Ensembles

Macroscopic system

example: gas of N atoms confined to volume V

$$\cancel{N \gg 1} \quad \log N \gg 1$$

$$V \gg \cancel{\text{volume } v_0 \text{ of atom}} \quad \log \frac{V}{v_0} \gg 1$$

macrostate characterized by macroscopic properties

equilibrium: macroscopic properties don't change with time

macrostate for gas in equilibrium
is characterized by 3 variables:

N, V, and energy E
or temperature T

microstates for classical gas

specified by position vector: $\vec{r}_n = (x_n, y_n, z_n)$
and momentum vector $\vec{p}_n = (p_{nx}, p_{ny}, p_{nz})$
for each of the atoms $n = 1, \ldots, N$

OR by 3N Cartesian coordinates: $x_1, x_2, \ldots, x_{3N}$
and 3N momentum components: $p_1, p_2, \ldots, p_{3N}$

$\Longrightarrow$ 6N continuous variables

microstate for quantum gas

specified by independent solutions
of Schroedinger equation

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

finite volume $\Longrightarrow$ energy eigenvalues E_i are discrete

$\Longrightarrow$ microstates can be enumerated

$|\psi_i\rangle, \; i = 1, 2, 3, \ldots$

ensemble: probability distribution
for microstates

quantum system: microstates can be enumerated

probability distribution is specified by
the probability P_i for each microstate

$$P_i \geq 0 \quad \text{for each } i$$

$$\sum_i P_i = 1$$

classical system

generalized coordinates: $q_1, q_2, \ldots q_N$
conjugate momenta: $p_1, p_2, \ldots, p_N$

integration measure on phase space

$$d\omega = dp_1 \, dq_1 \, dp_2 \, dq_2 \cdots dp_N \, dq_N$$

probability distribution is a function $P(p,q)$

$$P(p,q) \geq 0$$

$$\int d\omega \, P(p,q) = 1$$

Statistical Mechanics

derive thermodynamic variables
from probability distribution of ensemble

<u>information entropy</u> of ensemble

for discrete microstates

$$S_{info} = -\sum_i P_i \log P_i$$

for classical system.

$$S_{info} = -\int d\omega\, P(p,q) \log P(p,q)$$

all probability in one microstate: $P_1 = 1$
$P_i = 0$ for $i = 2, 3, ..$

$$\Longrightarrow S_{info} = 0$$

equal probability in all N microstate: $P_i = \frac{1}{N}$

$$\Longrightarrow S_{info} = \log N$$

energy E of macrostate

microstate i has discrete energy E_i

average over ensemble:

$$\langle E \rangle = \sum_i P_i E_i$$

classical system

microstate $(p, q) = (p_1, p_2, \ldots, p_N; q_1, q_2, \ldots, q_N)$

has energy $\mathcal{H}(p, q)$

$$\langle E \rangle = \int d\omega \, P(p, q) \, \mathcal{H}(p, q)$$