Chapter 7

Microcanonical Ensemble (E, V, N)

1. Definition

We consider an isolated system with $\boxed{N}$ particles and energy $\boxed{E}$ in a volume $\boxed{V}$. By definition, such a system exchanges neither particles nor energy with the surroundings and is known as Microcanonical Ensemble. Micro Canonical Ensemble is theoretical tool used to analyze an **isolated** thermo dynamic system.

Uniform distribution of microstates. The assumption, that thermal equilibrium implies that the distribution function $\rho(q, p)$ of the system is a function of its energy,

$$\rho(q,p)=\rho(H(q,p)),\quad \frac{d}{dt}\rho(q,p)=\frac{\partial\rho}{\partial H}\dot{E}\equiv 0$$

leads to a constant $\rho(q,p)$, which is manifestly consistent with the **ergodic** hypothesis and the postulate of a priori equal probabilities.

Schematically the system can be shown as,

NVE	NVE	NVE	NVE
NVE	NVE	NVE	NVE
NVE	NVE	NVE	NVE
NVE	NVE	NVE	NVE
NVE	NVE	NVE	NVE
NVE	NVE	NVE	NVE

In above table each cell considers as each microstate energy, volume and no of particle is fixed in each cell.

Energy Shell

We consider a small but finite shell $[E, E+\Delta]$ close to the energy surface.

The Microcanonical ensemble is then defined by,

$$\boxed{\begin{aligned} \rho(q,p) &= \begin{cases} \dfrac{1}{\Gamma(E,V,N)} & E < H(q,p) < E+\Delta \end{cases} \\ &= 0 \qquad\qquad\quad Otherwise \end{aligned}} \tag{1}$$

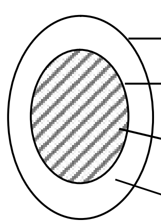
We define in (1) with,

$$\Gamma(E,V,N) = \iint\limits_{E<H(q,p)<E+\Delta} d^{3N}q d^{3N}p \tag{2}$$

the phase space volume occupied by the Microcanonical ensemble.

This is the volume of the shell bounded by the twoenergy surfaces with energies E and E + Δ

The dependence on the spatial volume V comes (2) from the limits of the integration over dq_i.



Infinitesimal shell. Let Φ (E, V) be the total volume of phase space enclosed by the energy surface E. We then have that

$$\Gamma(E) = \Phi(E + \Delta) - \Phi(E)$$

Taking with $\Delta \to 0$ the limit of an infinitesimal shell thickness we obtain

$$\Gamma(E) = \frac{\partial \phi}{\partial E}\Delta \equiv \Omega(E)\Delta, \quad \Delta \ll E$$

Density of states. The quantity $\Omega(E)$,

$$\boxed{\Omega(E) = \frac{\partial \phi(E)}{\partial E} = \int d^{3N}q \int d^{3N}p\, \delta(E - H(p,q))}$$

is the density of states at energy E. The distribution of microstates ρ is therefore given in terms of $\Omega(E)$, as

$$\rho(q,p) = \begin{cases} \dfrac{1}{\Gamma(E,V,N)} & E < H(q,p) < E + \Delta \\ = \ 0 & Otherwise \end{cases}$$

Note that the formal divergence of $\rho(q,p)$ with $1/\Delta$.