Nucl. Phys. **16** (1986), 1.

- [46] C. J. Horowitz and B. D. Serot: "Selfconsistent Hartree description of finite nuclei in a relativistic quantum field theory", Nucl. Phys. A **368** (1981), 503.
- [47] S. Coleman and E. Weinberg: "Radiative corrections as the origin of spontaneous symmetry breaking", Phys. Rev. D **7** (1973), 1888.
- [48] Ch. Schubert: "Perturbative quantum field theory in the string inspired formalism", Phys. Rep. **355** (2001), 73.
- [49] M. Reuter, M. G. Schmidt and Ch. Schubert: "Constant external fields in gauge theory and the spin 0, 1/2, 1 path integrals", Ann. Phys. **259** (1997), 313.
- [50] E. S. Fradkin and D. M. Gitman: "Path-integral representation for the relativistic particle propagators and BFV quantization", Phys. Rev. D **44** (1991), 3230.
- [51] C. Alexandrou, R. Rosenfelder and A. W. Schreiber: "Worldline path integral for the massive Dirac propagator: A four-dimensional approach", Phys. Rev. A **59** (1999), 1762.
- [52] R. M. Wilcox: "Exponential operators and parameter differentiation in quantum physics", J. Math. Phys. **8** (1967), 962.
- [53] L. Brink, S. Deser, B. Zumino, P. Di Vecchia and P. Howe: "Local supersymmetry for spinning particles", Phys. Lett. B **64** (1976), 435.
- [54] E. D'Hoker and D. G. Gagné: "Worldline path integrals for fermions with general couplings", Nucl. Phys. B **467** (1996), 297 [arXiv: hep-th/9512080v2].
- [55] F. A. Lunev: "Pure bosonic worldline path integral representation for the fermionic determinant, non-abelian Stokes theorem and quasiclassical approximation in QCD", Nucl. Phys. B **494** (1997), 433 [arXiv: hep-th/9609166].
- [56] K. Fujikawa: "Path-integral measure for gauge-invariant fermion theories", Phys. Rev. Lett. **42** (1979), 1195.
- [57] M. Reuter: "Chiral anomalies and zeta-function regularization", Phys. Rev. D **31** (1985), 1374.
- [58] J. Steinberger: "On the use of subtraction fields and the lifetimes of some types of meson decay", Phys. Rev. **76** (1949), 1180.
- [59] O. Bär and U.-J. Wiese: "Can one see the number of colors?", Nucl. Phys. B **609** (2001), 225.
- [60] G. P. Lepage: "Redesigning Lattice QCD", in: *Perturbative and nonperturbative aspects of quantum field theory*, Schladming 1996, Lecture Notes in Physics, vol. 479, p. 1 - 48, Springer.
- [61] G. Arnold, B. Bunk, T. Lippert and K. Schilling: "Compact QED under scrutiny: it's first order", Nucl. Phys. Proc. Suppl. **119** (2003), 864 [arXiv: hep-lat/0210010].
- [62] Ph. Pechukas: "Time-dependent semiclassical scattering theory. I. Potential scattering", Phys. Rev. **181** (1969) 166
- [63] Th. Mannel, W. Roberts and Z. Ryzak: "A derivation of the heavy quark effective lagrangian from QCD", Nucl. Phys. B **368** (1992) 204.

Exercises for the Lecture "Path Integrals in Quantum Physics"

Exercise 1

Problem 1 : Show that

- a)** the **free propagator** (the matrix element of the time-evolution operator) (1.51) fulfills the Schrödinger equation

$$i\hbar \frac{\partial U_0(b, a)}{\partial t_b} = -\frac{\hbar^2}{2m} \frac{\partial^2 U_0(b, a)}{\partial x_b^2} \quad (\text{P 1.1})$$

- b)** the **free Green function**

$$G_0(b, a) = -\frac{i}{\hbar} \Theta(t_b - t_a) U_0(b, a) \quad (\text{P 1.2})$$

obeys the equation

$$\left(i\hbar \frac{\partial}{\partial t_b} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_b^2} \right) G_0(b, a) = \delta(t_a - t_b) \delta(x_a - x_b). \quad (\text{P 1.3})$$

Show by Fourier transforming Eq. (P 1.2) that

$$G_0(b, a) = \int_{-\infty}^{+\infty} \frac{dE}{2\pi i\hbar} \int_{-\infty}^{+\infty} \frac{dp}{2\pi i\hbar} \frac{1}{E - p^2/(2m) + i0^+} e^{ip \cdot (x_b - x_a)/\hbar - iE(t_b - t_a)/\hbar} \quad (\text{P 1.4})$$

where $i0^+$ denotes a small positive imaginary part which at the end of the calculation is set to zero. Which Green function is obtained when a small *negative* imaginary part is taken?

Problem 2 : Determine the **classical action** for

- a)** a free particle (Lagrange function $L = m\dot{x}^2/2$),
- b)** a harmonic oscillator ($L = m\dot{x}^2/2 - m\omega^2 x^2/2$),
- c)** a harmonic oscillator with an external, time-dependent force ($L = m\dot{x}^2/2 - m\omega^2 x^2/2 - e(t)x$).

Problem 3 : For a **time-dependent potential** $V(x, t)$ the Schrödinger equation for the time-evolution operator reads

$$\frac{\partial \hat{U}(t, t_0)}{\partial t} = -\frac{i}{\hbar} \hat{H}(t) \hat{U}(t, t_0) \quad \text{with} \quad \hat{U}(t_0, t_0) = \hat{1} \quad (\text{P 3.1})$$

and the formal solution is not anymore $\exp\left(-i\hat{H}(t - t_0)/\hbar\right)$ but

$$\hat{U}(t, t_0) = \mathcal{T} \left\{ \exp \left(-i \int_{t_0}^t d\tau \hat{H}(\tau)/\hbar \right) \right\}, \quad (\text{P 3.2})$$

where \mathcal{T} is the time-ordering symbol.

- a)** Show that \hat{U} is unitary if $\hat{H}(t)$ is hermitean.
- b)** Prove the composition law $\hat{U}(t, t_0) = \hat{U}(t, t_1) \hat{U}(t_1, t_0)$.
- c)** Show with that and the usual time-slicing method that the path-integral representation of the matrix elements of \hat{U} retains the given form, i.e. that no time-ordering symbol is necessary.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 2

Problem 4 : Calculate

- a) the **functional derivative** $\frac{\delta S}{\delta x(\sigma)}$ for $S[x] = \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{x}^2(t) - V(x(t)) \right]$,
- b) the second functional derivative $\frac{\delta^2 S}{\delta x(\sigma) \delta x(\sigma')}$ of the action in **a)** and derive the functional Taylor expansion of the action S around the classical trajectory.
- c) Evaluate the functional derivative of the generating functional

$$Z[J] = \int \mathcal{D}x \exp \left(\frac{i}{\hbar} S[x] + \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt x(t) J(t) \right) \quad (\text{P 4.1})$$

w.r.t. the external source $J(\sigma)$.

Problem 5 : In 1932 **Wigner** introduced the **transformation** named after him

$$A_W(x, p) = \int_{-\infty}^{+\infty} dy \left\langle x - \frac{y}{2} \left| \hat{A} \right| x + \frac{y}{2} \right\rangle e^{ip \cdot y / \hbar} \quad (\text{P 5.1})$$

for an arbitrary quantum-mechanical operator \hat{A} . The Wigner transform $A_W(x, p)$ is the form of the quantum-mechanical operator which comes closest to the classical description.

- a) Calculate the Wigner transform of a (local) potential operator $V(\hat{x})$ and of the kinetic energy $T(\hat{p})$.
- b) By using the inverse transformation show that for the classical phase space function $A_W(x, p) = p^m x^n$ Weyl's quantization prescription follows for the quantum-mechanical operator \hat{A} .
- a) Calculate the Wigner transform of the density matrix $\hat{A} = |\psi_n\rangle \langle \psi_n|$ in the ground state ($n = 0$) and first excited state ($n = 1$) of the harmonic oscillator and examine whether these functions are everywhere positive so that they can be interpreted as genuine probabilities.

Problem 6 : Show that for a **classical motion** from (x_a, t_a) to (x_b, t_b) the energy of a particle at the initial point is given by

$$\frac{\partial S_{\text{cl}}}{\partial t_a} \quad (\text{P 6.1})$$

and its momentum by

$$-\frac{\partial S_{\text{cl}}}{\partial x_a} \quad (\text{P 6.2})$$

where $S_{\text{cl}}(x_b, t_b; x_a, t_a)$ is its classical action. Check for the free case and for the harmonic oscillator case.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 3

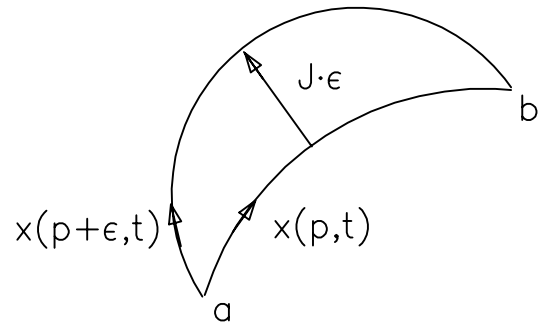
Problem 7 : For a charged particle in a magnetic field $\mathbf{B}(\mathbf{x}) = \text{rot } \mathbf{A}(\mathbf{x})$ the classical Hamilton function is

$$H(\mathbf{p}, \mathbf{x}) = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right)^2. \quad (\text{P 7.1})$$

- a) Starting from the phase-space path integral derive the Lagrange form of the path-integral for the time-evolution operator (propagator) of the particle.
- b) How does the propagator behave under a **gauge transformation** $\mathbf{A}(\mathbf{x}) \rightarrow \mathbf{A}(\mathbf{x}) + \text{grad } \Lambda(\mathbf{x})$?
- c) Show that only the mid-point rule in the discretized form of the path integral gives the correct Schrödinger equation if $\psi(\mathbf{x}, t + \epsilon) = \langle \mathbf{x} | \hat{U}(t + \epsilon, t) | \psi(t) \rangle$ is evaluated for small ϵ .

Problem 8 : Consider the family of (one-dimensional) classical paths leaving the point $x = a$ at time $t = 0$ with momentum p . Show that

$$J(p, t) = \frac{\partial x(p, t)}{\partial p} = \lim_{\epsilon \rightarrow 0} \frac{x(p + \epsilon, t) - x(p, t)}{\epsilon} \quad (\text{P 8.1})$$



- a) fulfills the **Jacobi equation**

$$\frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{x}^2} J \right) + \left[\frac{d}{dt} \left(\frac{\partial^2 L}{\partial x \partial \dot{x}} \right) - \frac{\partial^2 L}{\partial x^2} \right] J = 0 \quad (\text{P 8.2})$$

with $J(p, 0) = 0$, $\partial J(p, t) / \partial t \Big|_{t=0} = 1/m$;

- b) this is identical with the Gel'fand-Yaglom equation for a general quadratic Lagrange function;
- c) at the final point J can be expressed by the classical action $S(x_b, t_b; x_a, t_a)$ (with the help of the result in **Problem 6**) as follows:

$$\frac{1}{J(p, t_b)} = - \frac{\partial^2 S}{\partial x_a \partial x_b}. \quad (\text{P 8.3})$$

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 4

Problem 9 : Consider the 1-dimensional motion of a particle in a harmonic potential. Apply the composition law to (the explicit expression for) the propagator of the harmonic oscillator

$$U^{\text{h.o.}}(x_b, t_b; x_a, t_a) = \int_{-\infty}^{+\infty} dx_c U^{\text{h.o.}}(x_b, t_b; x_c, t_c) U^{\text{h.o.}}(x_c, t_c; x_a, t_a) \quad (\text{P 9.1})$$

and show that it indeed acquires a **Maslov phase** factor

$$-i = e^{-i\frac{\pi}{2}}, \quad (\text{P 9.2})$$

if $T_1 = t_c - t_a < \pi/\omega, T_2 = t_b - t_c < \pi/\omega$ holds but $T_1 + T_2 > \pi/\omega$, i.e. if the particle passes through a focal point in the time between t_a and t_b .

Problem 10* : In the limit $\beta \rightarrow \infty$ also $x_{\text{cl}}(\tau - \tau_0) = a \tanh \frac{\omega}{2}(\tau - \tau_0)$ is a solution of the classical equation of motion for an **instanton in the double-well potential** $V(x) = \frac{m\omega^2}{8a^2}(x^2 - a^2)^2$. Due to time-translation invariance the "position" τ_0 of the instanton is arbitrary.

- a) Derive Eq. (1.332) from Eq. (1.331) for the choice $x_1(\tau_0) = 0$.
- b) Show that the operator

$$\mathcal{O}_V = -m \frac{d^2}{d\tau^2} + V''(x_{\text{cl}}(\tau - \tau_0)), \quad (\text{P 10.1})$$

which describes the quadratic fluctuations around the classical solution, then possesses a **zero eigenvalue** (“zero mode”) with eigenfunction

$$y_0(\tau - \tau_0) = \frac{\text{const.}}{\cosh^2[\omega(\tau - \tau_0)/2]} = A_0 \frac{\partial x_1(\tau)}{\partial \tau_0}. \quad (\text{P 10.2})$$

Determine the normalization constant A_0 from $\langle y_0 | y_0 \rangle = 1$.

- c) Consider the **Gelfand-Yaglom equation** $\mathcal{O}_{V''} f_{\text{GY}} = 0$ with $f_{\text{GY}}(-\beta/2) = 0, \dot{f}_{\text{GY}}(-\beta/2) = 1$ and show that the Wronskian $W = f^{(1)}\dot{f}^{(2)} - f^{(2)}\dot{f}^{(1)}$ of two solutions is a constant.
- d) For finite, large β determine the would-be zero eigenvalue e_0 from the equation

$$Y_0(\tau) = f_{\text{GY}}(\tau) + e_0 \int_{-\beta/2}^{+\beta/2} d\tau' g(\tau, \tau') Y_0(\tau') \quad (\text{P 10.3})$$

where

$$g(\tau, \tau') = \frac{1}{mW} \Theta(\tau - \tau') \left[f^{(1)}(\tau)f^{(2)}(\tau') - f^{(2)}(\tau)f^{(1)}(\tau') \right] \quad (\text{P 10.4})$$

is a Green function: $\mathcal{O}_{V''} g(\tau, \tau') = \delta(\tau - \tau')$ and f_{GY} the solution of the Gel’fand-Yaglom equation with the correct initial conditions. Evaluate e_0 to leading order in $\exp(-\omega\beta)$ by requiring that the l.h.s of Eq. (P 10.3) also vanishes for $\tau = \beta/2$ and by approximating $Y_0(\tau') \simeq f_{\text{GY}}(\tau')$.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 5

Problem 11* : In Feynman’s variational approach for the polaron one obtains for the ground-state energy

$$E_0 \leq E_F = \frac{3}{4v}(v-w)^2 - \frac{\alpha}{\sqrt{\pi}} \int_0^\infty du \frac{e^{-u}}{\mu(u)} \quad (\text{P 11.1})$$

with

$$\mu(u) = \left[\frac{w^2}{v^2}u + \frac{v^2 - w^2}{v^3} (1 - e^{-vu}) \right]^{1/2}. \quad (\text{P 11.2})$$

Here v and w are two variational parameters for the strength ($v^2 = w^2 + 4C/w$) and the retardation of the trial action.

- a) Determine the variational minimum for small coupling constants α by the *ansatz* $v = w(1 + \epsilon)$, where $\epsilon = \mathcal{O}(\alpha)$. Show that the lowest energy $E_F = -\alpha - \alpha^2/81 - \mathcal{O}(\alpha^3)$ is reached for $w = 3$ and $\epsilon = 2\alpha/27$.
- b) Determine the variational minimum for large coupling constants α by the *ansatz* $v \gg w$. Show that the lowest energy $E_F = -\alpha^2/(3\pi)$ is reached for $v = 4\alpha^2/(9\pi)$.

Problem 12 : Show that the **coherent states** of the harmonic oscillator, which can be defined by

$$\hat{a}^\dagger |z\rangle = z |z\rangle \quad (\text{P 12.1})$$

are states of minimal uncertainty: Calculate

$$(\Delta x)^2 \equiv \frac{\langle z | \hat{x}^2 | z \rangle}{\langle z | z \rangle} - \left(\frac{\langle z | \hat{x} | z \rangle}{\langle z | z \rangle} \right)^2 \quad (\text{P 12.2})$$

$$(\Delta p)^2 \equiv \frac{\langle z | \hat{p}^2 | z \rangle}{\langle z | z \rangle} - \left(\frac{\langle z | \hat{p} | z \rangle}{\langle z | z \rangle} \right)^2. \quad (\text{P 12.3})$$

Problem 13 : Prove that

- a) $\det \mathbb{A} = \exp(\text{tr} \ln \mathbb{A})$,
- b) $\frac{\partial}{\partial \lambda} \det \mathbb{A}(\lambda) = \text{Tr} \left(\frac{\partial \mathbb{A}(\lambda)}{\partial \lambda} \mathbb{A}^{-1}(\lambda) \right) \cdot \det \mathbb{A}(\lambda)$,
- c) $\det(\mathbb{A}_0 + g\mathbb{A}_1) = \det(\mathbb{A}_0) \cdot \exp \left\{ \int_0^g dg' \text{Tr} \left[\mathbb{A}_1 (\mathbb{A}_0 + g'\mathbb{A}_1)^{-1} \right] \right\}$.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 6

Problem 14 : Consider a **Grassmann algebra** with one generator ξ . Show that for all analytic functions $f(\xi) = f_0 + f_1\xi$ the Grassmann- δ function is given by

$$\delta(\xi - \xi') = \int d\eta e^{-\eta(\xi - \xi')}, \tag{P 14.1}$$

i.e. that

$$\int d\xi' \delta(\xi - \xi') f(\xi') = f(\xi). \tag{P 14.2}$$

Problem 15 : Determine the partition function

$$Z_\omega(\beta) = \oint_{\text{a.p.}} \mathcal{D}\bar{\xi} \mathcal{D}\xi \exp \left\{ - \int_0^{\hbar\beta} d\tau \left[\bar{\xi}(\tau) \frac{\partial \xi(\tau)}{\partial \tau} + \omega \bar{\xi}(\tau) \xi(\tau) \right] \right\} \tag{P 15.1}$$

for the **fermionic harmonic oscillator**

a) by calculating the functional determinant

$$Z_\omega(\beta) = \mathcal{N} \cdot \text{Det} [\partial_\tau + \omega] \tag{P 15.2}$$

in the space of anti-periodic (“a.p.”) eigenfunctions of the operator $\partial_\tau + \omega$. Hint: Use the product representation (see, e.g. **{Gradshteyn-Ryzhik}**, eq. 1.431.4)

$$\cosh x = \prod_{k=0}^{\infty} \left(1 + \frac{4x^2}{(2k+1)^2\pi^2} \right). \tag{P 15.3}$$

b) Determine the normalization constant \mathcal{N} (as in the bosonic case) by comparing with the special case $\omega = 0$ when using the discretized form

$$Z_{\omega=0}(\beta) = \lim_{N \rightarrow \infty} \prod_{n=0}^N \left(\int d\bar{\xi}_n d\xi_n \right) \exp \left\{ - \sum_{n=1}^N [\bar{\xi}_n (\xi_n - \xi_{n-1})] \right\}. \tag{P 15.4}$$

c) Show that the result implies a negative ground-state energy

$$E_0 = -\frac{1}{2} \hbar\omega \tag{P 15.5}$$

of the fermionic harmonic oscillator which exactly cancels the positive ground-state energy of the (bosonic) harmonic oscillator. Does such a supersymmetry solve the problem of the (nearly) vanishing cosmological constant which frequently is considered as vacuum energy of the universe?

