CLASSICAL STATISTICS

- **TOPICS COVERED:**

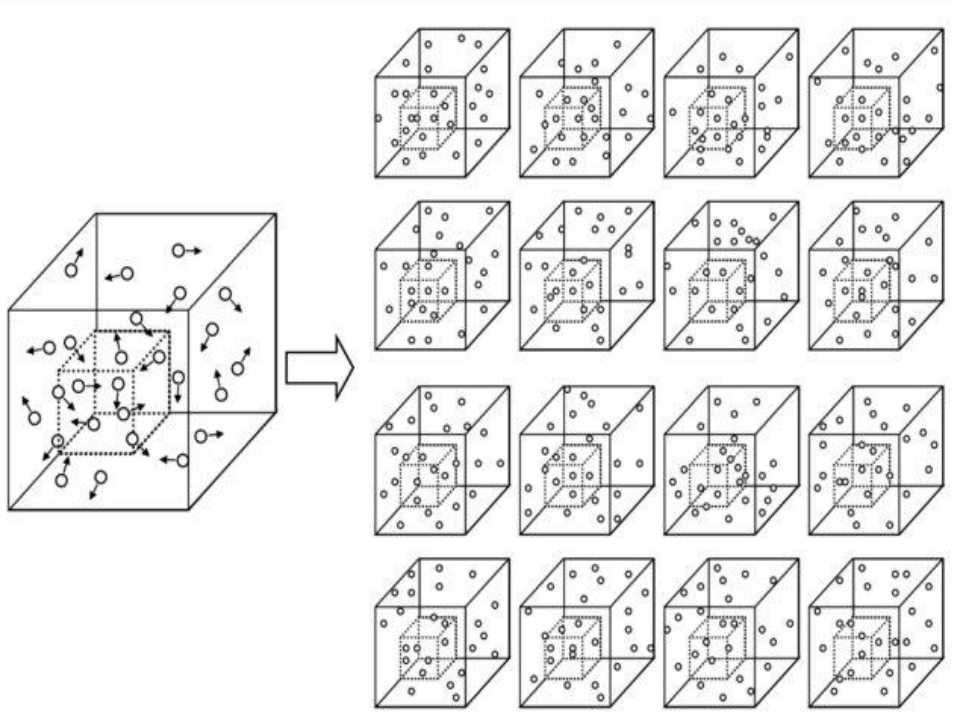
➢ **Elementary Concept of Ensemble**

ENSEMBLES

- An ensemble (also statistical ensemble) is an idealization consisting of a large number of virtual copies (sometimes infinitely many) of a system, considered all at once, each of which represents a possible state that the real system might be in.

- A thermodynamic ensemble is a specific variety of statistical ensemble that, among other properties, is in statistical equilibrium, and is used to derive the properties of thermodynamic systems from the laws of classical or quantum mechanics

ENSEMBLES

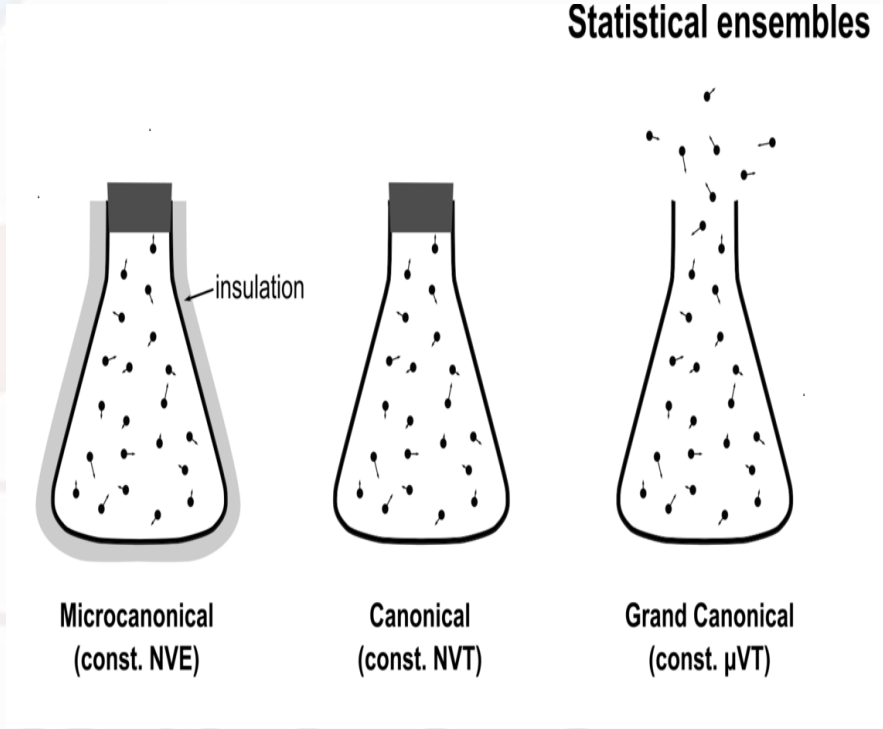


The fundamental idea of ensemble statistics is that **time average equals ensemble average !!!!**

We can therefore apply the same statistics to average a single snapshot of many identical systems as we would for multiple snapshots of a single system at different times

Types of Ensembles

ensemble	imposed variables (constraints)	fluctuating properties	corresponding thermodynamic system
microcanonical (NVE)	number of particles N volume V internal energy E	energy (quantum state) of each particle ε_i	isolated
canonical (NVT)	number of particles N volume V temperature T	internal energy E_i	closed
grand canonical (μVT)	chemical potential μ volume V temperature T	number of particles N_i internal energy E_i	open
isothermal-isobaric (NPT)	number of particles N pressure p temperature T	volume V_i internal energy E_i	-



Microcanonical ensemble or NVE ensemble

- a statistical ensemble where the total energy of the system and the number of particles in the system are each fixed to particular values.
- each of the members of the ensemble are required to have the same total energy and particle number.
- The system must remain totally isolated (unable to exchange energy or particles with its environment) in order to stay in statistical equilibrium

Canonical ensemble or NVT ensemble

- a statistical ensemble where the energy is not known exactly but the number of particles is fixed. In place of the energy, the temperature is specified.
- The canonical ensemble is appropriate for describing a closed system which is in, or has been in, weak thermal contact with a heat bath.
- In order to be in statistical equilibrium, the system must remain totally closed (unable to exchange particles with its environment) and may come into weak thermal contact with other systems that are described by ensembles with the same temperature

Grand canonical ensemble or μVT ensemble

- a statistical ensemble where neither the energy nor particle number are fixed.
- In their place, the temperature and chemical potential are specified.
- The grand canonical ensemble is appropriate for describing an open system: one which is in, or has been in, weak contact with a reservoir (thermal contact, chemical contact, etc.).
- The ensemble remains in statistical equilibrium if the system comes into weak contact with other systems that are described by ensembles with the same temperature and chemical potential.

REFERENCES

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- Statistical Mechanics, R.K. Pathria, Butterworth Heinemann: 2nd Ed., 1996, Oxford University Press
- Statistical and Thermal Physics, S. Lokanathan and R.S. Gambhir. 1991, Prentice Hall
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