Ensemble

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What is ensemble?

A single particle is called system & collection of particles called as a whole assembly. A large number of assembly is called ensemble. The number of ensemble are identical feature known as element. The element differ in their state i.e. coordinates and velocities. Thus an ensemble is defined as a collection of very large number of assemblies which are essentially independent of one another but which have been made macroscopically as identical as possible. By being macroscopically identical we mean that each assembly is characterized by same values of set of macroscopic parameters which uniquely determine the equilibrium state of assembly.

Ensembles are divided into three classes –

1) Microcanonical Ensembles
2) Canonical Ensembles
3) Grand Canonical Ensembles

Microcanonical Ensembles:

This ensembles consists of systems which are isolated from rest of the surroundings.

Such a system is also known as a closed isolated system & has a fixed volume, fixed total energy and fixed total number of particles.

The probability density $\rho(p, q)$ of such a system differs from zero only on the constant energy hyper surface.

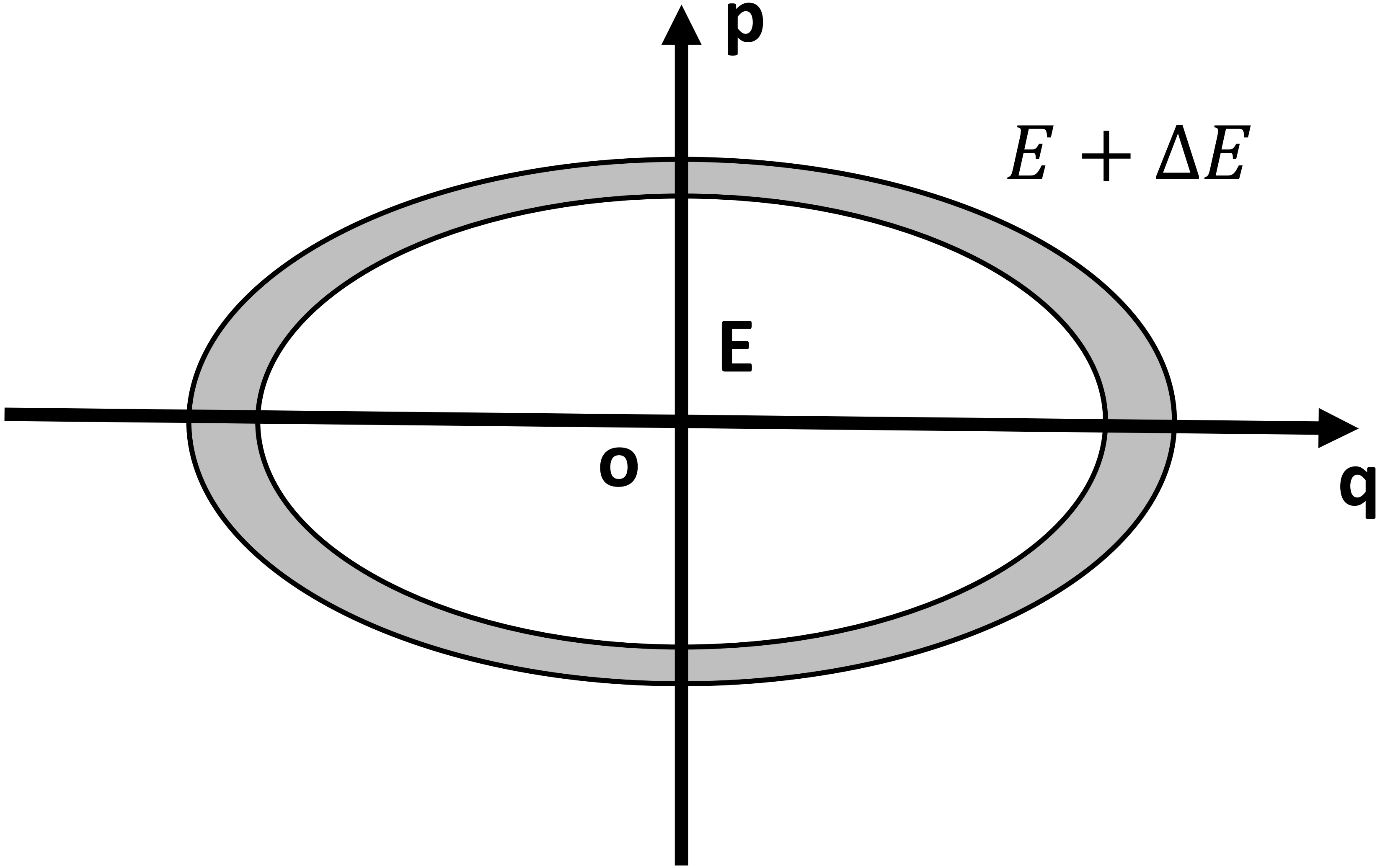
But in reality one cannot achieve complete isolation of system.