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 7

Problem 16 : Show that the **free energy** $F(\beta)$ of a system defined as

$$F(\beta) = -\frac{1}{\beta} \ln \left\{ \sum_{n=0}^{\infty} e^{-\beta E_n} \right\} \quad (\text{P 16.1})$$

is always smaller than the ground-state energy E_0 and increases monotonically:

$$F(\beta) \geq E_0, \quad F'(\beta) \geq 0 \quad \forall \beta \geq 0. \quad (\text{P 16.2})$$

Problem 17 : Derive the explicit form (2.176) of the interaction-free **one-particle Green function** in the basis which diagonalizes H_0 by solving the differential equation

$$(\partial_\tau + \epsilon_\alpha - \mu) G_0(\alpha, \tau | \alpha', \tau') = \delta_{\alpha\alpha'} \delta(\tau - \tau') \quad (\text{P 17.1})$$

with the boundary condition

$$G_0(\alpha, \beta | \alpha, 0) = \zeta G_0(\alpha, 0 | \alpha, 0), \quad \zeta = \begin{cases} +1 & : \text{bosons} \\ -1 & : \text{fermions} \end{cases}. \quad (\text{P 17.2})$$

Discuss why one has to set $\tau' \rightarrow \tau' + 0^+$, i.e. $\Theta(0) \rightarrow \Theta(-0^+) = 0$ in order to get the correct result for equal times.

Problem 18* : Calculate **Pekar’s constant** for the polaron ground-state energy at large coupling constant α ($E_0 \rightarrow \gamma_P \alpha^2$) from the minimum of the functional

$$\begin{aligned} \gamma_P &= \kappa^2 \min_{(y,y)=1} [\langle T \rangle + \langle V \rangle], \quad (y, y) = \int_0^\infty dr y^2(r) = 1, \quad \langle T \rangle = \int_0^\infty dr \frac{1}{2} y'^2(r), \\ \langle V \rangle &= -\frac{1}{\sqrt{2}\kappa} \int_0^\infty dr y^2(r) \int_0^\infty ds \frac{y^2(s)}{\max(r, s)} = -\frac{\sqrt{2}}{\kappa} \int_0^\infty dr y^2(r) \int_r^\infty ds \frac{1}{s} y^2(s) \end{aligned} \quad (\text{P 18.1})$$

a) with the help of the *ansatz*

$$y(r) = C_1 r e^{-r/a} \quad (\text{P 18.2})$$

b) with the help of the *ansatz*

$$y(r) = C_2 r e^{-r^2/(2b^2)}. \quad (\text{P 18.3})$$

by variation w.r.t. the free parameters a, b and show that the result is independent of the arbitrary scale parameter κ . [Help with the integrals: Use Euler’s integral representation of the Γ -function

$$\Gamma(x) = \int_0^\infty dt t^{x-1} e^{-t} \quad (\text{P 18.4})$$

and the properties $\Gamma(x+1) = x\Gamma(x)$, $\Gamma(1/2) = \sqrt{\pi}$.]

c) Modify the given program for the numerical calculation of γ_P to work with double-precision arithmetic and show that with FTOL = 10^{-8} and NMAX = 12 the more precise value

$$\gamma_P = -0.10851197(2) \quad (\text{P 18.5})$$

is obtained.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 8

Problem 19 : Calculate the divergent integral which in first-order perturbation theory determines the **selfenergy in Φ^4 -theory**

$$\Sigma^{(1)} = i \frac{\lambda}{2} \mu_0^{4-d} \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2 - m^2 + i0^+} \quad (\text{P 19.1})$$

in d dimensions (**dimensional regularization:** 1 time and $d - 1$ space dimensions). Here μ_0 is a mass parameter which one introduces to keep the coupling constant λ dimensionless for all d . In which dimension does this integral converge?

Hint: Use the **Fock-Schwinger representation** for the free propagator

$$\frac{1}{k^2 - m^2 + i0^+} = -i \int_0^\infty dT e^{iT(k^2 - m^2 + i0^+)} \quad (\text{P 19.2})$$

and the usual Gaussian integral (caution: Minkowski metric!). Show that the result

$$\Sigma^{(1)} = \frac{\lambda}{32\pi^2} m^2 \left(\frac{m^2}{4\pi\mu_0^2} \right)^{d/2-2} \Gamma(1 - d/2) \quad (\text{P 19.3})$$

is real. Set the dimension to $d = 4 - 2\epsilon$ and investigate the limit $\epsilon \rightarrow 0$ by using properties of the Gamma function $\Gamma(x)$.

Problem 20 : Consider a system of free scalar particles occurring in N species Φ_i (with equal masses) so that their Lagrangian reads

$$\mathcal{L}_0^{(N)} = \frac{1}{2} \sum_i^N \left[(\partial\Phi_i)^2 - m^2\Phi_i^2 \right]. \quad (\text{P 20.1})$$

Show for the special case $N = 2$ that for positively and negatively charged particles the free Lagrangian can be written as

$$\mathcal{L}_0^{(2)} = |\partial\Phi|^2 - m^2|\Phi|^2 \quad (\text{P 20.2})$$

where Φ is now a **complex field**. Evaluate the free generating functional

$$Z_0[J^*, J] = \int \mathcal{D}\Phi^* \mathcal{D}\Phi \exp \left[i \int d^4x \left(\mathcal{L}_0^{(2)} + J^*(x)\Phi(x) + \Phi^*(x)J(x) \right) \right] \quad (\text{P 20.3})$$

and the corresponding 2-point functions $\langle \Phi^*(x_1)\Phi(x_2) \rangle, \langle \Phi(x_1)\Phi(x_2) \rangle$.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 9

Problem 21 : Consider the Fourier transform of an ordinary function $f(x)$ expanded in moments

$$\tilde{f}(t) := \int dx f(x) e^{itx} = \sum_{n=0}^{\infty} m_n \frac{(it)^n}{n!}, \quad m_n \equiv \int dx x^n f(x), \quad (\text{P 21.1})$$

which all are supposed to exist. For $m_0 \neq 0$ the **cumulant expansion** of $\tilde{f}(t)$ is defined by

$$\tilde{f}(t) =: m_0 \exp \left\{ \sum_{n=1}^{\infty} \lambda_n \frac{(it)^n}{n!} \right\}. \quad (\text{P 21.2})$$

a) Show that the cumulants λ_n can be determined recursively from the moments m_n by

$$\lambda_{n+1} = \frac{m_{n+1}}{m_0} - \sum_{k=0}^{n-1} \binom{n}{k} \frac{m_{n-k}}{m_0} \lambda_{k+1}, \quad n = 0 \text{ (the sum is then empty)}, 1, \dots \quad (\text{P 21.3})$$

and give explicitly the first four (in statistics known under the names “**mean**”, “**variance**”, “**skewness**” and “**excess**”). Hint: Differentiate the moment and cumulant expansion w.r.t. the parameter t and compare respective powers of t .

b) Express the cumulants recursively in terms of the **central moments**

$$c_n := \int dx \left(x - \frac{m_1}{m_0} \right)^n f(x). \quad (\text{P 21.4})$$

c) Generalize the cumulant expansion to the functional representation of the generating functional and list the first four connected Green functions when the action is even ($S[-\Phi] = S[\Phi]$).

Problem 22* : Consider the **effective action**

$$\Gamma[\Phi] = W - \int d^4x J(x) \Phi_{\text{cl}}(x) \quad (\text{P 22.1})$$

of a scalar theory with the generating functional

$$Z[J] = \exp(iW[J]/\hbar) \quad \text{and} \quad \Phi_{\text{cl}}(x) = \frac{\delta W[J]}{\delta J(x)}. \quad (\text{P 22.2})$$

Prove that

$$\frac{\delta \Gamma[\Phi]}{\delta \Phi_{\text{cl}}(x)} = -J(x) \quad (\text{P 22.3})$$

and

$$\delta^4(x-y) = - \int d^4z \frac{\delta^2 \Gamma}{\delta \Phi_{\text{cl}}(z) \delta \Phi_{\text{cl}}(y)} \frac{\delta^2 W}{\delta J(z) \delta J(y)}. \quad (\text{P 22.4})$$

In momentum space the 2-point function can be written as $G^{(2)}(p) = i(p^2 - m^2 - \Sigma(p))^{-1}$. Show thereby that $\Gamma^{(2)}(p)$ gives the selfenergy $\Sigma(p)$ as sum of all one-particle irreducible contributions to the 2-point function.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 10

Problem 23* : Consider charged scalar particles described by the Lagrangian

$$\mathcal{L}_1 = |\partial\Phi|^2 - (m^2 + 2mV(x)) |\Phi|^2, \tag{P 23.1}$$

where $V(x)$ is an external potential.

a) Show with the help of the *ansatz*

$$\Phi(x_0 = t, \mathbf{x}) = \frac{1}{\sqrt{2m}} e^{-imt} \varphi(t, \mathbf{x}), \tag{P 23.2}$$

that in the limit $m \rightarrow \infty$ the action becomes the one of a non-relativistic system of particles in the external potential $V(t, \mathbf{x})$.

b) Calculate the exact generating functional for this system and show that the 2-point function (the propagator) is given by

$$\langle \Phi^*(x_2)\Phi(x_1) \rangle \equiv G_2(x_2, x_1) = i \left\langle x_2 \left| \frac{1}{-\partial^2 - m^2 - 2mV(x) + i0^+} \right| x_1 \right\rangle. \tag{P 23.3}$$

c) By using the **Fock-Schwinger representation**

$$\frac{1}{\hat{A} + i0^+} = -i\kappa \int_0^\infty dT \exp(i\kappa T \hat{A}), \quad \kappa > 0 \tag{P 23.4}$$

show that $G(x_2, x_1)$ can be written like a non-relativistic path integral:

$$G_2(x_2, x_1) = \frac{1}{2m} \int_0^\infty dT e^{-imT/2} \int_{x(0)=x_1}^{x(T)=x_2} \mathcal{D}x(\tau) e^{iS[x(\tau)]} \tag{P 23.5}$$

$$S[x(t)] = \int_0^T d\tau \left[-\frac{m}{2} \dot{x}(\tau)^2 + V(x(\tau)) \right]. \tag{P 23.6}$$

The paths $x_\mu(\tau)$ are now parametrized by the proper time τ which runs from 0 to T . Subsequently one has to integrate over T with the weight $\exp(-imT/2)$ (**worldline representation**).

Problem 24* : Verify

$$F \left(\frac{1}{i} \frac{\partial}{\partial x} \right) \exp \left(-\frac{i}{2} ax^2 \right) = \exp \left(-\frac{i}{2} ax^2 \right) \exp \left(-\frac{i}{2} a \frac{\partial^2}{\partial y^2} \right) F(y) \Big|_{y=ax}. \tag{P 24.1}$$

Hint: Use the Fourier transform $F(y) = \int_{-\infty}^{+\infty} dt \tilde{F}(t) \exp(-ity)/(2\pi)$ together with the fact that $\exp(t\partial/\partial x) f(x) = f(x+t)$ gives a shift of argument.

Generalizing that to functional derivatives show that the generating functional of a interacting scalar theory may be written as

$$Z[J] = \text{const.} \exp \left[-\frac{i}{2} (J, \Delta_F J) \right] \left\{ \exp \left[\frac{i}{2} \left(\frac{\delta}{\delta \varphi}, \Delta_F \frac{\delta}{\delta \varphi} \right) \right] \exp \left(-i \int d^4x V(\varphi) \right) \right\}_{\varphi=\Delta_F J} \tag{P 24.2}$$

where $\Delta_F(k) = 1/(k^2 - m^2 + i0^+)$ is the free propagator. Check in Φ^4 -theory whether the first correction to the free generating functional $\omega_1[J]$ (Eq. (3.28)) is obtained from this representation.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 11

Problem 25 : Consider, as in **Problem 20**, scalar particles which exist in N species Φ_i (with the same mass) but now have a self-interaction

$$\mathcal{L}^{(N)} = \frac{1}{2} \sum_i^N \left[(\partial\Phi_i)^2 - m^2 \Phi_i^2 \right] - \frac{\lambda}{4!} \left(\sum_i^N \Phi_i^2 \right)^2. \quad (\text{P 25.1})$$

(Since the action is invariant under a orthogonal transformation in the N -dimensional space of fields. this is called a “**O(N)-symmetric Φ^4 -theory**” in theoretical parlance).

In addition to the usual sources $J_i(x)$ introduce a source $K(x)$ which couples to $\sum_i^N \Phi_i^2$:

$$Z[J_i, K] := \left(\prod_{i=1}^N \int \mathcal{D}\Phi_i \right) \exp \left\{ i \int d^4x \left[\mathcal{L}^{(N)} - \frac{1}{2} K(x) \sum_i^N \Phi_i^2(x) + \sum_i^N J_i(x) \Phi_i(x) \right] \right\} \quad (\text{P 25.2})$$

a) Show that the generating functional of the interacting theory is given by

$$Z[J_i] = \exp \left(\frac{i\lambda}{6} \int d^4x \frac{\delta^2}{\delta K(x)^2} \right) Z_0[J_i, K] \Big|_{K=0}. \quad (\text{P 25.3})$$

b) Prove that

$$Z_0[J_i, K] = \text{const.} \exp \left(-\frac{i}{2} \sum_i^N \langle J_i | \mathcal{O}_K^{-1} | J_i \rangle - \frac{N}{2} \text{tr} \ln \mathcal{O}_K \right) \equiv e^{iW_0[J_i, K]} \quad (\text{P 25.4})$$

with $\mathcal{O}_K = -\partial^2 - m^2 - K$.

c) Show that the first-order correction for the generating functional $Z[J_i]$ now is

$$\omega_1[J_i] = \frac{i}{6} \int d^4x \left[i \frac{\delta^2 W_0}{\delta K(x)^2} - \left(\frac{\delta W_0}{\delta K(x)} \right)^2 \right]_{K=0}. \quad (\text{P 25.5})$$

Determine with that the symmetry factors for the individual first-order graphs depending on the number N of components of the field Φ_i .

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 12

Problem 26 : a) Consider the free Lagrangian (3.58) for a **massive spin-1 particle** (vector particle) $V_\mu(x)$. Evaluate the path integral for the free generating functional

$$\begin{aligned} Z_0[J_\mu] &= \int \prod_\mu \mathcal{D}V_\mu \exp \left\{ i \int d^4x [\mathcal{L}_0^V + J_\mu(x)V^\mu(x)] \right\} \\ &= \text{const.} \exp \left\{ -\frac{i}{2} \int d^4x d^4y J_\mu(x) D_V^{\mu\nu}(x-y) J_\nu(y) \right\}. \end{aligned} \quad (\text{P 26.1})$$

As in the scalar case determine the propagator by transforming into momentum space and thereby verify Eq. (3.59).

b) Do the same for the **massless** photon propagator in a covariant gauge with gauge fixing parameter λ given by

$$\Delta_{\mu\nu}(x, y) = \left\langle x \left| \left[g^{\mu\nu} \square - \left(1 - \frac{1}{\lambda} \right) \partial^\mu \partial^\nu \right]^{-1} \right| y \right\rangle. \quad (\text{P 26.2})$$

Problem 27 : Generalize **Noether’s theorem** derived in **chapter 1.8** from quantum mechanics to field theory: Assume that the Lagrangian $\mathcal{L}(\Phi, \partial_\mu \Phi)$ of a theory is invariant under an infinitesimal transformation

$$\Phi(x) \longrightarrow \Phi(x) + \alpha \Delta\Phi(x), \quad \alpha = \text{const.} \implies \mathcal{L} \longrightarrow \mathcal{L} + \alpha \partial_\mu \Lambda^\mu \quad (\text{P 27.1})$$

up to a total derivative. As in Eq. (1.280) show then by a transformation with a x -dependent parameter $\alpha(x)$ that there exists a conserved current, i.e. that

$$\partial_\mu \langle J^\mu \rangle = \mathcal{N} \int \mathcal{D}\Phi \partial_\mu \left\{ \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} \Delta\Phi - \Lambda^\mu \right\} e^{iS[\Phi]} = 0 \quad (\text{P 27.2})$$

holds.

a) For complex fields, in particular, derive this current from the invariance under the transformation

$$\Phi \longrightarrow e^{i\alpha} \Phi, \quad \Phi^* \longrightarrow \Phi^* e^{-i\alpha} \quad (\text{P 27.3})$$

for the following theories:

a1) A charged scalar field with the Lagrangian (3.56)

a2) A free Dirac field with the Lagrangian(3.60)

a3)* The nucleons in the Walecka model with Lagrangian (3.65a)

a4) A non-relativistic theory in which the particles interact via a *local* two-particle potential $\langle \mathbf{x}'_1, \mathbf{x}'_2 | \hat{V} | \mathbf{x}_1, \mathbf{x}_2 \rangle = V(\mathbf{x}_1 - \mathbf{x}_2) \delta(\mathbf{x}_1 - \mathbf{x}'_1) \delta(\mathbf{x}_2 - \mathbf{x}'_2)$ (Lagrangian (2.131) and (2.107)).

b) Consider for simplicity again a neutral scalar field $\Phi(x)$. Under the shift $x_\mu \longrightarrow x_\mu + a_\mu$ (a_μ constant) the action is invariant, i.e. the Lagrangian changes by a total derivative. For an infinitesimal shift calculate this total derivative and $\Delta\mathcal{L}$ from the field change $\Delta\Phi(x) = a_\mu \partial^\mu \Phi(x)$. Determine from the invariance the conserved energy-momentum tensor as

$$T^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial(\partial_\nu \Phi)} \partial^\mu \Phi - g^{\mu\nu} \mathcal{L}. \quad (\text{P 27.4})$$

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 13

Problem 28* : Consider a Dirac particle moving in external scalar and vector potentials

$$\mathcal{L} = \bar{\Psi} (i\mathcal{D} - M^*) \Psi, \quad D_\mu = \partial_\mu + iA_\mu(x), \quad M^*(x) := M + U_S(x). \quad (\text{P 28.1})$$

Given a constant four-velocity v_μ ($v^2 = 1$) of the system one can decompose

$$\phi(x) := \frac{1}{2} (1 + \not{v}) e^{iMv \cdot x} \Psi(x), \quad \chi(x) := \frac{1}{2} (1 - \not{v}) e^{iMv \cdot x} \Psi(x) \quad (\text{P 28.2})$$

$$D_\mu = v_\mu (v \cdot D) + D_\mu^\perp, \quad D_\mu^\perp = (g_{\mu\nu} - v_\mu v_\nu) D^\nu. \quad (\text{P 28.3})$$

a) Prove

$$\not{v}\phi = \phi, \quad \not{v}\chi = -\chi, \quad [\mathcal{D}^\perp, \not{v}]_+ = 0. \quad (\text{P 28.4})$$

Hint: Use

$$\gamma_\mu \gamma_\nu = \frac{1}{2} [\gamma_\mu, \gamma_\nu]_+ + \frac{1}{2} [\gamma_\mu, \gamma_\nu]_- = g_{\mu\nu} - i\sigma_{\mu\nu} \quad (\text{P 28.5})$$

with $\sigma_{\mu\nu} := \frac{i}{2} [\gamma_\mu, \gamma_\nu]_-$.

b) With these properties show that the action takes the form

$$S[\phi, \chi] = \int d^4x \left[\bar{\phi} (iv \cdot D + M - M^*) \phi - \bar{\chi} (iv \cdot D + M + M^*) \chi + \bar{\chi} i\mathcal{D}^\perp \phi + \bar{\phi} i\mathcal{D}^\perp \chi \right]. \quad (\text{P 28.6})$$

In the heavy-mass (non-relativistic) limit integrate out the ”small” component χ and expand in inverse powers of M .

c) Take the system at rest, i.e. $v_\mu = (1, \mathbf{0})$, and specialize to a situation where there is no preferred direction (e.g. a spherical or unpolarized system), i.e. $A_\mu(x) = (U_V(\mathbf{x}), \mathbf{0})$. Assume time-independent potentials depending only on $r = |\mathbf{x}|$. Show that in leading order one obtains a **non-relativistic Hamiltonian** with a **central potential** $V_c(r)$ and a **spin-orbit potential** V_{LS} given by

$$V_c(r) = U_V(r) + U_S(r), \quad V_{LS} = \frac{1}{2M^2} \frac{1}{r} \frac{d}{dr} \left[U_S(r) + U_V(r) \right] \mathbf{L} \cdot \mathbf{S} \quad (\text{P 28.7})$$

where $\mathbf{L} = \mathbf{x} \times \nabla/i$ is the orbital momentum and $\mathbf{S} = \vec{\sigma}/2$ the spin of the particle.

Hint: Use

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix} \quad (\text{P 28.8})$$

and the following relation for the Pauli matrices $\vec{\sigma}$

$$\vec{\sigma} \cdot \mathbf{a} \vec{\sigma} \cdot \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + i\vec{\sigma} \cdot (\mathbf{a} \times \mathbf{b}). \quad (\text{P 28.9})$$

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 14

Problem 29 : Evaluate – by Fourier transformation in d dimensions – the **free propagator in x -space**

a) for a scalar particle (use Eq. (3.20))

b) for a photon in covariant gauge with gauge fixing parameter λ (use Eq. (3.139)).

As in **Problem 19**) one may utilize the Schwinger representation for the individual denominators and the Gaussian integral in Minkowski space. How do these propagators behave if the relative space-time distance becomes small or large?

Problem 30* : Derive the full (interacting) propagator of a electron by functional differentiation of the generating functional of QED and show that one obtains

$$\bar{G}_2(p) = \int d^4(x-y) e^{-ip \cdot (x-y)} \int \mathcal{D}A \langle x | \mathcal{O}^{-1} | y \rangle \text{Det } \mathcal{O} e^{iS_0[A]}, \quad \mathcal{O} = i\not{\partial} - e\not{A}(x) - m + i0^+ \quad (\text{P 30.1})$$

with $S_0[A]$ as photon action.

The **Bloch-Nordsieck approximation** for the interacting electron propagator consists of neglecting the determinant in the path integral (which describes vacuum polarization) and of replacing the Dirac matrices by a constant four-vector

$$\gamma_\mu \longrightarrow v_\mu \equiv \frac{p_\mu}{m_{\text{phys}}}, \quad (\text{P 30.2})$$

such that the relation $\not{p} = m_{\text{phys}}$ is conserved on the mass shell.

a) Use again the Schwinger representation to show that

$$\exp \left[iT (iv \cdot \partial - ev \cdot A(x) - m) \right] = \exp \left[iT (iv \cdot \partial - m) \right] \cdot \exp \left[-ie \int_0^T d\tau u \cdot A(x + v\tau) \right]. \quad (\text{P 30.3})$$

With this result perform the functional integration over the photon field and prove

$$\bar{G}_2(p) \simeq \bar{G}_2^{\text{BN}}(p) = \int_0^\infty dT \exp [i (v \cdot p - m) T + X(T)] \quad (\text{P 30.4})$$

where

$$X(T) = -i \frac{e^2}{2} \int_0^T d\tau d\tau' v^\mu v^\nu \Delta_{\mu\nu} (v(\tau - \tau')) \quad (\text{P 30.5})$$

is determined by the photon propagator $\Delta_{\mu\nu}(x-y)$ in x -space.

b) Calculate $X(T)$ in dimensional regularization ($e^2 \rightarrow e^2 \mu_0^{4-d}$) by using the result in **Problem 29 b)** in $d = 4 - 2\epsilon$ dimensions. Expand the result up to order ϵ^0 and show thereby

$$\bar{G}_2^{\text{BN}}(p) = \int_0^\infty dT \exp \left[i \frac{p^2 - m^2}{m} T + \kappa \ln \mu_0 T + c \right] = iZ_2 \frac{m^{1+2\kappa}}{(p^2 - m^2 + i0^+)^{1+\kappa}}. \quad (\text{P 30.6})$$

Determine Z_2, m in this approximation and show that the exponent κ depends on the gauge fixing parameter λ . Show that the $\ln T$ -dependence in the proper-time integral and accordingly the essential singularity of the electron propagator at $p^2 = m_{\text{phys}}^2$ has its origin in the fact that the photons are massless.

Problems for the Lecture “Path Integrals in Quantum Physics”

Exercise 15

Problem 31* : To quantize a gauge theory one needs to fix the gauge and to introduce Faddeev-Popov ghosts which take away unphysical degrees of freedom. Show that the Lagrangian (3.146a)

$$\mathcal{L} = \mathcal{L}_f + \mathcal{L}_g + \mathcal{L}_{gauge\ fix} + \mathcal{L}_{FP}, \quad \mathcal{L}_{gauge\ fix} = \frac{\lambda}{2} B^a B^a - B^a \partial \cdot A^a \quad (\text{P 31.1})$$

of a non-abelian gauge theory with covariant gauge fixing, Faddeev-Popov ghosts and auxiliary field B^a is invariant under the **Becchi-Rouet-Stora-Tyutin (BRST) transformation**:

$$\begin{aligned} \delta A_\mu^a &= \omega (D^\mu \chi)^a, & \delta \psi &= ig \omega \chi^a T^a \psi \\ \delta \bar{\chi}^a(x) &= \omega B^a, & \delta \chi^a &= -\frac{g}{2} \omega f^{abc} \chi^b \chi^c, & \delta B^a &= 0 \end{aligned} \quad (\text{P 31.2})$$

with a constant Grassmann-valued parameter ω . Show first that the BRST transformation is a special, local gauge transformation with the parameter $\Theta^a(x) = \omega \chi^a(x)$. Calculate then the variation of $D_\mu^{ab} \chi^b$ and with that the variation of $\mathcal{L}_{gauge} + \mathcal{L}_{FP}$.

Hint: Use the Jacobi identity for the structure constants

$$f^{ade} f^{bcd} + f^{bde} f^{cad} + f^{cde} f^{abd} = 0. \quad (\text{P 31.3})$$

Problem 32* : Calculate the **free 2-point function on a Euclidean space-time lattice**.

a) Verify Eq. (3.247) for a **scalar field**.

Hint: Calculate first (as in the continuum) the generating functional

$$Z_0(J_l) = \prod_k \left(\int d^4 \Phi_k \right) \exp \left[-S_E^{(0)}(\Phi) + \sum_l J_l \Phi_l \right] \quad (\text{P 32.1})$$

with the ($\lambda = 0$)-action from Eq. (3.244) by Gaussian integration and then the 2-point function by differentiation w.r.t. the external source. For the inversion of the kernel K , which determines the quadratic part of the action, use the Fourier representation

$$K(l-l') = a^4 \int_{-\pi/a}^{+\pi/a} \frac{d^4 k}{(2\pi)^4} \tilde{K}(k) e^{ik \cdot (l-l')a}. \quad (\text{P 32.2})$$

b) Derive Eq. (3.250) for a **fermionic field**. In doing so, use the Euclidean action

$$S_E[\bar{\psi}, \psi] = \int d^4 x \bar{\psi}(x) \left[\sum_\mu \gamma_\mu^E \partial_\mu + m \right] \psi(x), \quad (\text{P 32.3})$$

with the (Hermitean) Euclidean Dirac matrices γ_μ^E (satisfying $[\gamma_\mu^E, \gamma_\nu^E]_+ = 2\delta_{\mu\nu}$) and the naive discretization of the derivative

$$\partial_\mu \psi(n) = \frac{1}{2a} [\psi(n+\mu) - \psi(n-\mu)]. \quad (\text{P 32.4})$$

Solutions for the Problems in "Path Integrals in Quantum Physics"

Note: These are only **sketches** of the solutions – straightforward calculational details are omitted.

Problem 1:

a) Perform the differentiations in the explicit form (1.51).

b) When doing the same for the free Green function there is now an additional term

$$\left[\frac{\partial}{\partial t_b} \Theta(t_b - t_a) \right] U_0(x_b, t_b; x_a, t_a) = \delta(t_b - t_a) U_0(x_b, t_b; x_a, t_b) = \delta(t_b - t_a) \delta(x_b - x_a), \quad (\text{S } 1.1)$$

since $U(x_b, t_b; x_a, t_b) = \langle x_b | \hat{U}(t_b, t_b) | x_a \rangle = \langle x_b | x_a \rangle = \delta(x_b - x_a)$. Alternatively, one can use the fact that

$$\lim_{a \rightarrow \infty} \sqrt{\frac{a}{\pi}} e^{-a(x_b - x_a)^2} = \delta(x_b - x_a) \quad (\text{S } 1.2)$$

with $a = -im/(2\hbar(t_b - t_a))$ is a (well-known) representation of Dirac's δ -function.

The inverse Fourier transform of $G_0(x = x_b - x_a, T = t_b - t_a)$ is

$$\begin{aligned} \tilde{G}_0(E, p) &= \int_{-\infty}^{+\infty} dT dx \left(-\frac{i}{\hbar} \right) \Theta(T) \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left(\frac{im}{2\hbar T} x^2 \right) e^{-ip \cdot x / \hbar + iET / \hbar} = \int_0^{+\infty} dT \exp\left[\frac{i}{\hbar} \left(E + i\epsilon - \frac{p^2}{2m} \right) T \right] \\ &= \frac{1}{E - p^2/(2m) + i\epsilon} \end{aligned} \quad (\text{S } 1.3)$$

where the Gaussian x -integral has been performed first and the T -integral after adding a small positive imaginary part $i\epsilon$ for convergence at the upper limit of the integral. The sign of this imaginary part determines whether one has forward or backward propagation in time: By closing the integration contour in the upper and lower E -plane, respectively, one finds from the theorem of residues

$$\int_{-\infty}^{+\infty} dE \frac{1}{E - p^2/(2m) \pm i\epsilon} e^{-iET/\hbar} = \mp 2\pi i \Theta(\pm T) e^{-ip^2 T / (2m\hbar)}. \quad (\text{S } 1.4)$$

Problem 2:

a) The classical trajectory obeying the boundary conditions is a straight-line path $x(t) = x_a + (x_b - x_a)(t - t_a)/(t_b - t_a)$. Since the velocity is constant one obtains

$$S_{\text{cl}}^{\text{free}} = \int_{t_a}^{t_b} dt \frac{m}{2} \dot{x}^2 = \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}. \quad (\text{S } 2.1)$$

b) The solution of the classical equation of motion $\ddot{x} + \omega^2 x = 0$ may be written as any combination of $\sin \omega t$ and $\cos \omega t$ but taking

$$x_{\text{cl}}(t) = A \sin[\omega(t_b - t)] + B \sin[\omega(t - t_a)] \quad (\text{S } 2.2)$$

has the advantage that the boundary conditions determine the coefficients easily: $A = x_a / \sin \omega T$, $B = x_b / \sin \omega T$, ($T \equiv t_b - t_a$). Inserting that into the expression for the action, using trigonometric identities ($\sin 2x = 2 \sin x \cos x$, $\cos(x + y) = \cos x \cos y - \sin x \sin y$) gives

$$S_{\text{cl}}^{\text{h.o.}} = \frac{m}{2} \omega^2 \int_{t_a}^{t_b} dt \left\{ A^2 \cos[2\omega(t_b - t)] + B^2 \cos[2\omega(t - t_a)] - 2AB \cos[\omega(t_a + t_b - 2t)] \right\}. \quad (\text{S } 2.3)$$

Performing the integrations and inserting the values for the coefficients A, B one obtains with little algebra

$$S_{\text{cl}}^{\text{h.o.}} = \frac{m\omega}{2 \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right], \quad (\text{S } 2.4)$$

i.e. Eq. (1.64).

c) The general solution of the equation of motion

$$\ddot{x}_{\text{cl}}(t) + \omega^2 x_{\text{cl}}(t) = -\frac{e(t)}{m} \quad (\text{S } 2.5)$$

is a particular solution + the general solution of the homogenous equation. A particular solution is obtained by Fourier transformation $x(t) = \int_{-\infty}^{+\infty} dE \tilde{x}(E) \exp(iEt)$ etc. as

$$\tilde{x}(E)_{\text{part}} = -\mathcal{P} \frac{\tilde{e}(E)/m}{\omega^2 - E^2} \implies x_{\text{part}}(t) = -\int_{-\infty}^{+\infty} d\tau \frac{e(\tau)}{m} \frac{\sin \omega|t - \tau|}{2\omega}. \quad (\text{S } 2.6)$$

Here \mathcal{P} denotes the principal value which may be chosen to get a real particular solution (one also could take the $\pm i0^+$ -prescription in the denominator but this would render the particular solution complex which is then compensated by a complex homogeneous solution). Since one is only considering the time evolution in the interval $[t_a, t_b]$ one may cut off $e(\tau)$ for $\tau < t_a$ and $\tau > t_b$. Indeed, $g(t - \tau) := \sin[\omega|t - \tau|]/(2\omega)$ is a Green function of the harmonic oscillator obeying $\ddot{g} + \omega^2 g = \delta(t - \tau)$. The calculational effort is reduced by writing $g(t - \tau) = \tilde{g}(t - \tau) - \sin[\omega(t - \tau)]/(2\omega)$ and realizing that the last term just leads to a modification of the homogenous solution. In other words: One can use the Green function $\tilde{g}(t - \tau) = \Theta(t - t_a) \sin[\omega(t - \tau)]/\omega$ and take

$$x_{\text{cl}}(t) = A \sin \omega(t_b - t) + B \cos \omega(t - t_a) - f(t), \quad f(t) := \int_{t_a}^t d\tau \frac{e(\tau)}{m} \frac{\sin \omega(t - \tau)}{\omega} \quad (\text{S } 2.7)$$

as *ansatz* for the classical solution of the forced harmonic oscillator (it can be verified that it also fulfills the equation of motion (S 2.5)). Here the homogenous solution has been written again in such a way that the boundary conditions are easily implemented: $A = x_a/\sin \omega T$, $B = (x_b + f(t_b))/\sin \omega T$. Note that use of the (less symmetric) Green function \tilde{g} implies $f(t_a) = \dot{f}(t_a) = 0$, i.e. generates less terms for the coefficients A, B . It is now a straight-forward, albeit tedious calculational task to evaluate the classical action by inserting Eq. (S 2.7) into the corresponding expression and performing the time integrations when possible. Some simplification arises if the equation of motion (S 2.5) is used after an integration by parts

$$\begin{aligned} S_{\text{cl}} &= \frac{m}{2} x_{\text{cl}}(t) \dot{x}_{\text{cl}}(t) \Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} dt \left[\frac{m}{2} x_{\text{cl}}(t) \ddot{x}_{\text{cl}}(t) + \frac{m}{2} \omega^2 x_{\text{cl}}^2(t) + e(t) x_{\text{cl}}(t) \right] = \frac{m}{2} \left[x_{\text{cl}}(t_b) \dot{x}_{\text{cl}}(t_b) - x_{\text{cl}}(t_a) \dot{x}_{\text{cl}}(t_a) \right] - \int_{t_a}^{t_b} dt \frac{e(t)}{2} x_{\text{cl}}(t) \\ &= \frac{m}{2 \sin \omega T} x_b \left[-x_a \omega + (x_b + f(t_b)) \omega \cos \omega T - \dot{f}(t_b) \sin \omega T \right] - \frac{m}{2 \sin \omega T} x_a \left[-x_a \omega \cos \omega T + (x_b + f(t_b)) \omega \right] \\ &\quad - \frac{1}{2 \sin \omega T} \int_{t_a}^{t_b} dt e(t) \left\{ x_a \sin[\omega(t_b - t)] + (x_b + f(t_b)) \sin[\omega(t - t_a)] - f(t) \sin \omega T \right\}. \end{aligned} \quad (\text{S } 2.8)$$

It is seen that the terms which do not contain the external force $e(t)$ (or $f(t)$) add up to the classical harmonic oscillator action (S 2.4). The terms linear in $e(t)$ are

$$\frac{m\omega}{2 \sin \omega T} x_b f(t_b) \omega \cos \omega T - \frac{m}{2} x_b \dot{f}(t_b) - \frac{m\omega}{2 \sin \omega T} f(t_b) - \frac{1}{2 \sin \omega T} \int_{t_a}^{t_b} dt e(t) \left[x_a \sin[\omega(t_b - t)] + x_b \sin[\omega(t - t_a)] \right]. \quad (\text{S } 2.9)$$

Using the definition of $f(t)$ in Eq. (S 2.7) this can be brought into the form $-\int_{t_a}^{t_b} dt e(t) \left\{ x_a \sin[\omega(t_b - t)] + x_b \sin[\omega(t - t_a)] \right\} / \sin \omega T$, in agreement with the corresponding term in Eq. (1.98). Finally the term quadratic in $e(t)$ is

$$-\frac{1}{2 \sin \omega T} \int_{t_a}^{t_b} dt e(t) \left\{ f(t_b) \sin[\omega(t - t_a)] - f(t) \sin \omega T \right\} =: -\frac{1}{2m\omega \sin \omega T} \int_{t_a}^{t_b} dt e(t) \int_0^t d\tau e(\tau) G(t, \tau, T) \quad (\text{S } 2.10)$$

with

$$G(t, \tau, T) = \sin[\omega(t_b - t)] \sin[\omega(\tau - t_a)] + \sin[\omega(t_b - \tau)] \sin[\omega(t - t_a)] - \sin \omega T \sin[\omega(t - \tau)]. \quad (\text{S } 2.11)$$

Here the relation $\int_{t_a}^{t_b} dt d\tau F(t, \tau) = \int_{t_a}^{t_b} dt \int_{t_a}^t d\tau [F(t, \tau) + F(\tau, t)]$ and the definition (S 2.7) have been used. Rewrite this in terms of the variables $x = \omega(t - t_a)$, $y = \omega(\tau - t_a)$, $z = \omega T$ as $G(x, y, z) = \sin(z - x) \sin y + \sin(z - y) \sin x - \sin z \sin(x - y)$ and use the addition theorems for the trigonometric functions. This leads to

$$\begin{aligned} G(x, y, z) &= 2 \sin z \sin y \cos x - 2 \cos z \sin x \sin y = 2 \sin y (\sin z \cos x - \cos z \sin x) = 2 \sin y \sin(z - x) \\ &\equiv 2 \sin[\omega(t_b - t)] \sin[\omega(\tau - t_a)], \end{aligned} \quad (\text{S } 2.12)$$

i.e. to the last term of Eq. (1.98).

Problem 3:

a) From Eq. (P 3.1) one finds for $\hat{H}^\dagger(t) = \hat{H}(t)$

$$i\hbar \frac{\partial}{\partial t} \left(\hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) \right) = \left[\hat{H}(t), \hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) \right], \quad (\text{S } 3.1)$$

for which $\hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) = \text{const.}$ is a solution. From the initial condition $\hat{U}(t_0, t_0) = \hat{1}$ one determines that $\hat{U}^\dagger \hat{U} = 1$. Similarly for $\hat{U} \hat{U}^\dagger = 1$. Conversely, if \hat{U} is unitary then $\hat{U}^{-1} = \hat{U}^\dagger$ and $\hat{H}^\dagger = (i\hbar \partial_t \hat{U}) \hat{U}^\dagger = -i\hbar \hat{U} \partial_t \hat{U}^\dagger = i\hbar (\partial_t \hat{U}) \hat{U}^\dagger - i\hbar \partial_t (\hat{U} \hat{U}^\dagger) = i\hbar (\partial_t \hat{U}) \hat{U}^\dagger = \hat{H}$, i.e. \hat{H} is hermitean.

b) $\hat{U}(t, t_1) \hat{U}(t_1, t_0)$ is a solution of the Schrödinger equation (P 3.1). For it to be equal to $\hat{U}(t, t_0)$ for any value of t , it is sufficient that it be equal for a particular value of t , say $t = t_1$ which is obvious because then the first factor $\hat{U}(t_1, t_1) = \hat{1}$.

c) Use of the composition law allows to write the time-sliced time-evolution operator as in Eq. (1.19): $\hat{U}(t_b, t_a) = \lim_{N \rightarrow \infty} \prod_{k=1}^N \hat{U}(t_k, t_{k-1})$, ($t_k = t_a + k\epsilon$, $\epsilon = (t_b - t_a)/N$). Instead of Eq. (1.20) we now have for small time-steps $\hat{U}(t_k, t_{k-1}) \simeq \exp[-i\epsilon \hat{T}/\hbar] \exp[-i\epsilon V(\hat{x}, t_{k-1})/\hbar]$. Proceeding as before we end up with the (slightly generalized) Lagrange form (1.29) of the path integral

$$\begin{aligned} U(x_b, t_b; x_a, t_a) &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{N/2} \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1} \cdot \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{j=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j, t_j) \right] \right\} \\ &\equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{x}^2 - V(x, t) \right] \right\}. \end{aligned} \quad (\text{S } 3.2)$$

Problem 4:

a) Applying the chain rule gives

$$\frac{\delta S}{\delta x(\sigma)} = \int_{t_a}^{t_b} dt \left[m\dot{x}(t) \frac{\delta \dot{x}(t)}{\delta x(\sigma)} - V'(x(t)) \frac{\delta x(t)}{\delta x(\sigma)} \right]. \quad (\text{S } 4.1)$$

The last functional derivative is $\delta(t - \sigma)$, while the first one may be written as $\frac{d}{dt} \frac{\delta x(t)}{\delta x(\sigma)} = \frac{d}{dt} \delta(t - \sigma) = -\frac{d}{d\sigma} \delta(t - \sigma)$. This gives

$$\frac{\delta S}{\delta x(\sigma)} = -\frac{d}{d\sigma} \int_{t_a}^{t_b} dt m\dot{x}(t) \delta(t - \sigma) - \int_{t_a}^{t_b} dt V'(x(t)) \delta(t - \sigma) = -m\dot{x}(\sigma) - V'(x(\sigma)) \quad (\text{S } 4.2)$$

and Newton's equation when demanding $\delta S = 0$.

b) Differentiate Eq. (S 4.2) again functionally and use the basic rule (1.62d) to obtain

$$\frac{\delta^2 S}{\delta x(\sigma)\delta x(\sigma')} = \left[-m \frac{d^2}{d\sigma^2} - V''(x(\sigma)) \right] \delta(\sigma - \sigma'). \quad (\text{S } 4.3)$$

The functional Taylor expansion (1.63) around the classical path then becomes

$$S[x_{cl}(t) + y(t)] = S[x_{cl}(t)] + \int d\sigma \left[\frac{m}{2} \dot{y}^2 - \frac{1}{2} V''(x_{cl}(\sigma)) y^2(\sigma) \right] + \dots \quad (\text{S } 4.4)$$

c) Apply the chain rule and the basic rule (1.62d) of functional differentiation to get the generalized result

$$\frac{\delta^n Z[J]}{\delta J(\sigma_1) \dots \delta J(\sigma_n)} = \left(\frac{i}{\hbar} \right)^n \int \mathcal{D}x \, x(\sigma_1) \dots x(\sigma_n) \exp \left(\frac{i}{\hbar} S[x(t)] + \frac{i}{\hbar} \int dt x(t) J(t) \right). \quad (\text{S } 4.5)$$

If after differentiation the source is set to zero, the result allows to calculate integrals of arbitrary monomials of x weighted with the exponential of the action (the Green functions).