So it must allow for some interaction energy ΔE though it is very small.

The elements of the microcanonical ensemble thus lie within the range between E and $E + \Delta E$.

Let ellipse *E* represents a system with total energy *E*. This system is just one member of the ensemble.

The other members may have energy between E and $E + \Delta E$.



$Fig\ 1$

Hence their corresponding phase points will be lie between two ellipses. The thin elliptic cloud is the energy shell.

As if ΔE as smaller and smaller the energy shell between the two surface would be just a surface in the limit as $\Delta E \to 0$

According to the fundamental postulate of equal priori probability under the condition of equilibrium the system is equally likely to be found in one of its accessible states.

In the case of microcanonical ensemble all states between E and $E + \Delta E$ are equally accessible.

Therefore if the system is in state of X, corresponding energy E_X, probability P_X of finding the system in the state is given by –

$$P_X = C, \qquad if\ E < E_X < E + \Delta E$$
$$P_X = 0, \qquad otherwise$$

Where C is constant, the value of which can be determined from normalization condition $\sum P_X = 1$ when summed over all accessible states in the range between E and $E + \Delta E$.

Canonical Ensemble:

Microcanonical ensemble is fundamental, in which the constituent system are isolated and not influenced in any way by external disturbance.

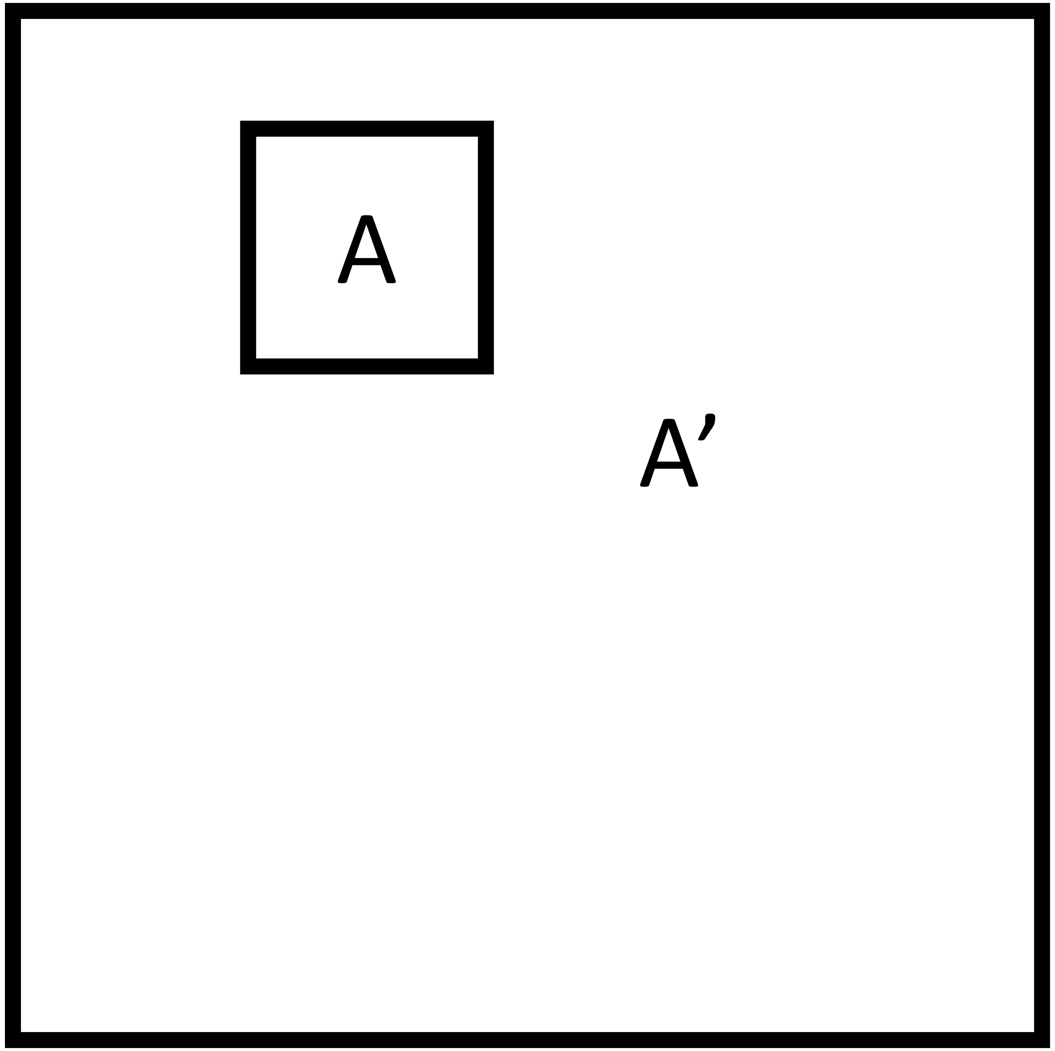
Microcanonical ensemble are best suited for isolated system, but when we deal with a complete isolated system, there is some always energy exchange with surroundings.