Problem 5:

a) In the definition (1.56) of the Wigner transform, the matrix element is $\langle x - \frac{y}{2} | V(\hat{x}) | x + \frac{y}{2} \rangle = V(x + y/2) \delta(x - \frac{y}{2} - (x + \frac{y}{2})) = V(x + \frac{y}{2}) \delta(-y) = V(x) \delta(y)$ and therefore $V_W(x, p) = V(x)$. For momentum-dependent operators transform (1.56) into

$$A_W(x, p) = \int dy dk dk' \left\langle x - \frac{y}{2} \left| k \right. \right\rangle \left\langle k \left| \hat{A} \right| k' \right\rangle \left\langle k' \left| x + \frac{y}{2} \right. \right\rangle e^{ipy/\hbar} = \int dq \left\langle p - \frac{q}{2} \left| \hat{A} \right| p + \frac{q}{2} \right\rangle \exp(-iqx/\hbar) \quad (\text{S } 5.1)$$

using the transformation bracket $\langle x|p\rangle = \exp(ipx)/(2\pi\hbar)^{1/2}$ between position and momentum eigenstates. From Eq. (S 5.1) it is then clear that $T_W(x, p) = T(p)$, in particular for the non-relativistic kinetic energy $T(p) = p^2/(2m)$.

b) Eq. (1.56) is a Fourier transformation w.r.t. y and therefore can be inverted in the usual way: Multiply by $\exp(-ipz/\hbar)$ and integrate over p . Shifting the arguments in the matrix element gives Eq. (1.57). Insert $A_W(\frac{x+x'}{2}, p) = \left(\frac{x+x'}{2}\right)^m p^n$ and use the binomial theorem. This gives

$$\langle x | \hat{A} | y \rangle = \frac{1}{2^m} \sum_{l=0}^m \binom{m}{l} \int_{-\infty}^{+\infty} dp \frac{\exp(ipx/\hbar)}{\sqrt{2\pi\hbar}} x^l p^n y^{m-l} \frac{\exp(-ipy/\hbar)}{\sqrt{2\pi\hbar}} \equiv \frac{1}{2^m} \sum_{l=0}^m \binom{m}{l} \langle x | \hat{x}^l \hat{p}^n \hat{x}^{m-l} | y \rangle \quad q.e.d. \quad (\text{S } 5.2)$$

Problem 6:

The path $x(t)$ depends parametrically on x_a, t_a, x_b, t_b . Using the rules for differentiation of integrals one therefore has for the (partial, not functional!) derivative of the classical action w.r.t. the initial time

$$\frac{\partial S_{cl}}{\partial t_a} = -L(x_a, \dot{x}_a) + \int_{t_a}^{t_b} dt \left[\frac{\partial L}{\partial x} \frac{\partial x(t)}{\partial t_a} + \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}(t)}{\partial t_a} \right] \quad (\text{S } 6.1)$$

where $\dot{x}_a = \dot{x}|_{t=t_a}$. Write the last factor in the last term as $\frac{d}{dt} \frac{\partial x(t)}{\partial t_a}$, perform an integration by parts and use the Euler-Lagrange equations to obtain

$$\frac{\partial S_{cl}}{\partial t_a} = -L(x_a, \dot{x}|_{t=t_a}) + \frac{\partial L}{\partial \dot{x}} \Big|_{t_b} \lim_{t \rightarrow t_b} \frac{\partial}{\partial t_a} x(t) - \frac{\partial L}{\partial \dot{x}} \Big|_{t_a} \lim_{t \rightarrow t_a} \frac{\partial}{\partial t_a} x(t) = -L(x_a, \dot{x}_a) + \frac{\partial L}{\partial \dot{x}} \Big|_{t_a} \equiv H \Big|_{t_a} = E_a. \quad (\text{S } 6.2)$$

Here the Taylor expansion of the paths near initial and final time $x(t) = x_{a/b} + \dot{x}_{a/b}(t - t_{a/b}) + \dots$ has been used to determine $\frac{\partial}{\partial t_a} x(t)|_{t_b} = 0$ and $\frac{\partial}{\partial t_a} x(t)|_{t_a} = -\dot{x}_a$. Similarly for

$$\frac{\partial S}{\partial x_a} = \frac{\partial L}{\partial \dot{x}} \frac{\partial x(t)}{\partial x_a} \Big|_{t_a}^{t_b} = -\frac{\partial L}{\partial \dot{x}} \Big|_{t_a} \lim_{t \rightarrow t_a} \frac{\partial}{\partial x_a} [x_a + \dot{x}_a(t - t_a) + \dots] = -\frac{\partial L}{\partial \dot{x}} \Big|_{t_a} \equiv -p_a. \quad (\text{S } 6.3)$$

With the explicit expressions for the classical action determined in **Problem 2 a)** and **b)**, it is easy to verify these relations for the free particle and the particle in a harmonic potential.

Problem 7:

a) Minimal substitution for a particle in an electromagnetic field \mathbf{A} means replacing the momentum of the particle by the canonical momentum: $\mathbf{p} \rightarrow \mathbf{\Pi} = \mathbf{p} - e\mathbf{A}/c$. To derive the path-integral representation complete the square in the exponent of the phase space path integral

$$\mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{\Pi}) = -\frac{\mathbf{p}^2}{2m} + \mathbf{p} \cdot \left(\dot{\mathbf{x}} + \frac{e}{mc} \mathbf{A} \right) - \frac{e^2}{2mc^2} \mathbf{A}^2 = -\frac{1}{2m} \left(\mathbf{p} - \left(m\dot{\mathbf{x}} + \frac{e}{c} \mathbf{A} \right) \right)^2 + \frac{m}{2} \dot{\mathbf{x}}^2 + \frac{e}{c} \mathbf{A} \cdot \dot{\mathbf{x}} \quad (\text{S } 7.1)$$

and perform the Gaussian integral over $\mathbf{\Pi} - m\dot{\mathbf{x}}$. This gives a constant while the remaining path integral reads $\int \mathcal{D}^3 x(t) \exp(iS[\mathbf{x}]/\hbar)$ with the action

$$S[\mathbf{x}(t)] = \int_{t_a}^{t_b} dt \left[\frac{m}{2} \dot{\mathbf{x}}^2 + \frac{e}{c} \mathbf{A} \cdot \dot{\mathbf{x}} \right]. \quad (\text{S } 7.2)$$

b) Under the gauge transformation $\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda$ the action (S 7.2) changes into

$$S[\mathbf{x}(t)] \rightarrow S[\mathbf{x}(t)] + \int_{t_a}^{t_b} dt \frac{e}{c} \nabla\Lambda(\mathbf{x}) \cdot \dot{\mathbf{x}} = S[\mathbf{x}(t)] + \int_{t_a}^{t_b} dt \frac{e}{c} \frac{d}{dt} \Lambda(\mathbf{x}) = S[\mathbf{x}(t)] + \frac{e}{c} [\Lambda(\mathbf{x}_b) - \Lambda(\mathbf{x}_a)]. \quad (\text{S } 7.3)$$

This means that

$$U(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \sum_n \psi_n^*(\mathbf{x}_b) e^{-iE_n(t_b - t_a)/\hbar} \psi_n(\mathbf{x}_a) \rightarrow U(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) \cdot \exp \left\{ \frac{ie}{\hbar c} [\Lambda(\mathbf{x}_b) - \Lambda(\mathbf{x}_a)] \right\}, \quad (\text{S } 7.4)$$

i.e. that the wave functions acquire a (position-dependent) phase factor

$$\psi_n(\mathbf{x}) \rightarrow \psi_n(\mathbf{x}) \cdot e^{\frac{ie}{\hbar c} \Lambda(\mathbf{x})}. \quad (\text{S } 7.5)$$

c) Following the derivation of Schrödinger's equation for a particle in a potential in chapter 1.2 one may use

$$S = \epsilon \sum_{j=0}^N \left[\frac{m}{2} \left(\frac{\mathbf{x}_{j+1} - \mathbf{x}_j}{\epsilon} \right)^2 + \frac{e}{c} \mathbf{A}(\lambda \mathbf{x}_j + (1 - \lambda)\mathbf{x}_{j+1}) \cdot \frac{\mathbf{x}_{j+1} - \mathbf{x}_j}{\epsilon} \right] \quad (\text{S } 7.6)$$

as discretized version of the action (S 7.2). Here the parameter $\lambda \in [0, 1]$ determines the ordering prescription: $\lambda = 1/2$ gives the midpoint rule. In 3 dimensions Eq. (1.36) now reads

$$\psi(\mathbf{x}, t + \epsilon) = \left(\frac{m}{2\pi i \epsilon \hbar} \right)^{3/2} \int_{-\infty}^{+\infty} d^3 \xi \exp \left(\frac{im \xi^2}{2\epsilon \hbar} \right) \exp \left[-\frac{ie}{\hbar c} \xi \cdot \mathbf{A}(x + \lambda \xi) \right] \psi(\mathbf{x} + \xi, t). \quad (\text{S } 7.7)$$

and again one has to expand in powers of ϵ and ξ . Use the Gaussian integrals $\int d^3 \xi (1, \xi_k, \xi_k \xi_l) \exp(-a \xi^2) = \left(1, 0, \frac{\delta_{kl}}{2a}\right) \left(\frac{\pi}{a}\right)^{3/2}$, where $a = -\frac{im}{2\epsilon \hbar}$ and k, l are cartesian components, to derive

$$\psi(\mathbf{x}, t + \epsilon) = \psi(\mathbf{x}, t) + \epsilon \frac{i\hbar}{2m} \Delta \psi(\mathbf{x}, t) + \epsilon \frac{\lambda e}{mc} (\nabla \cdot \mathbf{A}(\mathbf{x})) \psi(\mathbf{x}, t) - \epsilon \frac{ie^2}{2\hbar mc^2} \mathbf{A}^2(\mathbf{x}) \psi(\mathbf{x}, t) + \epsilon \frac{e}{mc} \mathbf{A}(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}, t) + \mathcal{O}(\epsilon^2). \quad (\text{S } 7.8)$$

In the limit $\epsilon \rightarrow 0$ one thus obtains

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \Delta + \frac{i\hbar e}{mc} \mathbf{A}(\mathbf{x}) \cdot \nabla + \lambda \frac{i\hbar e}{mc} (\nabla \cdot \mathbf{A}(\mathbf{x})) + \frac{e^2}{2mc^2} \mathbf{A}^2(\mathbf{x}) \right] \psi(\mathbf{x}, t) \quad (\text{S } 7.9)$$

and one sees that only for $\lambda = 1/2$ the r.h.s. can be written as

$$\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right)^2 \psi(\mathbf{x}, t) \equiv \frac{1}{2m} \hat{\Pi}^2 \psi(\mathbf{x}, t) \quad (\text{S } 7.10)$$

(be careful when squaring the differential operator: $(d/dx + f)^2 g = g'' + 2fg' + g'f + f^2g$). Note that "outer averaging" $(\mathbf{A}(\mathbf{x}_j) + \mathbf{A}(\mathbf{x}_{j+1}))/2$ would lead to the same result.

Problem 8:

a) Differentiate the Euler-Lagrange eq. $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0$ w.r.t. to the momentum p . This gives

$$\frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{x}^2} j \right) + \left[\frac{d}{dt} \left(\frac{\partial^2 L}{\partial x \partial \dot{x}} \right) - \frac{\partial L}{\partial x^2} \right] J = 0, \tag{S 8.1}$$

i.e. the Jacobi equation. The initial conditions are $x(p, t) \rightarrow x_a + \frac{p}{m}t + \dots \implies J(p, t) \rightarrow \frac{1}{m}t + \dots$ for $t \rightarrow 0$ and therefore $J(p, 0) = 0$ and $\partial J / \partial t|_{t=0} = 1/m$.

b) For $L = m\dot{x}^2/2 - c(t)x^2/2 - e(t)x$ we find from Eq. (S 8.1) $m\ddot{J} + c(t)J = 0$, i.e. the Gel'fand-Yaglom equation for $mJ(t)$. Since $mJ(p, 0) = 0$ and $m\dot{J}(p, t)|_{t=0} = 1$ are precisely the initial conditions to determine the functional determinant in the prefactor as solution of the GY equation, one obtains the result $mJ(p, t) \equiv f_{\text{GY}}(t)$.

c) From **Problem (6)** we know that the initial momentum is given by $p = p(0) = -\frac{\partial S}{\partial x_a}$. Then

$$\frac{\partial p}{\partial x_b} = \frac{1}{\partial x_b / \partial p} = \frac{1}{J(p, t_b)} = -\frac{\partial^2 S}{\partial x_a \partial x_b} \quad \text{q.e.d.} \tag{S 8.2}$$

Combined with the previous result this verifies Eq. (1.99).

Problem 9:

Plugging the harmonic oscillator result (1.64) for the time-evolution operator into the r.h.s., one has

$$\frac{m\omega}{2\pi i \hbar} \frac{1}{\sqrt{s_1 s_2}} \int_{-\infty}^{+\infty} dx_c \exp \left\{ \frac{i m \omega}{2 s_2 \hbar} \left[(x_b^2 + x_c^2) c_2 - 2 x_b x_c \right] \right\} \exp \left\{ \frac{i m \omega}{2 s_1 \hbar} \left[(x_c^2 + x_a^2) c_1 - 2 x_c x_a \right] \right\} \tag{S 9.1}$$

where $s_k := \sin \omega T_k$, $c_k := \cos \omega T_k$, $k = 1, 2$. By assumption both s_1 and s_2 are positive. The x_c -integral is of the form of Eq. (1.25g) with

$$a = \frac{m\omega}{2s_2\hbar} \left(\frac{c_2}{s_2} + \frac{c_1}{s_1} \right) = \frac{m\omega}{2s_2\hbar} \frac{s_{1+2}}{s_1 s_2}, \quad b = -\frac{m\omega}{s_2\hbar} \left(\frac{x_b}{s_2} + \frac{x_a}{s_1} \right). \tag{S 9.2}$$

It now depends on the sign of $s_{1+2} \equiv \sin \omega(T_1 + T_2)$ whether the phase of the prefactor is $\pi/4$ (for $s_{1+2} > 0$, i.e. the focal point has not been reached) or $-\pi/4 = \pi/4 - \pi/2$ (for $s_{1+2} < 0$, i.e. the particle has passed the first focal point) as Eq. (1.25a) clearly shows. Careful algebra then also demonstrates that all trigonometric functions on the r.h.s. have the argument $\omega(T_1 + T_2) = \omega(t_b - t_a)$ - no dependence on the intermediate time t_c is left - and that indeed

$$U^{\text{h.o.}}(x_b, t_b; x_a, t_c) = \sqrt{\frac{m\omega}{2\pi i \hbar |s_{1+2}|}} e^{-in\pi/2} e^{iS_{\text{cl}}^{\text{h.o.}}} \tag{S 9.3}$$

acquires a Maslov phase ($n = 1$) if a focal point is passed (cf. Ref.[62])

Problem 10*:

a) Inserting $V(x) = (m\omega(x^2 - a^2)/a)^2/8$ into Eq. (1.331) one obtains for $|x| < a$

$$\tau - \tau_0 = \frac{2a}{\omega} \int_{x_1(\tau_0)}^{x_1(\tau)} dx \frac{1}{a^2 - x^2} = \frac{1}{\omega} \ln \frac{a+x}{a-x} \Big|_{x_1(\tau_0)}^{x_1(\tau)} \tag{S 10.1}$$

from which $x(\tau) = a(A \exp[\omega(\tau - \tau_0)] - 1)/(A \exp[\omega(\tau - \tau_0)] + 1)$ follows. Here $A = (a + x_1(\tau_0))/(a - x_1(\tau_0))$. Thus

$$x_1(\tau) = a \tanh \left[\frac{\omega}{2}(\tau - \tau_0) + \gamma \right], \quad \gamma = \frac{1}{2} \ln \left(\frac{a + x_1(\tau_0)}{a - x_1(\tau_0)} \right). \tag{S 10.2}$$

If one chooses $x_1(\tau_0) = 0$, i.e. the particle should traverse the axis at time τ_0 , then $\gamma = 0$ and Eq. (S 10.2) turns into Eq. (1.332).

b) Use $V''(x) = m\omega^2(3x^2/a^2 - 1)/2$ and evaluate $m\partial^2 x_0(\tau - \tau_0)/\partial \tau^2$ to verify that $\mathcal{O}_{V''} y_0 = 0$. Observe that this also follows if the classical equation of motion (1.328) for the instanton is differentiated again w.r.t. τ_0 :

$$m \frac{d^2}{d\tau^2} \frac{\partial x_1}{\partial \tau_0} - V''(x_1) \frac{\partial x_1}{\partial \tau_0} = 0. \tag{S 10.3}$$

Normalizing the zero mode

$$y_0(\tau) = A_0 \partial x_1 / \partial \tau_0 = -A_0 \dot{x}_1 = \frac{A_0 a \omega}{2 \cosh^2[\omega(\tau - \tau_0)]} \tag{S 10.4}$$

to unity one finds

$$A_0^2 \int_{-\infty}^{+\infty} d\tau \left(\frac{dx_1(\tau)}{d\tau} \right)^2 = A_0^2 \frac{1}{m} S_1 = 1 \implies A_0 = \sqrt{\frac{m}{S_1}} \tag{S 10.5}$$

by means of Eq. (1.333) in which the action S_1 of the one-instanton solution has been calculated. Note that (in the $\beta \rightarrow \infty$ -limit) the zero mode is orthogonal to the instanton solution

$$\int_{-\infty}^{+\infty} d\tau y_0(\tau) x_1(\tau) = \int_{-\infty}^{+\infty} d\tau (-A_0) \frac{dx_1(\tau)}{d\tau} x_1(\tau) = -A_0 \int_{-\infty}^{+\infty} d\tau \frac{d}{d\tau} \frac{1}{2} (x_1(\tau))^2 = -\frac{1}{2} A_0 (x_1(\tau))^2 \Big|_{\tau \rightarrow -\infty}^{\tau \rightarrow +\infty} = 0. \quad (\text{S } 10.6)$$

c) Write down the linear differential equations $-m\ddot{f}^{(i)}(\tau) + V''(x_{\text{cl}}) f^{(i)}(\tau) = 0$ for $i = 1, 2$, multiply the first equation by $f^{(2)}(\tau)$, the second one by $f^{(1)}(\tau)$ and subtract. This gives

$$0 = -m\ddot{f}^{(1)}(\tau)f^{(2)}(\tau) + m\ddot{f}^{(2)}(\tau)f^{(1)}(\tau) = m\frac{d}{d\tau} \left[f^{(1)}(\tau)\dot{f}^{(2)}(\tau) - \dot{f}^{(1)}(\tau)f^{(2)}(\tau) \right] \equiv m\frac{d}{d\tau} W \left(f^{(1)}, f^{(2)} \right). \quad (\text{S } 10.7)$$

Integration then shows that the Wronskian is a constant whose value $8\omega^3 a^2 A_0^2$ is determined from the asymptotic behaviour of the functions $f^{(1)}, f^{(2)}$.

d) Differentiating $g(\tau, \tau) =: \Theta(\tau - \tau') \tilde{g}(\tau, \tau')$ twice w.r.t. τ , using $\delta(\tau - \tau') \tilde{g}(\tau, \tau') = \delta(\tau - \tau') \tilde{g}(\tau, \tau) = 0$ and the definition of the Wronskian shows that $\mathcal{O}_{V''} g(\tau, \tau') = \delta(\tau - \tau')$ (similar as in **Problem 2 c)** for the forced harmonic oscillator). Thus Eq. (P 10.3) is an integral equation for the would-be-zero-mode eigen function $Y_0(\tau)$ which by construction fulfills the boundary condition at $\tau = -\beta/2$ but not at $\tau = \beta/2$. Requiring that, one obtains for the eigenvalue

$$\frac{f_{\text{GY}}(+\beta/2)}{e_0} = - \int_{-\beta/2}^{+\beta/2} d\tau' g(\beta/2, \tau') Y_0(\tau') \simeq - \int_{-\beta/2}^{+\beta/2} d\tau' g(\beta/2, \tau') f_{\text{GY}}(\tau') \quad (\text{S } 10.8)$$

in a first-order expansion in powers of the exponentially small eigenvalue e_0 (similar as the Born approximation in the Lippmann-Schwinger equation). Inserting the expressions for the Green function and the Gel'fand-Yaglom function, the r.h.s. of the equation becomes

$$\begin{aligned} & -\frac{1}{mW} \int_{-\beta/2}^{+\beta/2} d\tau' \left[f^{(1)}(\beta/2) f^{(2)}(\tau') - f^{(2)}(\beta/2) f^{(1)}(\tau') \right] \frac{1}{W} \left[f^{(1)}(-\beta/2) f^{(2)}(\tau') - f^{(2)}(-\beta/2) f^{(1)}(\tau') \right] \\ &= -\frac{1}{mW^2} \left[f^{(1)}(-\beta/2) f^{(1)}(\beta/2) \langle f^{(2)} | f^{(2)} \rangle - f^{(2)}(-\beta/2) f^{(2)}(\beta/2) \langle f^{(1)} | f^{(1)} \rangle \right] \\ &\xrightarrow{\beta \rightarrow \infty} -\frac{1}{m} \left(\frac{2\omega a A_0}{W} \right)^2 \left[e^{-\omega\beta} \langle f^{(2)} | f^{(2)} \rangle - e^{\omega\beta} \langle f^{(1)} | f^{(1)} \rangle \right] \end{aligned} \quad (\text{S } 10.9)$$

since the mixed terms $\langle f^{(1)} | f^{(2)} \rangle$ vanish because of the different parity of the solutions. In the last line their asymptotic behaviour has been inserted which also allows to estimate the normalization $\langle f^{(2)} | f^{(2)} \rangle \sim \int^{\beta/2} d\tau' \exp(2\omega\tau') \sim \exp(\omega\beta)$ while in the second term $\langle f^{(1)} | f^{(1)} \rangle = \langle y_0 | y_0 \rangle = 1$ has already been normalized to unity as zero-mode solution. Thus at large β the second term is dominant and with $W = 8\omega^3 a^2 A_0^2$, $A_0^2 = m/S_1 = 3/(2\omega a^2)$ one obtains

$$\text{Det}' \mathcal{O}_{V''} = \frac{f_{\text{GY}}(+\beta/2)}{e_0} \rightarrow \frac{1}{m} \left(\frac{2\omega a A_0}{W} \right)^2 e^{\omega\beta} = \frac{1}{16m\omega^4 a^2 A_0^2} e^{\omega\beta} = \frac{1}{24m\omega^3} e^{\omega\beta}. \quad (\text{S } 10.10)$$

Problem 11*:

a) For $v = w(1 + \epsilon)$ one obtains by expanding in ϵ , $\mu^2(u) = u - 2\epsilon u + 2\epsilon(1 - e^{-wu})/w + \mathcal{O}(\epsilon^2)$ and therefore

$$E_F(w, \epsilon) = \frac{3}{4} w\epsilon^2 - \frac{2\alpha}{\sqrt{\pi}} \int_0^\infty dt e^{-t^2} \left[1 + \epsilon - \frac{\epsilon}{wt^2} \left(1 - e^{-wt^2} \right) + \dots \right] = -\alpha + \frac{3}{4} w\epsilon^2 - \frac{\alpha\epsilon}{w} (1 - \sqrt{1+w})^2 + \mathcal{O}(\epsilon^3, \alpha\epsilon^2). \quad (\text{S } 11.1)$$

Here the substitution $u = t^2$ and an integration by part have been made to reduce the occurring integrals to the (ubiquitous) Gaussian one. Variation w.r.t. ϵ is straightforward since Eq. (S 11.1) is a quadratic form in ϵ and gives $e_0 = 2\alpha(1 - \sqrt{1+w})^2/(3w^2)$. Plugging that back into the expression (S 11.1) for the Feynman energy gives

$$E_F(w) = -\alpha - \frac{\alpha^2}{3w^3} (1 - \sqrt{1+w})^4 + \dots \quad (\text{S } 11.2)$$

which can be varied w.r.t. w . This leads to the equation $w_0^2 = 3w_0$ with two solutions: $w_0 = 0$ (no retardation) leads to the first-order result $E_F = -\alpha$ whereas the second solution $w_0 = 3$ gives the lower ground-state energy $E_F = -\alpha - \alpha^2/81 - \dots$.

b) Assuming $v \gg w$ for large coupling immediately leads to $\mu^2(u) = 1/\sqrt{v} + \mathcal{O}(1/v^{3/2})$ and thus

$$E_F(v) = \frac{3}{4} v - \frac{\alpha}{\sqrt{\pi}} v^{1/2} + \dots \quad (\text{S } 11.3)$$

is only a function of v in this limit. Variation is "kinderleicht" (easy as pie) and gives $v_0 = 4\alpha^2/(9\pi)$ and therefore

$$E_F \xrightarrow{\alpha \rightarrow \infty} -\frac{\alpha^2}{3\pi}. \quad (\text{S } 11.4)$$

Problem 12:

Using

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^\dagger - \hat{a}) \quad (\text{S 12.1})$$

gives, for example

$$\langle z | \hat{x} | z \rangle = \sqrt{\frac{\hbar}{2m\omega}} (z + z^*) \langle z | z \rangle, \quad \langle z | \hat{p} | z \rangle = i\sqrt{\frac{m\hbar\omega}{2}} (z^* - z) \langle z | z \rangle \quad (\text{S 12.2})$$

and similar for the squared operators:

$$(\Delta x)^2 = \frac{\hbar}{2m\omega} [z^2 + z^{*2} + 2zz^* + 1 - (z + z^*)^2] = \frac{\hbar}{2m\omega}, \quad (\Delta p)^2 = -\frac{m\hbar\omega}{2} [z^2 + z^{*2} - 2zz^* - 1 - (z - z^*)^2] = \frac{m\hbar\omega}{2}. \quad (\text{S 12.3})$$

Therefore the equality sign holds in the uncertainty relation

$$\Delta x \cdot \Delta p = \sqrt{\frac{\hbar}{2m\omega}} \cdot \sqrt{\frac{m\hbar\omega}{2}} = \frac{\hbar}{2}. \quad (\text{S 12.4})$$

Problem 13:

a) Assume that the matrix \mathbb{A} can be diagonalized: $\mathbb{A} =: \text{diag}(a_1, a_2, \dots)$. Then

$$\det \mathbb{A} = \prod_k a_k = \exp \left[\sum_k \ln(a_k) \right] = \exp[\text{tr} \ln \mathbb{A}]. \quad (\text{S 13.1})$$

b) Differentiate Eq. (S 13.1) w. r. t. the parameter λ to obtain

$$\frac{\partial}{\partial \lambda} \det \mathbb{A}(\lambda) = \left(\sum_k \frac{1}{a_k(\lambda)} \frac{\partial a_k(\lambda)}{\partial \lambda} \right) \cdot \det \mathbb{A}(\lambda) = \text{tr} \left(\mathbb{A}^{-1}(\lambda) \frac{\partial \mathbb{A}(\lambda)}{\partial \lambda} \right) \cdot \det \mathbb{A}(\lambda). \quad (\text{S 13.2})$$

c) Use the previous result (S 13.2) to evaluate

$$\frac{\partial}{\partial g'} \ln \det (\mathbb{A}_0 + g' \mathbb{A}_1) = \text{tr} \left[(\mathbb{A}_0 + g' \mathbb{A}_1)^{-1} \mathbb{A}_1 \right]. \quad (\text{S 13.3})$$

Integrate both sides of this equation w.r.t. g' from 0 to g with the initial condition $\det (\mathbb{A}_0 + g' \mathbb{A}_1) \Big|_{g'=0} = \det \mathbb{A}_0$; this proves the assertion. If g is a small (coupling) constant one may expand in powers of it and obtains

$$\det (\mathbb{A}_0 + g \mathbb{A}_1) = \det (\mathbb{A}_0) \cdot \exp \left\{ g \text{tr} (\mathbb{A}_1 \mathbb{A}_0^{-1}) - \frac{g^2}{2} \text{tr} (\mathbb{A}_1 \mathbb{A}_0^{-1} \mathbb{A}_1 \mathbb{A}_0^{-1}) + \dots \right\}. \quad (\text{S 13.4})$$

Problem 14:

Calculate

$$\int d\eta e^{-\eta(\xi - \xi')} = \int d\eta [1 - \eta(\xi - \xi')] = -(\xi - \xi') \quad (\text{S 14.1})$$

using the property that the square of a Grassmann variable vanishes and the Berezin integration rules. That this is indeed a Grassmann δ -function can be seen by evaluating its integral with a general function $f(\xi') = f_0 + f_a \xi'$

$$\int d\xi' (-)(\xi - \xi') [f_0 + f_1 \xi'] = - \int d\xi' \xi f_1 \xi' + \int d\xi' \xi' f_0 = f_1 \xi + f_0 \equiv f(\xi). \quad (\text{S 14.2})$$

Problem 15:

a) Eq. (2.158) with $H = \hbar\omega \bar{\xi} \xi$ leads to the expression (P 15.1) for the partition function of the harmonic oscillator. Berezin integration gives $Z_\omega = \text{const. Det } \mathcal{O}_\omega$ where $\mathcal{O}_\omega := \frac{\partial}{\partial \tau} + \omega$. The determinant is calculated as product of the eigenvalues λ_n of the operator \mathcal{O}_ω in the space of functions with anti-periodic boundary conditions at $\tau = 0$ and $\tau = \hbar\beta$. The eigenfunctions are $\text{const. exp}[(\lambda - \omega)\tau]$ and therefore the eigenvalues $\lambda_n = \omega + \frac{2n+1}{\hbar\beta} \pi i, n = 0, \pm 1, \dots$. This leads to

$$\text{Det } \mathcal{O}_\omega = \text{Det } \mathcal{O}_0 \prod_{n=0, \pm 1, \pm 2, \dots} \left(1 - \frac{\omega \hbar \beta}{(2n+1)\pi} i \right) = \text{Det } \mathcal{O}_0 \prod_{n=0}^{\infty} \left(1 + \frac{\omega^2 \hbar^2 \beta^2}{(2n+1)^2 \pi^2} \right) = \text{Det } \mathcal{O}_0 \cosh \left(\frac{1}{2} \hbar \omega \beta \right). \quad (\text{S 15.1})$$

b) In the discretized version one has to evaluate

$$Z_0(\beta) = \lim_{N \rightarrow \infty} \prod_{n=0}^N \left(\int d\bar{\xi}_n d\xi_n \right) \exp \left[-\epsilon \sum_{n=1}^N \bar{\xi}_n \frac{\xi_n - \xi_{n-1}}{\epsilon} \right] = \lim_{N \rightarrow \infty} \det_{N+1} \mathbb{H} \quad (\text{S 15.2})$$

where the determinant can be calculated by an expansion along the first row

$$\det_{N+1} \mathbb{H} = \begin{vmatrix} 1 & 0 & \dots & 0 & 1 \\ -1 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 1 \end{vmatrix} = 1 + 1^{N+1} = 2. \quad (\text{S 15.3})$$

Thus $Z_0 = 2$ and

$$Z_\omega = 2 \cosh \left(\frac{1}{2} \hbar \omega \beta \right). \quad (\text{S 15.4})$$

c) From Eq. (S 15.4) one finds

$$Z_\omega(\beta \rightarrow \infty) \rightarrow \exp \left(\frac{1}{2} \hbar \omega \beta \right) \implies E_0 = -\frac{1}{2} \hbar \omega. \quad (\text{S 15.5})$$

That the fermionic "partners" cancel the (infinite) ground-state energy of the (infinite) harmonic oscillators (representing the scalar fields) in the Universe is a nice idea. However, "the great tragedy of Science is the slaying of a beautiful hypothesis by an ugly fact" (T. H. Huxley). Here the "ugly facts" are (i) The fermionic (or more generally, supersymmetric) partners have not been found experimentally. (ii) The cosmological constant is not zero but has a small, non-zero value determined from the observed acceleration of far-away galaxies (Nobel prize in Physics 2011).

Problem 16:

Write the free energy as

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta) = -\frac{1}{\beta} \ln \left[e^{-\beta E_0} + \sum_{n=1} e^{-\beta E_n} \right] = E_0 - \frac{1}{\beta} \ln \left[1 + \sum_{n=1} e^{-\beta(E_n - E_0)} \right] \quad (\text{S 16.1})$$

and observe that $\ln(1+x) \geq 0$ for $x \geq 0$ as can be seen from a graph of the function. Differentiating Eq. (S 16.1) w.r.t β one obtains

$$F'(\beta) = \frac{1}{\beta^2} \ln \left[1 + \sum_{n=1} e^{-\beta(E_n - E_0)} \right] + \frac{1}{\beta} \sum_{n=1} ((E_n - E_0) e^{-\beta(E_n - E_0)}) \left[1 + \sum_{n=1} e^{-\beta(E_n - E_0)} \right]^{-1} \quad (\text{S 16.2})$$

and sees that all terms are positive since $E_n > E_0$. Thus the free energy is monotonically growing from $F(0) = -\infty$ to $F(\infty) = E_0$.

Problem 17:

Because of time-translation invariance and the absence of interactions one can write $G_0(\alpha, \tau; \alpha', \tau') = \delta_{\alpha\alpha'} g_\alpha(\tau - \tau')$ where $g_\alpha(t := \tau - \tau')$ fulfills

$$(\partial_t + \epsilon_\alpha - \mu) g_\alpha = \delta(t). \quad (\text{S 17.1})$$

One can solve this differential equation by the method of "variation of the constant", i.e. by the ansatz

$$g_\alpha(t) = C(t) \cdot \exp[-(\epsilon_\alpha - \mu)t]. \quad (\text{S 17.2})$$

This gives $\dot{C}(t) = \delta(t) \cdot \exp[(\epsilon_\alpha - \mu)t] = \delta(t)$, i.e. $C(t) = a + \Theta(t)$. The boundary condition $g_\alpha(\beta) = \zeta g_\alpha(0)$ determine the constant as $a = n_\alpha \{ \zeta - \Theta(0) \exp[(\epsilon_\alpha - \mu)\beta] \}$ where n_α is the occupation probability (2.170). It remains to give a meaning to the step function at zero argument, i.e. to consider the time-ordered product at equal time. This is defined to be equal to a normal-ordered product at equal time so that in the time-sliced expression for $\langle \hat{a}_{\alpha'}^\dagger(\tau') \hat{a}_\alpha(\tau) \rangle$ one has terms like

$$e^{-\epsilon \hat{H}} |z_k\rangle \langle z_k | \hat{a}_\alpha^\dagger \hat{a}_{\alpha'} e^{-\epsilon \hat{H}} |z_{k-1}\rangle \langle z_{k-1} | \dots = e^{-\epsilon \hat{H}} |z_k\rangle \left(z_{\alpha,k}^* z_{\alpha',k-1} e^{-\epsilon H(z_k^*, z_{k-1})} + \mathcal{O}(\epsilon) \right) \langle z_{k-1} | \dots \quad (\text{S 17.3})$$

In other words: The creation operator is evaluated one time step later than the annihilation operator ($\tau' = \tau + \epsilon$) and therefore $\Theta(0) \longrightarrow \lim_{\epsilon \rightarrow 0} \Theta(\tau - (\tau + \epsilon)) = 0$. The discretized version of the path integral thus gives the unambiguous result

$$g_\alpha(t) = e^{-(\epsilon_\alpha - \mu)t} \{ (1 + \zeta n_\alpha) \Theta(t - \epsilon) + \zeta n_\alpha \Theta(\epsilon - t) \}. \quad (\text{S 17.4})$$

Problem 18*:

a) From Eq. (P 18.4) one finds $\int_0^\infty dy y^n \exp(-\lambda y) = n!/\lambda^{n+1}$. Some algebra then gives the normalization as $C_1 = \sqrt{2/a}$ and determines the kinetic and potential terms as $\langle T \rangle = 1/(2a^2)$, $\langle V \rangle = -5\sqrt{2}/(16\kappa a)$, respectively. Therefore the lowest value of $\langle T \rangle + \langle V \rangle$ occurs at $a_0 = 8\sqrt{2}\kappa/5$ and the optimal value of Pekar's constant is independent of the scaling parameter κ

$$\gamma_P(a_0) = -\frac{25}{256}. \tag{S 18.1}$$

b) Substitute in Eq. (P 18.4) $t = \lambda^2 y^2$ to derive

$$\int_0^\infty dy y^{2n} \exp(-\lambda^2 y^2) = \frac{1 \cdot 3 \dots (2n-1)}{2^{n+1} \lambda^{2n+1}} \sqrt{\pi} \tag{S 18.2}$$

and find thereby $C_2^2 = 4/(\sqrt{\pi}b^3)$, $\langle T \rangle = 3/(4b^2)$ (compare with the virial theorem for the 3-dim. harmonic oscillator!) and $\langle V \rangle = -1/(\sqrt{\pi}\kappa b)$. This gives the optimal value

$$b_0 = \frac{3}{2}\sqrt{\pi}\kappa \implies \gamma_P(b_0) = -\frac{1}{3\pi}. \tag{S 18.3}$$

c) Declare all real-valued variables in the beginning of the program as "DOUBLE PRECISION" or insert "IMPLICIT REAL*8 (A-H,O-Z)" which declares all variables as double-precision unless they begin with "I,J,K,L,M,N" in which case they are integer. To avoid loss of accuracy replace numerical constants by their double-precision value, e.g. "1. → 1.d0" etc.