Therefore it is realistic that to use an ensemble in which statistical equilibrium is attained not by isolation, but by free interaction.

Canonical ensembles have been found to be more appropriate for description of such system.

Besides canonical approach gives result which apply even when components interact strongly.

Let to study the statistical properties of thermodynamical system A, Let there is a possibility an assembly of a very large number of system *N* identical in volume and molecular composition with A. Each system of assembly is considered to be thermal contact with a huge heat reservoir, whose heat capacity is so much higher than that of sub system in contact with it.


A
A’

So heat flow from or to the heat reservoir does not change its temperature significantly.

The assembly can be thought of as contained within a microcanonical ensemble.

Each system of assembly is in contact with other elements of microcanonical ensemble, but isolated from outside.

The wall of container of the system of assembly which allow heat to flow through them, but do not allow the exchange of mass.

An assembly of this kind is called a canonical ensemble of system of type A

The number of system in a canonical ensemble is constant but their energy is not fixed.

Let us find the probability that a canonical system under the condition of equilibrium is in a particular state with specific energy $E_A^{/}$.

Considering a canonical system A in a microcanonical ensemble $A^{/}$ ($A << A^{/}$)

The wall of A and $A^{/}$ are such that free to exchange energy.

The microcanonical ensemble is isolated & its total energy E_0 is constant.

A large number of microstate corresponding to macroscopic state of microcanonical ensemble with energy E_0.

Let Ω_0 be the total number of microstate of microcanonical ensemble with energy E_0.

By postulate of equal priori probability all microstate are equally probable.

Therefore of each microstate is $\frac{1}{\Omega_0}$

It is obvious that different microstate of microcanonical ensemble $A^{/}$ will give rise to different microstate of A with energy E_A $(E_A << E_0)$

Hence energy of remaining part of the complete system is $(E_0 - E_A)$.

This is one microstate of A with energy E_A attained through other microstate of $A^/$.

Let number of states of the microcanonical ensemble $A^/$ through which the states of small system A corresponding to energy E_A are attained be $\Omega_A(E_0 - E_A)$.

Therefore the probability that the small system A is in a state with energy E_A is

$$P_A = \frac{\Omega_A(E_0 - E_A)}{\Omega_0}$$