Problem 19:

Use the Schwinger representation (P 19.2) to perform the Gaussian k -integration in Minkowski space

$$\begin{aligned} \int \frac{d^d k}{(2\pi)^d} e^{iak^2 + ib \cdot k} &= e^{-ib^2/(4a)} \int \frac{d^d k'}{(2\pi)^d} e^{iak'^2} = e^{-ib^2/(4a)} \int \frac{dk'_0}{2\pi} e^{iak'_0{}^2} \prod_{i=1}^{d-1} \left(\int \frac{d^i k'_i}{(2\pi)^i} e^{-iak'_i{}^2} \right) \\ &= e^{-ib^2/(4a)} \frac{1}{2\pi} \sqrt{\frac{\pi}{-ia}} \frac{1}{(2\pi)^{d-1}} \sqrt{\frac{\pi}{ia}}^{d-1} = \frac{i}{(4\pi ia)^{d/2}} e^{-ib^2/(4a)} \end{aligned} \tag{S 19.1}$$

with $a = T$ and $b_\mu = 0$. The T -integral is of the form $\int_0^\infty dT T^{-d/2} \exp(-im^2 T)$ and can be performed by means of Eq. (P 18.4). This gives the result (P 19.3). As the Gamma function has poles at argument = 0, -1, -2... the integral diverges not only for the relevant case $d = 4$ but also for $d = 2$. This signals a quadratic divergence when the momentum integral is cut off at $k = \Lambda$:

$$\int^\Lambda d^4 k \frac{1}{k^2 - m^2 + i0^+} \sim \int^\Lambda dk k^3 \frac{1}{k^2} \sim \Lambda^2. \tag{S 19.2}$$

Near the physical dimension one sets $d = 4 - 2\epsilon$ and finds with $\Gamma(1 - d/2) = \Gamma(-1 + \epsilon) = \Gamma(\epsilon)/(-1 + \epsilon)$ and the expansions $\Gamma(\epsilon) = 1/\epsilon - \gamma_E + \mathcal{O}(\epsilon)$, $x^{-\epsilon} = \exp(-\epsilon \ln x) = 1 - \epsilon \ln x + \mathcal{O}(\epsilon^2)$ ($\gamma_E = 0.57721566\dots$ is Euler's constant) that the first-order self energy in Φ^4 theory is given in dimensional regularization by

$$\Sigma^{(1)}(p) = -\frac{\lambda}{32\pi^2} \frac{m^2}{\epsilon} \left[1 - \epsilon \left(\gamma_E - 1 + \ln \frac{m^2}{4\pi\mu_0^2} \right) + \mathcal{O}(\epsilon^2) \right], \tag{S 19.3}$$

consisting of a divergent and a finite part when $\epsilon \rightarrow 0$.

Problem 20:

For $N = 2$ define

$$\Phi := \frac{1}{\sqrt{2}} (\Phi_1 + i\Phi_2), \quad \Phi^* := \frac{1}{\sqrt{2}} (\Phi_1 - i\Phi_2) \tag{S 20.1}$$

so that $\Phi_1 = (\Phi + \Phi^*)/\sqrt{2}$, $\Phi_2 = (\Phi - \Phi^*)/(\sqrt{2}i)$. Then

$$\mathcal{L}_0^{(2)} = \frac{1}{2} [(\partial_\mu \Phi + \partial \Phi^*)^2 - (\partial_\mu \Phi - \partial \Phi^*)^2] - \frac{m^2}{2} [(\Phi + \Phi^*)^2 - (\Phi - \Phi^*)^2] = |\partial_\mu \Phi|^2 - m^2 |\Phi|^2, \tag{S 20.2}$$

i.e. the factor 1/2 of the neutral case has been removed. The Jacobian of the transformation (S 20.1) is

$$\begin{vmatrix} \frac{\partial \Phi_1}{\partial \Phi} & \frac{\partial \Phi_2}{\partial \Phi} \\ \frac{\partial \Phi_1}{\partial \Phi^*} & \frac{\partial \Phi_2}{\partial \Phi^*} \end{vmatrix} = \begin{vmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}i} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}i} \end{vmatrix} = i \tag{S 20.3}$$

which just modifies the irrelevant normalization of the path integral for the generating functional

$$\begin{aligned} Z_0[J^*, J] &= \int \mathcal{D}\Phi^* \mathcal{D}\Phi \exp [i(\Phi^*, K\Phi) + (J^*, \Phi) + (\Phi^*, J)] = \text{const.} \int \mathcal{D}\chi^* \mathcal{D}\chi \exp [i(\chi^*, K^{-1}\chi) - i(J^*, K^{-1}J)] \\ &= \text{const.}' \exp [-i(J^*, K^{-1}J)], \end{aligned} \quad (\text{S 20.4})$$

where the square in the exponent has been completed with $\chi := K\Phi + J$, $\chi^* := \Phi^*K + J^*$. $K := \partial^2 - m^2$ is the same kernel as in the neutral case and its inversion just gives the usual scalar propagator Δ_F . Thus by functional differentiation w.r.t. the sources J and J^* one obtains

$$\langle \Phi^*(x_1) \Phi(x_2) \rangle = (-i)^2 \frac{\delta^2}{\delta J(x_1) \delta J^*(x_2)} Z_0[J^*, J] \Big|_{J^*=J=0} \frac{1}{Z_0[0, 0]} = i \Delta(x_1, x_2). \quad (\text{S 20.5})$$

In the same way one finds $\langle \Phi(x_1) \Phi(x_2) \rangle = \langle \Phi^*(x_1) \Phi^*(x_2) \rangle = 0$.

Problem 21:

a) Differentiate Eqs. (P 21.1) and (P 21.2) w.r.t. the variable t and equate

$$\sum_{n=1} m_n i n \frac{(it)^{n-1}}{n!} = \sum_{k=0} m_k \frac{(it)^k}{k!} \cdot \sum_{l=1} \lambda_l i l \frac{(it)^{l-1}}{l!}. \quad (\text{S 21.1})$$

Writing the product of the two sums on the r.h.s. as

$$\sum_{n=0} (it)^n \sum_{m=0}^n \lambda_{n+1} m_{n-m} \frac{i(m+1)}{(n-m)!(m+1)!} \quad (\text{S 21.2})$$

and comparing powers of t on both sides establishes Eq. (P 21.3).

Writing $\langle x^n \rangle := m_n/m_0$ one finds

$$\begin{aligned} \lambda_1 &= \langle x \rangle, \quad \lambda_2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle (x - \langle x \rangle)^2 \rangle, \quad \lambda_3 = \langle x^3 \rangle - 3 \langle x^2 \rangle \langle x \rangle + 2 \langle x \rangle^3 = \langle (x - \langle x \rangle)^3 \rangle \\ \lambda_4 &= \langle x^4 \rangle - 4 \langle x^3 \rangle \langle x \rangle + 12 \langle x^2 \rangle \langle x \rangle^2 - 3 \langle x^2 \rangle^2 - 6 \langle x \rangle^4 = \langle (x - \langle x \rangle)^4 \rangle - 3 \langle (x - \langle x \rangle)^2 \rangle^2. \end{aligned} \quad (\text{S 21.3})$$

The simple structure of the first cumulants suggests a simpler relation in terms of the central moments (see below).

b) Multiply Eqs. (P 21.1) and (P 21.2) both by $\exp(-i \langle x \rangle t)$ and equate: The l.h.s. then becomes the expansion in central moments whereas on the r.h.s only the first cumulant is modified. Thus one can take over the final moment result (P 21.3) with the modifications $m_n \rightarrow c_n$, $\lambda_n \rightarrow \lambda_n - \langle x \rangle \delta_{n,1}$. Since by construction $c_0 \equiv m_0$ and $c_1 = 0$, one obtains $\lambda_1 = \langle x \rangle$ and

$$\lambda_{n+1} = \frac{c_{n+1}}{c_0} - \sum_{k=1}^{n-2} \binom{n}{k} \frac{c_{n-k}}{c_0} \lambda_{k+1}, \quad n = 1, 2 \text{ (the sum is then empty)}, 3 \dots \quad (\text{S 21.4})$$

Thus $\lambda_2 = c_2/c_0$, $\lambda_3 = c_3/c_0$, $\lambda_4 = c_4/c_0 - 3(c_2/c_0)^2$, $\lambda_5 = c_5/c_0 - 10 c_2 c_3/c_0^2$ etc.

c) The moment and cumulant expansion of the generating functional (3.13) for the Green functions in a scalar theory read

$$Z[J] = \sum_{n=0} \frac{i^n}{n!} \int d^4 x_1 \dots d^4 x_n m_n(x_1 \dots x_n) J(x_1) \dots J(x_n) = m_0 \exp \left[\sum_{n=1} \frac{i^n}{n!} \int d^4 x_1 \dots d^4 x_n G_c^{(n)}(x_1 \dots x_n) J(x_1) \dots J(x_n) \right] \quad (\text{S 21.5})$$

where the moments

$$m_n(x_1 \dots x_n) = \int \mathcal{D}\Phi \Phi(x_1) \dots \Phi(x_n) e^{iS[\Phi]}, \quad m_0 = \int \mathcal{D}\Phi e^{iS[\Phi]} \quad (\text{S 21.6})$$

are the Green functions up to a normalization: $G_n(x_1 \dots x_n) = m_n(x_1 \dots x_n)/m_0 =: \langle 1 \dots n \rangle$. The connected Green functions are then just the corresponding cumulants (see Eq. (3.31)) and for an even action where all odd moments/Green functions vanish, the first ones are found as

$$\begin{aligned} G_c^{(1)}(x_1) &= \langle 1 \rangle = 0, \quad G_c^{(2)}(x_1, x_2) = \langle 12 \rangle, \quad G_c^{(3)}(x_1, x_2, x_3) = 0 \\ G_c^{(4)}(x_1, x_2, x_3, x_4) &= \langle 1234 \rangle - \langle 12 \rangle \langle 34 \rangle - \langle 13 \rangle \langle 24 \rangle - \langle 14 \rangle \langle 23 \rangle. \end{aligned} \quad (\text{S 21.7})$$

Problem 22*:

Differentiate Eq. (P 22.1) w.r.t. $\Phi_{\text{cl}}(x)$ and use the chain rule to obtain

$$\frac{\delta \Gamma}{\delta \Phi_{\text{cl}}(x)} = \frac{\delta W}{\delta \Phi_{\text{cl}}(x)} - \int d^4 y \frac{\delta J(y)}{\delta \Phi_{\text{cl}}(x)} \Phi_{\text{cl}}(y) - J(x) = \int d^4 y \frac{\delta W[J]}{\delta J(y)} \frac{\delta J(y)}{\delta \Phi_{\text{cl}}(x)} - \int d^4 y \frac{\delta J(y)}{\delta \Phi_{\text{cl}}(x)} \Phi_{\text{cl}}(y) - J(x) = -J(x) \quad (\text{S 22.1})$$

due to the definition in Eq. (P 22.2).

Next differentiate the defining Eq. (P 22.2) for the classical field w.r.t. $\Phi_{\text{cl}}(y)$. This gives

$$\delta^{(4)}(x-y) = \frac{\delta^2 W}{\delta J(x)\delta\Phi_{\text{cl}}(y)} = \int d^4 z \frac{\delta J(z)}{\delta\Phi_{\text{cl}}(y)} \frac{\delta^2 W[J]}{\delta J(z)\delta J(x)}, \quad (\text{S 22.2})$$

where again the chain rule has been applied. One can now use the result $\delta\Gamma/\delta\Phi_{\text{cl}} = -J$ (just derived) and find

$$\delta^{(4)}(x-y) = - \int d^4 z \frac{\delta^2 \Gamma[\Phi_{\text{cl}}]}{\delta\Phi_{\text{cl}}(y)\delta\Phi_{\text{cl}}(z)} \frac{\delta^2 W[J]}{\delta J(z)\delta J(x)}. \quad (\text{S 22.3})$$

Recall that the connected Green functions are obtained from Eq. (3.31) as $G_c^{(n)} = (1/i)^n \delta^n iW$. Hence, if one sets $\Phi_{\text{cl}} = 0$ one finds that the connected 2-point function $G_c^{(2)}(x_1, x_2) = -i[\delta^2 W/\delta J(x_1)\delta J(x_2)]_{J=0}$ is the inverse (in operator sense) of $-\Gamma^{(2)}(x_1, x_2) = -[\delta^2 \Gamma/\delta\Phi_{\text{cl}}(x_1)\delta\Phi_{\text{cl}}(x_2)]_{\Phi_{\text{cl}}=0}$. Due to translation invariance these functions only depend on the difference $x_1 - x_2$ so that in momentum space the relation reads

$$\tilde{\Gamma}^{(2)}(p) = i \left[\tilde{G}^{(2)}(p) \right]^{-1} \implies \tilde{\Gamma}_2(p) = p^2 - m^2 - \Sigma(p) \quad (\text{S 22.4})$$

where $\Sigma(p)$ is the self-energy defined in Eq. (3.37). From the expansion of the 2-point function

$$\tilde{G}^{(2)}(p) = \frac{i}{p^2 - m^2} + \frac{i}{p^2 - m^2} \frac{1}{i} \Sigma(p) \frac{i}{p^2 - m^2} + \frac{i}{p^2 - m^2} \frac{1}{i} \Sigma(p) \frac{i}{p^2 - m^2} \frac{1}{i} \Sigma(p) \frac{i}{p^2 - m^2} + \dots \quad (\text{S 22.5})$$

one sees that $-i\Sigma$ is the 1-particle irreducible perturbative contribution to the 2-point function. The interpretation of higher functions Γ_n as 1-particle irreducible (proper) functions can be derived by successive differentiations of Eq. (S 22.3) at $\Phi_{\text{cl}} = 0$.

Problem 23*:

a) With the ansatz (P 23.2) the action becomes

$$S_a = \frac{1}{2m} \int d^4 x \left[-im\varphi + \dot{\varphi} \right]^2 - \left(m^2 + 2mV(x) \right) |\varphi|^2 = \frac{1}{2m} \int d^4 x \left[im\varphi^* \dot{\varphi} - im\dot{\varphi}^* \varphi - |\nabla\varphi|^2 - 2mV(x) |\varphi|^2 + |\dot{\varphi}|^2 \right]. \quad (\text{S 23.1})$$

Neglecting the last term in the square bracket for large mass and performing appropriate integration by parts gives the non-relativistic action

$$S_a [\varphi^*, \varphi] = \int dt \int d^3 x \varphi^*(\mathbf{x}, t) \left[i\partial_t + \frac{\Delta}{2m} - V(\mathbf{x}, t) \right] \varphi(\mathbf{x}, t) \quad (\text{S 23.2})$$

for a particle in a potential.

b) The generating functional can be calculated exactly by completing the square and performing the Gaussian integral since the full action is quadratic in the fields

$$Z[J^*, J] = \int \mathcal{D}\Phi^* \mathcal{D}\Phi \exp \left\{ i \left[S_a[\Phi^*, \Phi] + \int d^4 x (J^* \Phi + \Phi^* J) \right] \right\} = \text{const.} \exp \left[-i \left(J^*, \frac{1}{-\square - m^2 - 2mV(x)} J \right) \right]. \quad (\text{S 23.3})$$

Here the usual short-hand notation is used. This gives for the 2-point function (the only non-vanishing n -point function)

$$G_2(x_2, x_1) = (-i)^2 \frac{\delta^2}{\delta J^*(x_2)\delta J(x_1)} \frac{Z[J^*, J]}{Z[0, 0]} \Big|_{J^*=J=0} = i \left\langle x_2 \left| \frac{1}{-\square - m^2 - 2mV(x)} \right| x_1 \right\rangle. \quad (\text{S 23.4})$$

c) The Fock-Schwinger representation for the 2-point function reads

$$G_2(x_2, x_1) = \kappa \int_0^\infty dT e^{i\kappa(-m^2 + i0^+ T)} \left\langle x_2 \left| e^{-iT H} \right| x_1 \right\rangle, \quad H := \kappa \square + 2m\kappa V(x). \quad (\text{S 23.5})$$

Choose $\kappa = 1/(2m)$, then $H = -\hat{p}^2/(2m) + V(x)$ with $\hat{p}_\mu = \partial/(i\partial x^\mu)$ is formally the Hamiltonian of a non-relativistic particle moving in 4 dimensions with a mass $-m$. Therefore one can use the standard path-integral representation for the matrix element of the time-evolution operator and immediately obtain Eqs. (P 23.5), (P 23.6)

Problem 24*:

Fourier transformation gives

$$F \left(\frac{1}{i} \frac{\partial}{\partial x} \right) e^{-iax^2/2} = \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \tilde{F}(t) \underbrace{e^{t \frac{\partial}{\partial x}} e^{-iax^2/2}}_{=\exp[-ia(x+t)^2/2]} \quad (\text{S 24.1})$$

using the shift property of $\exp(t\partial/\partial x)$. Writing

$$\exp \left[-\frac{i}{2}(x+t)^2 \right] = e^{-iax^2/2} \exp \left[-i \left(at^2/2 + axt \right) \right] = e^{-iax^2/2} \exp \left[-\frac{i}{2} a \left(\frac{1}{a} \frac{\partial}{\partial x} \right)^2 \right] e^{-iaxt} \quad (\text{S 24.2})$$

one finds Eq. (P 24.1). Generalizing this result to the infinite-dimensional case and applying it to the generating functional in Eq. (3.24) one just has to set $F[y] = \exp[-i \int d^4x V(y(x))]$ and $a \rightarrow \Delta_F$ to obtain Eq. (P 24.2).

In Φ^4 -theory one has $S_{\text{int}}[\Phi] := -\lambda \int d^4x \Phi^4(x)/4!$ and up to first order

$$Z[J] = Z_0[J] \left[1 + A + \frac{1}{2}A^2 + \dots \right] \left[1 + i S_{\text{int}}[\Phi] + \mathcal{O}(\lambda^2) \right] = Z_0[J] \left[1 + \lambda \omega_1[J] + \dots \right], \quad (\text{S 24.3})$$

where the operator $A := (i \frac{\delta}{\delta \Phi}, \Delta_F \frac{\delta}{\delta \Phi})/2$ contains 2 functional derivatives – in first order one therefore only needs terms up to A^2 . Performing these derivatives one obtains $A S_{\text{int}} = -i \lambda \Delta_{xx} \Phi_x^2/4$ and $A^2 S_{\text{int}} = \lambda \Delta_{xx}^2/4$ in the abbreviated notation used when calculating the second order $\omega_2[J]$. When inserting $\Phi_x = \Delta_{xy} J_y$ this gives Eq. (3.28).

Problem 25:

a) As

$$\frac{\delta}{\delta K(x)} \exp \left[-\frac{i}{2} \int d^4y K(y) \sum_i^N \Phi_i^2(y) \right] = -\frac{i}{2} \sum_i^N \Phi_i^2(x) \cdot \exp \left[-\frac{i}{2} \int d^4y K(y) \sum_i^N \Phi_i^2(y) \right] \quad (\text{S 25.1})$$

Eq. (P 25.3) is (nearly) self-evident.

b) With vanishing interaction the generating functional is just the N -fold product of a Gaussian integral where the prefactor (the determinant, see **Problem 13 a)**) cannot be subsumed in an irrelevant constant since it depends on the source K

$$Z_0[J_i, K] = \text{const.} \prod_i^N \left(\exp \left[-\frac{i}{2} \langle J_i | \mathcal{O}_K^{-1} | J_i \rangle - \frac{1}{2} \text{tr} \ln \mathcal{O}_K \right] \right). \quad (\text{S 25.2})$$

c) Expand Eq. (P 25.3) to first order in λ and use the analogue of the relation $(e^{if})'' = (if'' - f'^2)e^{if}$ for the case of functional derivatives in order to verify Eq. (P 25.5). Normalizing the determinant to the no-source case, i.e. $\ln \mathcal{O}_K \rightarrow \ln [\mathcal{O}_0^{-1} \mathcal{O}_K] = \ln [1 - \mathcal{O}_0^{-1} K]$, and expanding the different terms up to $\mathcal{O}(K^2)$ one obtains explicitly

$$W_0[J_i, K] = -\frac{1}{2} \langle J_i | \Delta_F + \Delta_F K \Delta_F + \Delta_F K \Delta_F \Delta_F K \Delta_F + \dots | J_i \rangle + \frac{iN}{2} \text{tr} \left[-\Delta_F K - \frac{1}{2} \Delta_F K \Delta_F K - \dots \right]. \quad (\text{S 25.3})$$

Here $\mathcal{O}_0^{-1} \equiv \Delta_F$. Functional differentiation w.r.t. $K(x)$ is just a matter of book-keeping and one obtains

$$\left. \frac{\delta W_0}{\delta K(x)} \right|_{K=0} = -\frac{1}{2} \sum_i^N \langle J_i | \Delta_F | x \rangle \langle x | \Delta_F | J_i \rangle - \frac{iN}{2} \Delta_F(0) \quad (\text{S 25.4})$$

$$\left. \frac{\delta^2 W_0}{\delta K(x)^2} \right|_{K=0} = -\sum_i^N \langle J_i | \Delta_F | x \rangle \langle x | \Delta_F | J_i \rangle \Delta_F(0) - \frac{iN}{2} \Delta_F^2(0). \quad (\text{S 25.5})$$

This gives the following symmetry factors in first-order perturbation theory: For the vacuum energy density $N^2 + 2N$ (in agreement with Eq. (3.28) for $N = 1$), for the 2-point function $2N + 4$ ($= 6$ for $N = 1$) and 1 for the 4-point function (unchanged).

Problem 26:

a) Multiplying out the field-strength term in the Lagrangian one has

$$S_0[V] = -2 \frac{1}{4} \int d^4x \left[\partial_\mu V_\nu \partial^\mu V^\nu - \partial_\mu V_\nu \partial^\nu V^\mu - m_V^2 V_\mu V^\mu \right] = \frac{1}{2} \int d^4x V_\mu \left[(\square + m_V^2) g^{\mu\nu} - \partial^\mu \partial^\nu \right] V_\nu \quad (\text{S 26.1})$$

with the help of an integration by parts. Thus the Gaussian integration gives for the free generating functional

$$\begin{aligned} Z_0[J_\mu] &= \int \left(\prod_\rho \mathcal{D}V_\rho \right) \exp \left\{ i S_0[V] + i \int d^4x J_\mu(x) V^\mu(x) \right\} \\ &= \text{const.} \exp \left\{ -\frac{i}{2} \int d^4x d^4y J^\mu(y) \left\langle y \left| \left[(\square + m_V^2) g^{\mu\nu} - \partial^\mu \partial^\nu \right]^{-1} \right| x \right\rangle J^\nu(x) \right\}. \end{aligned} \quad (\text{S 26.2})$$

In momentum space the free propagator therefore is

$$\tilde{D}_{\mu\nu}(k) = \left[(-k^2 + m_V^2) g^{\mu\nu} + k^\mu k^\nu \right]^{-1}. \quad (\text{S 26.3})$$

For the inversion in Lorentz space one can make the *ansatz* $\tilde{D}_{\mu\nu}(k) = A(k) g_{\mu\nu} + B(k) k_\mu k_\nu$ (these are the only available Lorentz structures). Requiring that $[(-k^2 + m_V^2) g_{\mu\rho} + k_\mu k_\rho] (A(k) g^{\rho\nu} + B(k) k^\rho k^\nu) = \delta_\mu^\nu$ one finds $A(k) = -1/(k^2 - m_V^2)$, $B(k) = -A(k)/m_V^2$ leading to Eq. (3.59).

b) For the photon propagator in covariant gauge one has to evaluate

$$\tilde{\Delta}_{\mu\nu}(k) = \left[-k^2 g^{\mu\nu} + \left(1 - \frac{1}{\lambda} \right) k^\mu k^\nu \right]^{-1} \stackrel{!}{=} A(k) g_{\mu\nu} + B(k) k_\mu k_\nu \quad (\text{S 26.4})$$

and finds by a similar procedure $A(k) = -1/k^2$, $B(k) = (\lambda - 1)A(k)/k^2$. Note the different behaviour of the massive and massless vector propagators for large k , i.e. the different terms $B(k)$.

Problem 27:

If the transformation parameter depends on the spacetime then the Lagrangian changes as follows

$$\mathcal{L}(\Phi, \partial_\mu \Phi) \longrightarrow \mathcal{L}(\Phi, \partial_\mu \Phi) + (\partial_\mu \alpha(x)) \Delta\Phi(x) \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} + \alpha(x) \partial_\mu \Lambda^\mu, \quad (\text{S 27.1})$$

since terms which do not contain derivatives of $\alpha(x)$ vanish due to the assumed invariance under constant transformations or combine into the total derivative. Assume that the symmetry transformation is not "anomalous", i.e. that the Jacobian of the transformation is unity, then one has

$$\int \mathcal{D}\Phi i \int d^4x \Delta \mathcal{L} e^{iS[\Phi]} = \int \mathcal{D}\Phi i \int d^4x \left[(\partial_\mu \alpha(x)) \Delta\Phi(x) \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} + \alpha(x) \partial_\mu \Lambda^\mu \right] e^{iS[\Phi]} = 0. \quad (\text{S 27.2})$$

Perform an integration by parts in the term containing $\partial_\mu \alpha(x)$ and conclude from the arbitrariness of $\alpha(x)$ that

$$\partial_\mu \langle J^\mu(x) \rangle = 0, \quad \text{with} \quad J^\mu(x) := C \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} \Delta\Phi - \partial_\mu \Lambda^\mu \right]. \quad (\text{S 27.3})$$

The normalization C of this conserved current is arbitrary.

a1) For $\mathcal{L}_0 = |\partial\Phi|^2 - m^2|\Phi|^2$ one has $\Delta\Phi = i\Phi$, $\Delta\Phi^* = -i\Phi^*$, $\Lambda_\mu = 0$ and therefore (summing over the two independent fields)

$$J_\mu(x) = (\partial_\mu \bar{\Phi}^*(x)) i\Phi(x) - i\Phi^*(x) (\partial_\mu \bar{\Phi}(x)). \quad (\text{S 27.4})$$

If $C = 1/(2m)$ is taken, the result is in agreement with **{Itzykson-Zuber}** eq. (2-5). This current is obviously also conserved if there is an interaction of the form $V(\Phi^* \Phi)$.

a2) For $\mathcal{L}_0 = i\bar{\psi}\gamma \cdot \partial\psi/2 - m\bar{\psi}\psi$ one has $\Delta\Psi = i\psi$, $\Delta\bar{\psi} = -i\bar{\psi}$, $\Lambda_\mu = 0$ and thus

$$J_\mu = i\frac{i}{2}\bar{\psi}\gamma_\mu\psi + (-i)\frac{-i}{2}\bar{\psi}\gamma_\mu\psi = -\bar{\psi}\gamma_\mu\psi. \quad (\text{S 27.5})$$

The same result is obtained if the equivalent Lagrangian $\mathcal{L}_0 = \bar{\psi}(i\gamma \cdot \partial - m)\psi$ is used. The normalization $C = -1$ gives the standard result (see, e.g. **{Itzykson-Zuber}** eq. (2-13)).

a3)* For the Walecka Lagrangian the nucleonic parts $\bar{\Psi}(i\rlap{/}\partial - M)\Psi - g_\sigma\bar{\Psi}\Psi\sigma - g_\omega\bar{\Psi}\gamma_\mu\Psi\omega^\mu$ do not contain additional derivatives of the nucleon field. Hence the same Dirac current $\bar{\Psi}\gamma_\mu\Psi$ remains conserved.

a4) For the non-relativistic Lagrangian for particles interacting via a local 2-body potential one can write $\mathcal{L} = \Phi^*(\mathbf{x}, t)i\hbar\partial_t\Phi(\mathbf{x}, t) - \mathcal{T} - \mathcal{V}$. After an integration by parts in the Lagrange function the kinetic energy density reads $\mathcal{T} = \hbar^2(\nabla\Phi^*(\mathbf{x}, t)) \cdot (\nabla\Phi(\mathbf{x}, t))/(2m)$, and the potential energy density is $\mathcal{V} = -(1/2)\int d^3x' \Phi^*(\mathbf{x}, t)\Phi^*(\mathbf{x}', t)V(\mathbf{x}-\mathbf{x}')\Phi(\mathbf{x}', t)\Phi(\mathbf{x}, t)$. Therefore the Lagrangian is invariant under the global phase transformation (P 27.3) although it is non-local, i.e. does not depend only on the field $\Phi(\mathbf{x}, t)$ and its derivative as was assumed when deriving the Noether current (S 27.3). However, for a local potential the x -dependent transformation does not give a contribution and one can apply the same procedures:

$$\frac{\partial \mathcal{L}}{\partial(\partial_t \Phi)} = i\hbar\Phi^*, \quad \frac{\partial \mathcal{L}}{\partial(\nabla\Phi)} = -\frac{\hbar^2}{2m}\nabla\Phi^*, \quad \frac{\partial \mathcal{L}}{\partial(\nabla\Phi^*)} = -\frac{\hbar^2}{2m}\Phi. \quad (\text{S 27.6})$$

It then follows that

$$J_0 = -\hbar\Phi^*\Phi, \quad J_k = i\frac{\hbar^2}{2m}[\Phi^*\nabla_k\Phi - (\nabla_k\Phi^*)\Phi], \quad k = 1, 2, 3 \quad (\text{S 27.7})$$

is conserved: $\partial J_0 + \nabla_k J_k = 0$. If the normalization is taken as $C = -1/\hbar$ one has agreement with standard quantum-mechanical results (see, e.g. **{Messiah 1}**, eqs. (IV.9) and (IV.11)).

In the most general case of a (non-local) interaction $V = \int d^3x_1 d^3x_2 d^3x_3 d^3x_4 \Phi^*(\mathbf{x}_1, t)\Phi^*(\mathbf{x}_2, t)V(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)\Phi(\mathbf{x}_4)\Phi(\mathbf{x}_3)$ there is a new source of contributions for a x -dependent transformation – the current is modified by a non-local interaction. This is well-known in Nuclear Physics where special non-local (so-called Yamaguchi) potentials have been frequently used to describe the two-nucleon bound state, the deuteron.

b) The shift operator is $\exp(a_\mu \partial^\mu)$. Therefore the change of the Lagrangian for infinitesimal, constant a_μ is a total derivative $\Delta\mathcal{L}\Big|_a = a_\mu \partial^\mu \mathcal{L}$. Thus expanding $\mathcal{L}(\Phi + \Delta\Phi, \partial\Phi + \partial\Delta\Phi)$ one obtains

$$\Delta\mathcal{L}\Big|_{a(x)} = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} (\partial_\mu a_\nu) \partial^\nu \Phi + a_\mu \partial^\mu \mathcal{L}. \quad (\text{S 27.8})$$

The only difference to Eq. (S 27.2) is that the infinitesimal parameter now has a Lorentz index so that after an integration by parts one obtains

$$0 = \int \mathcal{D}\Phi e^{iS[\Phi]} \int d^4x (-\Delta \mathcal{L}) \Big|_{a(x)} = \int \mathcal{D}\Phi e^{iS[\Phi]} \int d^4x a_\nu(x) \partial_\mu \underbrace{\left[\frac{\partial \mathcal{L}}{\partial (\partial_\mu \Phi)} \partial^\nu \Phi - g^{\mu\nu} \mathcal{L} \right]}_{=: T^{\mu\nu}}. \quad (\text{S 27.9})$$

For a Lagrangian of the form (3.1) the energy-momentum tensor is symmetric $T^{\mu\nu} = \partial^\mu \Phi \partial^\nu \Phi - g^{\mu\nu} \mathcal{L}$. In particular, one finds $T^{00} = [(\partial_0 \Phi)^2 + (\nabla \Phi)^2 + m^2 \Phi^2]/2 + V(\Phi) \equiv \mathcal{H}$, i.e. the Hamilton density is a special component of the energy-momentum tensor. In contrast, the Lagrange density (Lagrangian) is a Lorentz scalar.

Problem 28*:

a) Since $\not{\psi} \psi = v^2 = 1$ it is clear that Φ, χ are eigenfunctions of $\not{\psi}$ with eigenvalue $+1, -1$, respectively. Similarly, one also has $\bar{\psi} / \bar{\chi} \not{\psi} = \pm \bar{\psi} / \bar{\chi}$ from the corresponding definitions of $\bar{\Phi}, \bar{\chi}$ (note that this cannot be “derived” as $\bar{\Phi}, \bar{\chi}$ are independent Grassmann-valued fields over which one has to integrate and **not** $\Phi^\dagger \gamma_0, \chi^\dagger \gamma_0$!). Using Eq. (P 28.5) the anticommutator becomes

$$[\not{D}^\perp, \not{\psi}]_+ = (\not{D} - v \cdot D \not{\psi}) \not{\psi} + \not{\psi} (\not{D} - v \cdot D \not{\psi}) = \not{D} \not{\psi} + \not{\psi} \not{D} - 2v \cdot D = -i\sigma_{\mu\nu} D^\mu v^\nu - i\sigma_{\mu\nu} v^\mu D^\nu = 0 \quad (\text{S 28.1})$$

due to the antisymmetry of $\sigma_{\mu\nu}$ (cf. Ref. [63]).

b) Substitute $\Psi = \exp(-iMv \cdot x) (\Phi + \chi)$ into Eq. (P 28.1) and use $i\not{D} \exp(-iMv \cdot x) \phi / \chi = \exp(-iMv \cdot x) (i\not{D} + M)\phi / \chi = (i\not{D} \pm M)\phi / \chi$. This gives $S = S_{\bar{\psi}, \psi} + S_{\bar{\chi}, \chi} + S_{\bar{\psi}, \chi} + S_{\bar{\chi}, \psi}$. With $\not{D} = \not{\psi} v \cdot D + \not{D}^\perp$ the first term is

$$S_{\bar{\psi}, \psi} = \left(\bar{\psi}, \left[i(\not{\psi} v \cdot D + \not{D}^\perp) + M - M^* \right] \psi \right) = \left(\bar{\psi}, [iv \cdot D + M - M^*] \psi \right) \quad (\text{S 28.2})$$

as $\bar{\psi} \not{D}^\perp \psi = \bar{\psi} \not{D}^\perp \not{\psi} \psi = -\bar{\psi} \not{\psi} \not{D}^\perp \psi = -\bar{\psi} \not{D}^\perp \psi \implies \bar{\psi} \not{D}^\perp \psi = 0$. Similar one finds

$$S_{\bar{\chi}, \chi} = \left(\bar{\chi}, \left[i(\not{\psi} v \cdot D + \not{D}^\perp) - M - M^* \right] \chi \right) = - \left(\bar{\chi}, [iv \cdot D + M + M^*] \chi \right). \quad (\text{S 28.3})$$

The mixed terms simplify to $S_{\bar{\psi}, \chi} = \left(\bar{\psi}, i\not{D}^\perp \chi \right)$, $S_{\bar{\chi}, \psi} = \left(\bar{\chi}, i\not{D}^\perp \psi \right)$ since, e.g. $\bar{\chi} (M \text{ or } M^*) \phi = \bar{\chi} (M \text{ or } M^*) \not{\psi} \phi = \bar{\chi} \not{\psi} (M \text{ or } M^*) \phi = -\bar{\chi} (M \text{ or } M^*) \phi \implies \bar{\chi} (M \text{ or } M^*) \phi = 0$. Altogether this gives Eq. (P 28.6). One may integrate out the “small” component χ by using the extended Gaussian Grassmann integral (2.149). This leads to

$$S_{\text{eff}}[\bar{\Phi}, \phi] = \int d^4x \bar{\Phi} \left[iv \cdot D + M - M^* - \not{D}^\perp \frac{1}{iv \cdot D + M + M^*} \not{D}^\perp \right] \Phi - i \text{tr} \ln [iv \cdot D + M + M^*], \quad (\text{S 28.4})$$

where the last term from the determinant is a constant for external potentials which drops out when calculating Green functions as ratios of path integrals.

Now assume that the mass is large compared to the potentials and the derivatives and that one can expand

$$S_{\text{eff}}[\bar{\Phi}, \phi] = \int d^4x \bar{\Phi} \left[iv \cdot \partial - v \cdot A(x) - U_S(x) - \frac{\not{D}_\perp^2}{2M} + \frac{1}{4M^2} \not{D}^\perp (iv \cdot D + U_S(x) - v \cdot A(x)) \not{D}^\perp + \mathcal{O}(1/M^3) \right] \Phi. \quad (\text{S 28.5})$$

c) For $v_\mu = (1, \mathbf{0})$ and $A_\mu(x) = (U_V(\mathbf{x}), \mathbf{0})$ one has $\not{D}_\perp = -\vec{\gamma} \cdot \nabla \implies \not{D}_\perp^2 = -\Delta$ and Eq. (S 28.5) simplifies to

$$S_{\text{eff}}[\bar{\Phi}, \Phi] = \int d^4x \bar{\Phi} \hat{L} \Phi \quad \text{with} \quad \hat{L} = i\partial_t - U_+ + \frac{\Delta}{2M} + \frac{1}{4M^2} (i\partial_t \Delta + \vec{\sigma} \cdot \nabla U_- \vec{\sigma} \cdot \nabla) \quad (\text{S 28.6})$$

where the explicit form (P 28.8) of the Dirac matrices and the abbreviation $U_\pm := U_S \pm U_V$ has been used. In the $\mathcal{O}(1/M^2)$ -term there is an additional time-derivative which can be removed by a rescaling of the fields: $\Phi = (1 - \Delta/(4M^2))^{-1/2} \varphi$, $\bar{\Phi} =: \bar{\varphi} (1 - \Delta/(4M^2))^{-1/2}$ (the Jacobian is an irrelevant constant) so that one can read off the equivalent Hamiltonian $\hat{L} =: i\partial_t - \hat{H}$ as

$$\hat{H} = -\frac{\Delta}{2M} + U_+ + \frac{1}{8M^2} (\Delta U_+ + U_+ \Delta) + \frac{1}{4M^2} \vec{\sigma} \cdot \nabla U_- \vec{\sigma} \cdot \nabla + \mathcal{O}(1/M^3). \quad (\text{S 28.7})$$

acting between $\bar{\varphi}$ and φ . The 3rd term arises from the transformation $\Phi \rightarrow \varphi$ and explicitly reads $[(\Delta U_+) + 2(\nabla U_+) \cdot \nabla + 2U_+ \Delta]/(8M^2)$ when taking into account that the derivatives also act on the field. Similar, the last term has the form $[(\nabla U_-) \cdot \nabla + i\vec{\sigma} \cdot ((\nabla U_-) \times \nabla)]/(4M^2)$ and contains the spin-orbit interaction. Altogether one finds

$$\hat{H} = -\frac{\Delta}{2M} + \frac{1}{2M^2} [U_S \Delta + (\nabla U_S) \cdot \nabla] + U_+ + \frac{1}{8M^2} (\Delta U_+) + V_{LS} \quad (\text{S 28.8})$$

where for spherically symmetric potentials

$$V_{LS} = \frac{1}{4M^2} \frac{1}{r} \frac{\partial}{\partial r} [U_V(r) - U_S(r)] \vec{\sigma} \cdot \left(\mathbf{r} \times \frac{\nabla}{i} \right). \quad (\text{S 28.9})$$

The first three terms in Eq. (S 28.8) can be concisely written as $-\nabla(M + U_S)^{-1} \cdot \nabla/2$ (up to $\mathcal{O}(1/M^3)$), i.e. as kinetic energy with an effective, position-dependent mass so that one finally obtains

$$\hat{H} = -\frac{1}{2} \nabla \frac{1}{M^*(r)} \cdot \nabla + \underbrace{U_S(r) + U_V(r)}_{=: V_c(r)} + \frac{1}{8M^2} \Delta [U_S(r) + U_V(r)] + V_{LS} + \mathcal{O}(1/M^3) \quad (\text{S 28.10})$$

in agreement with **{Bjorken-Drell 1}**, eqs. (4.5),(4.6) (no scalar potential there, no vector potential \mathbf{A} here!). The term $\Delta U_+/(8M^2)$ is the so-called Darwin term. Since U_V arises from the exchange of vector particles it is repulsive (i.e. positive) whereas the scalar potential is attractive (i.e. negative). Thus these potentials mostly cancel in the central potential but add in magnitude in the spin-orbit potential.

Problem 29:

a) By Fourier transformation and Schwinger's trick one has

$$\begin{aligned} \Delta_F(x-y) &= \int \frac{d^d k}{(2\pi)^d} e^{ik \cdot (x-y)} \frac{1}{k^2 - m^2 + i0^+} = -i \int_0^\infty dT e^{-im^2 T} \int \frac{d^d k}{(2\pi)^d} \exp \left[ik^2 T + ik \cdot (x-y) \right] \\ &= \frac{1}{(4\pi i)^{d/2}} \int_0^\infty dT \frac{1}{T^{d/2}} \exp \left(-im^2 T - i \frac{(x-y)^2}{4T} \right). \end{aligned} \quad (\text{S 29.1})$$

Here the Gaussian integral in Minkowski space (S 19.1) has been used with $a = T$ and $b_\mu = (x-y)_\mu$. The remaining T -integral can be expressed by a modified Bessel function of second kind (see **{Gradsteyn-Ryzhik}**, eq. 8.432.6) so that

$$\Delta_F(x-y) = \frac{-i}{(2\pi)^{d/2}} \left(\frac{m^2}{z} \right)^{d/2-1} K_{d/2-1}(z), \quad z := \sqrt{-m^2(x-y)^2}. \quad (\text{S 29.2})$$

Note that the argument of this Bessel function is real for space-like separation and purely imaginary for time-like $r = x-y$. For small arguments one has (see **{Handbook}**, eq. 9.6.9 and 9.6.8) $K_\nu(z) \rightarrow \frac{1}{2} \Gamma(\nu) \left(\frac{1}{2}z\right)^{-\nu}$ valid for $\text{Re } \nu > 0$ and $K_0(z) \rightarrow -\ln z$. Thus

$$\Delta_F(r) \xrightarrow{r \rightarrow 0} \begin{cases} \frac{-i}{4\pi^{d/2}} \Gamma(d/2-1) (-r^2)^{1-d/2} & \text{for } d \neq 2 \\ \frac{i}{4\pi} \ln(-m^2 r^2) & \text{for } d = 2. \end{cases} \quad (\text{S 29.3})$$

Notice that the small-distance behaviour is independent of the mass of the particle (for $d = 2$ the mass term is just a constant) which is to be expected as this corresponds to large momenta $|k^2| \gg m^2$. The dependence on (spacelike) r illustrates the frequent statement that the Coulomb potential – as solution of the Poisson equation with a point-like source, i.e. as inverse Laplacian – is linear in one dimension, logarithmic in two, of $1/r$ -type in three dimensions etc.

For large distances one can use (see **{Handbook}**, eq. 9.7.2) the asymptotic expansion $K_\nu(z) \rightarrow \sqrt{\pi/(2z)} \exp(-z)$ to obtain an oscillatory (time-like r) or exponentially decaying (spacelike r) behaviour of the free Feynman propagator.

b) For the calculation of the space-time behaviour of the photon propagator one proceeds in a similar way: Zero mass simplifies the algebra but for the gauge-dependent term in the propagator one has to use an extended Schwinger representation $1/(a+i0^+)^2 = -\int_0^\infty dT T \exp(iaT)$. Then

$$\Delta_{\mu\nu}(r) = \int_0^\infty dT \int \frac{d^d k}{(2\pi)^d} \left[ig_{\mu\nu} + (1-\lambda)T \frac{\partial^2}{\partial r^\mu \partial r^\nu} \right] e^{ik^2 T + ik \cdot r}, \quad (\text{S 29.4})$$

where the terms $k_\mu k_\nu$ have been written as derivatives w.r.t. r^μ and r^ν . The k -integration can then be performed as before and the final T -integration is even simpler: Substituting $\tau = 1/T$ one only encounters integrals of the type $\int_0^\infty d\tau \tau^{\nu-1} e^{-a\tau} = \Gamma(\nu)/a^\nu$ in the massless case. After some algebra one obtains

$$\begin{aligned} \Delta_{\mu\nu}(r) &= \frac{i}{(4\pi i)^{d/2}} \left[ig_{\mu\nu} \Gamma\left(\frac{d}{2}-1\right) \left(\frac{4}{ir^2}\right)^{d/2-1} + (1-\lambda) \Gamma\left(\frac{d}{2}-2\right) \frac{\partial^2}{\partial r^\mu \partial r^\nu} \left(\frac{4}{ir^2}\right)^{d/2-2} \right] \\ &= \frac{i^{3-d}}{4\pi^{d/2}} \Gamma\left(\frac{d}{2}-1\right) \left(\frac{1}{r^2}\right)^{d/2-1} \left[\frac{1+\lambda}{2} g_{\mu\nu} + (1-\lambda) \left(\frac{d}{2}-1\right) \frac{r_\mu r_\nu}{r^2} \right]. \end{aligned} \quad (\text{S 29.5})$$

Problem 30*:

Integrating out the electron fields in the full generating functional of QED with no external photons ($J = 0$) one gets

$$Z[\bar{\eta}, \eta] = \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \{ iS_0[A] + i(\bar{\psi}, \mathcal{O}_A \psi) + i(\bar{\psi}, \eta) + i(\bar{\eta}, \psi) \} = \int \mathcal{D}A \text{Det} \mathcal{O}_A \exp \{ iS_0[A] - i(\bar{\eta}, \mathcal{O}_A^{-1} \eta) \} \quad (\text{S 30.1})$$

with $S_0[A] = (A^\mu, \Delta_{\mu\nu}^{-1} A^\nu)$ and $\mathcal{O}_A = \not{p} - eA - m$. The 2-point function (the electron propagator) therefore is

$$\bar{G}_2(p) = \int d^4(x-y) e^{-ip \cdot (x-y)} \int \mathcal{D}A e^{iS_0[A] + tr \ln \mathcal{O}_A} \int_0^\infty dT \langle y \left| e^{i\mathcal{O}_A T} \right| x \rangle, \quad (\text{S 30.2})$$

when the Fock-Schwinger representation is being used.

The Bloch-Nordsieck approximation consists in neglecting the trace terms (vacuum polarization) and to replace the Dirac matrices $\gamma_\mu \rightarrow v_\mu = p_\mu/m_{\text{phys}}$, i.e. by a constant velocity made up by the external momentum p_μ . Then

$$e^{i\mathcal{O}_A T} \simeq \exp [i(iv \cdot \partial - ev \cdot A(x) - m) T] =: e^{-imT} \exp(-Tv \cdot \partial) F(T) \quad (\text{S 30.3})$$

and by solving the differential equation $\partial F/\partial T = -iev \cdot A(x+vT) F$ one finds an eikonal-like expression

$$\langle y \left| e^{i\mathcal{O}_A^{\text{BN}} T} \right| x \rangle = e^{-imT} \delta(y-x-vT) \exp \left[-ie \int_0^T d\tau v \cdot A(x+v\tau) \right]. \quad (\text{S 30.4})$$

Inserting that into Eq. (S 30.2) one sees that the functional integral over the photon field is now a Gaussian and can be performed. In addition, due to the δ -function the Fourier transformation can be done as well. Some algebra then gives

$$\bar{G}_2^{\text{BN}}(p) = \int_0^\infty dT e^{i(p \cdot v - m + i0^+)T} e^{X(T)}, \quad X(T) = -\frac{ie^2}{2} \int_0^T d\tau_1 d\tau_2 v^\mu v^\nu \Delta_{\mu\nu}(v(\tau_1 - \tau_2)), \quad (\text{S 30.5})$$

where $\Delta_{\mu\nu}(r)$ is the free photon propagator in x -space studied in **Problem 29**. As the integrand only depends on $\tau^2 = (\tau_1 - \tau_2)^2$ one can replace $\int_0^T d\tau_1 d\tau_2 \rightarrow 2 \int_0^T d\tau (T - \tau)$. Using Eq. (S 29.5), $v^2 = 1$ and replacing in d dimensions $e^2 \rightarrow e^2 \mu_0^{d-4}$ one obtains

$$X(T) = -\mu_0^{4-d} e^2 \frac{i^{4-d}}{4\pi^{d/2}} \Gamma\left(\frac{d}{2} - 1\right) \left[\frac{1+\lambda}{2} + (1-\lambda) \left(\frac{d}{2} - 1\right) \right] \int_0^T d\tau (T - \tau) \tau^{2-d}. \quad (\text{S 30.6})$$

In dimensional regularization it is assumed that d is such that the integrals converge followed by an analytic continuation to $d = 4 - 2\epsilon$. Thus in the remaining τ -integral there is no contribution (or divergence) at the lower limit and one finds

$$X(T) = -\frac{e^2}{16\pi^2} (i\sqrt{\pi}\mu_0 T)^{2\epsilon} \frac{\Gamma(-\epsilon)}{1-2\epsilon} \left[3 - \lambda - 2(1-\lambda)\epsilon \right] = \frac{\kappa}{2\epsilon} + \kappa \ln(\mu_0 T) + C + \mathcal{O}(\epsilon), \quad (\text{S 30.7})$$

where

$$\kappa := \frac{e^2}{8\pi^2} (3 - \lambda), \quad C := \frac{e^2}{16\pi^2} [4 + (3 - \lambda)(\gamma_E + \ln(\pi) + i\pi)]. \quad (\text{S 30.8})$$

The proper-time integration can now be performed by means of Euler's Gamma-function integral (P 18.4) so that one has

$$\bar{G}_2^{\text{BN}}(p) = \frac{\Gamma(1 + \kappa)}{\mu_0} (i\mu_0 m_{\text{phys}})^{1+\kappa} \frac{\exp[\kappa/(2\epsilon) + C]}{(p^2 - m m_{\text{phys}} + i0^+)^{1+\kappa}}. \quad (\text{S 30.9})$$

One sees that the pole of the free propagator has turned into a branch cut unless the gauge fixing parameter is chosen as $\lambda = 3$ (Yennie gauge). There is no mass renormalization: Requiring the singularity to happen at $p^2 = m_{\text{phys}}^2$ implies $m = m_{\text{phys}}$. For the wave function renormalization constant one finds

$$Z_2 = \left(\frac{\mu_0}{m}\right)^\kappa \Gamma(1 + \kappa) \exp\left[\frac{\kappa}{2} \left(\frac{1}{\epsilon} + \gamma_E + \ln \pi + 2i\pi\right) + \frac{e^2}{4\pi^2}\right], \quad (\text{S 30.10})$$

an expression which contains all divergences for $\epsilon \rightarrow 0$ and becomes unity with no interaction ($e^2 = 0$).

The singularity of the electron propagator at $p^2 = m_{\text{phys}}^2$ (pole or branch point) is determined by the large- T behaviour of the proper-time integrand in Eq. (S 30.5), i.e. of the quantity $X(T)$. Disregarding irrelevant Lorentz structures this behaviour can be traced back to the short- or long-distance limits of the scalar Feynman propagator, viz. the corresponding limits of the modified Bessel functions: For massless ($\mu = 0$) photons the *logarithmic* behaviour of $X(T)$ is caused by the $\mu\tau \rightarrow 0$ -limit for the Feynman propagator as given in the first line of Eq. (S 29.3). This then leads to the $(T - \tau)\tau^{-2+2\epsilon}$ behaviour of the integrand in Eq. (S 30.6), i.e. after integration and the limit $\epsilon \rightarrow 0$ to the logarithmic growth of $X(T)$ and thereby to the branch-type singularity of the electron propagator. In contrast, for $\mu \neq 0$ the $\mu\tau \rightarrow \infty$ -limit of the Feynman propagator matters at large T and τ ; the integrand of $X(T)$ then behaves like $\sqrt{\mu}(T - \tau)\tau^{-3/2} \exp(-i\mu\tau)$ making the integral convergent for $T \rightarrow \infty$. This leads to $X(T) \xrightarrow{T \rightarrow \infty} C_1 T + C_0$. Thus for massive photons the electron propagator would still display a pole as the linear term in T just gives a mass renormalization whereas the constant C_0 contributes to the wave function renormalization constant.

Problem 31*:

Compare the infinitesimal gauge transformation for the fermion field in Eq. (3.105) $\delta\psi(x) = -ig\Theta^a(x)T^a\psi(x)$ with the BRST transformation $\delta\psi(x) = -ig\omega\chi^a(x)T^a\psi(x)$: This allows to identify the parameter of the gauge transformation as $\Theta^a(x) \equiv -\omega\chi^a(x)$. That value inserted into the gauge transformation (3.106) for the gauge field also reproduces the BRST transformation of the field:

$$\delta A_\mu^a = \partial_\mu [\omega\chi^a(x)] - gf^{abc}\omega\chi^b A_\mu^c = \omega \underbrace{[\partial_\mu\delta^{ab} + gf^{acb}A_\mu^c]}_{\equiv D_\mu^{ab}} \chi^b. \quad (\text{S 31.1})$$

Here $D_\mu^{ab}(x)$ exactly is the covariant derivative (3.111) in the adjoint representation under which the gauge fields transform. As by construction the fermionic and gauge-field part of the Lagrangian are invariant under a local gauge transformation, one therefore also has invariance of $\mathcal{L}_f + \mathcal{L}_g$ under BRST transformations.

Consequently one only has to prove the invariance of the gauge-fixing Lagrangian $\mathcal{L}_{\text{gauge}}$ and of the Faddeev-Popov part \mathcal{L}_{FP} :

$$\delta(\mathcal{L}_{\text{gauge}} + \mathcal{L}_{FP}) = \delta \left[-B^a \partial^\mu A_\mu^a - (\partial^\mu \bar{\chi}^a) (D_\mu \chi)^a \right] = -B^a \omega \partial^\mu (D_\mu \chi)^a - \omega (\partial^\mu B^a) (D_\mu \chi)^a + (\partial^\mu \bar{\chi}^a) \delta((D_\mu \chi)^a). \quad (\text{S 31.2})$$

The first two terms cancel (after an integration by parts in the action) and thus one has to evaluate

$$\begin{aligned} \delta((D_\mu \chi)^a) &= D_\mu^{ab} \delta\chi^b + D_\mu^{ab} \delta\chi^b + gf^{acb} \delta A_\mu^c \chi^b = \left[\partial_\mu \delta^{ab} + gf^{acb} A_\mu^c \right] \left[-\frac{g}{2} \omega f^{bed} \chi^e \chi^d \right] \\ &+ gf^{abc} \omega \left[(\partial_\mu \delta^{cd} + gf^{ced} A_\mu^e) \chi^d \right] \chi^b =: \frac{g}{2} \omega X_1^a + \frac{g^2}{2} \omega X_2^a. \end{aligned} \quad (\text{S 31.3})$$

The terms $\mathcal{O}(g)$

$$X_1^a = -f^{acd} \partial_\mu (\chi^c \chi^d) + 2f^{acb} (\partial_\mu \chi^c) \chi^b = 0 \quad (\text{S 31.4})$$

cancel if product rule and anticommutativity of the ghost fields χ are used. The terms $\mathcal{O}(g^2)$ read

$$X_2^a = -f^{acb} f^{bed} \chi^e \chi^d A_\mu^c + 2f^{abc} f^{ced} A_{m\mu}^e \chi^d \chi^b. \quad (\text{S } 31.5)$$

By carefully renaming indices one finds

$$X_2^a = \left[2f^{acd} f^{deb} + f^{aed} f^{dbc} \right] \chi^b \chi^c A_\mu^e = \left[-f^{ade} f^{bcd} - 2f^{bde} f^{cad} \right] \chi^b \chi^c A_\mu^e \quad (\text{S } 31.6)$$

where the antisymmetry properties of the structure constants again has been used. Finally in the last term one can exchange $b \leftrightarrow c$ and use $\chi^c \chi^b = -\chi^b \chi^c$. Adding it to the unchanged term and dividing by two gives

$$X_2^a = \left[-f^{ade} f^{bcd} - f^{bde} f^{cad} - f^{cde} f^{abd} \right] \chi^b \chi^c A_\mu^e \equiv 0 \quad (\text{S } 31.7)$$

due to the Jacobi identity (P 31.3).

Problem 32*:

a) The free lattice action may be written as (the factor a^2 is needed to make the action dimensionless)

$$S_E^{(0)} =: \frac{a^2}{2} \sum_{l, l'} \Phi_l K_{ll'} \Phi_{l'}, \quad \text{with} \quad K_{ll'} = - \sum_{\mu} (\delta_{l', l+\mu} + \delta_{l', l-\mu}) + \delta_{ll'} (8 + m^2 a^2). \quad (\text{S } 32.1)$$

(Note $l = (l_1, l_2, l_3, l_4)$ is an euclidean 4-vector made of integer numbers and μ stands for a similar unit vector in direction μ). Thus the free partition function is given by

$$Z_0[J] = \prod_k d\Phi_k \exp \left[-S_E^{(0)} + \sum_l J_l \Phi_l \right] = \text{const.} \exp \left[\frac{1}{2a^2} \sum_{l, l'} J_l K_{ll'}^{-1} J_{l'} \right] \quad (\text{S } 32.2)$$

and the free correlation function by

$$\langle \Phi_n \Phi_{n'} \rangle_0 = \frac{\partial^2 \ln Z_0(J)}{\partial J_n \partial J_{n'}} = \frac{1}{a^2} K_{nn'}^{-1}. \quad (\text{S } 32.3)$$

As in the continuum case the inverse is calculated by Fourier transform methods which have to be slightly modified as x -space is now discrete: The inversion of the Fourier transform of the propagator is achieved by multiplying both sides of Eq. (P 32.2) by $\exp(-ip \cdot ja)$ and summing over $j = l - l'$. Use of Poisson's summation formula (see, e.g. **{Lighthill}**, ch. 5.4) for the 4-dimensional case

$$\sum_{j=-\infty}^{+\infty} e^{\pm i(k-p) \cdot ja} = \left(\frac{2\pi}{a} \right)^4 \sum_{j=-\infty}^{+\infty} \delta^{(4)} \left(k - p \pm \frac{2\pi j}{a} \right) \quad (\text{S } 32.4)$$

gives

$$\sum_j K_j e^{-ip \cdot ja} = \int_{-\pi/a}^{+\pi/a} d^4 k \tilde{K}(k) \sum_j \delta^{(4)} \left(k - p - \frac{2\pi j}{a} \right) = \tilde{K}(p), \quad (\text{S } 32.5)$$

since only the term $j = 0$ contributes in the sum on the r.h.s. if $|p| < \pi/a$ which is the case one is interested in Eq. (P 32.2). Inserting Eq. (S 32.1) on the l.h.s gives $\tilde{K}(p) = 8 + m^2 a^2 - \sum_{\mu} [\exp(ip_{\mu} a) + \exp(-ip_{\mu} a)]$ and thus one obtains Eq. (3.247).

b) Here one writes (the Dirac fields ψ and $\bar{\psi}$ have dimension length $^{-3/2}$)

$$S_E^{(0)}[\bar{\psi}, \psi] = a^3 \sum_{l, l', \alpha, \beta} \bar{\psi}_{\alpha}(l) K_{\alpha\beta}(l, l') \psi_{\beta}(l') \quad (\text{S } 32.6)$$

with

$$K_{\alpha\beta}(l, l') = \frac{1}{2} \sum_{\mu} \left(\gamma_{\mu}^E \right)_{\alpha\beta} [\delta_{l, l'+\mu} - \delta_{l, l'-\mu}] + ma \delta_{ll'} \delta_{\alpha\beta}. \quad (\text{S } 32.7)$$

The free generating functional is easily calculated by performing the Grassmann Gaussian integral and the free 2-point function is obtained as

$$\langle \psi_{\alpha}(n) \bar{\psi}_{\beta}(n') \rangle_0 = \frac{1}{a^3} \left(K^{-1} \right)_{\alpha\beta} (n, n'). \quad (\text{S } 32.8)$$

As in the scalar case the inverse of the kernel K can be calculated in Fourier space and one gets $\tilde{K}^{-1}(p) = 1/\tilde{K}(p)$ with

$$\tilde{K}_{\alpha\beta}(p) = \sum_j K_{\alpha\beta}(j) e^{-ip \cdot ja} = ma \delta_{\alpha\beta} + \frac{1}{2} \sum_{\mu} \left(\gamma_{\mu}^E \right)_{\alpha\beta} [\exp(ip_{\mu} a) - \exp(-ip_{\mu} a)]. \quad (\text{S } 32.9)$$

Similar as in the continuum case, the inverse in Dirac matrix space can be found by multiplying both the denominator and numerator by $\tilde{K}^{\dagger}(p) = (ma - i \sum_{\mu} \gamma_{\mu}^E \sin(p_{\mu} a))$. The denominator then becomes diagonal

$$\tilde{K}^{\dagger}(p) \tilde{K}(p) = m^2 a^2 + \sum_{\mu, \nu} \gamma_{\nu}^E \gamma_{\nu}^E \sin(p_{\mu} a) \sin(p_{\nu} a) = m^2 a^2 + \sum_{\mu, \nu} \frac{1}{2} \left[\gamma_{\nu}^E \gamma_{\nu}^E + \gamma_{\nu}^E \gamma_{\mu}^E \right] \sin(p_{\mu} a) \sin(p_{\nu} a) = m^2 a^2 + \sum_{\mu} \sin^2(p_{\mu} a) \quad (\text{S } 32.10)$$

leading to

$$\left(\tilde{K}^{-1} \right)_{\alpha\beta} (p) = \frac{\tilde{K}^{\dagger}_{\alpha\beta}(p)}{[\tilde{K}^{\dagger}(p) \tilde{K}(p)]} \quad (\text{S } 32.11)$$

i.e. Eq. (3.250).