Lecture 2 (Eq. Stat Mech)

Statistical Ensembles

Fundamental Postulates

- Energy is conserved
- System is ergodic

$\Rightarrow$ Isolated system

$\Rightarrow$ fixed energy

$\Rightarrow$ all microstates are equally likely (consequence of ergodicity)

$$P_\nu(E) = \frac{1}{\Omega(E)}$$

Example of an ensemble (microcanonical)

Ensembles are characterized by a-priori probability distributions

If I know $\Omega(E)$ for a system (follows from the Hamiltonian)

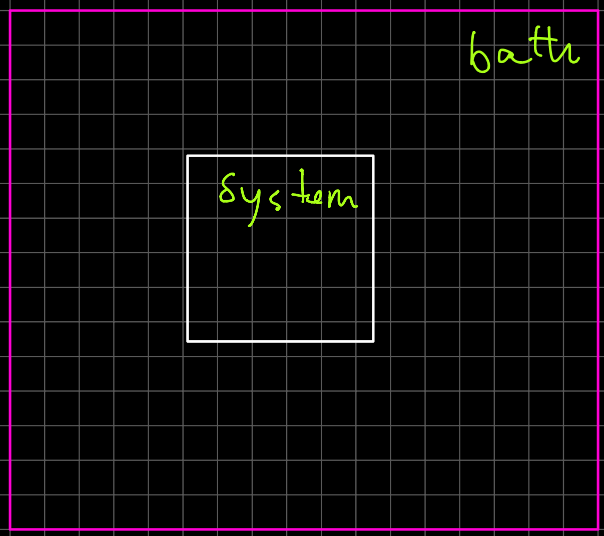
$\Rightarrow$ I know $P_\nu(E)$

More interesting is the canonical ensemble where we need to introduce the notion of an intensive variable (temperature) which is conjugate to Energy

Two systems brought in contact and allowed to equilibrate reach the same temperature

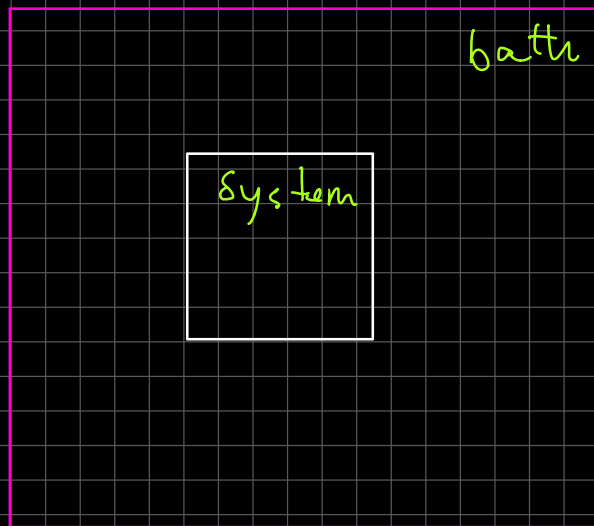
$$P_\nu(\beta) = e^{-\beta E_\nu} / Z$$

Exercise 1



E of bath + system is fixed

- derive an expression for β
- derive $P_\nu(\beta)$ using two methods



$$\Omega_s(E_s)\,\Omega_{bath}(E - E_s) = \Omega(E)$$

$$S = -\ln \Omega(E)$$

$$S = S_s + S_{bath}$$

$$\frac{\partial S}{\partial E_S} = 0$$ maximizes entropy

$$\frac{\partial \ln \Omega_S}{\partial E_S} - \frac{\partial \ln \Omega_{bath}}{\partial E_S} = 0$$

$$\beta = \frac{\partial \ln \Omega_S}{\partial E_S}$$

$\Rightarrow$ inverse T

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make $E_s \to E_\nu$

$P(E_\nu)$?

Prob bath $\to E - E_\nu$

$$\Omega(E - E_\nu) = \Omega(E) - E_\nu \frac{\partial \Omega}{\partial E}$$

$$\ln \Omega(E - E_\nu)$$

$$= \ln \Omega - E_\nu \frac{\partial \ln \Omega}{\partial E}$$

$$= \ln \Omega - \beta E_\nu$$

$$\Omega \sim e^{-\beta E_\nu}$$

Gibbs

$$S[P] = \sum_\nu P_\nu \ln P_\nu$$

subject to constraints

$$\langle E \rangle = \sum_\nu E_\nu P_\nu \quad \text{(fixed)}$$

$$\sum_\nu P_\nu = 1$$

Maximize S subject to these constraints

$$P_\nu \propto e^{-\beta E_\nu}$$

$$\beta^{-1} = \frac{\partial \langle E \rangle}{\partial S}$$

Let's look at assumptions behind the first (bath + system) approach

- Ergodicity : certainly violated in athermal
- Energy is conserved : again not true

Maximizing $S[p]$ more of an information theoretic approach

Proposal by Sam Edwards
to construct an ensemble
for granular materials
(infinitely rigid grains)

I. Slowly driven systems:
collective behavior controlled
by the ensemble of "Blocked"
states: configurations where
a grain cannot move

Jammed : modern parlance

II. These blocked states
under repeated experimentation
are sampled according to
the a-priori probability

$$P_\nu \sim e^{-V_\nu / X}$$

Volume V_ν replaces E_ν

$$X \sim T \; : \; \frac{1}{X} = \frac{\partial S}{\partial V}$$

Volume ensemble

[Work with Daan Frenkel shown that hard-particles are indeed described by this ensemble]

What is S (the entropy)?

Edwards $\quad S(V) = -\ln \Omega(V)$

$$\Omega(V) = \sum_\nu \delta(V - V_\nu)$$

Generalize

$$\Omega = \sum_\nu \omega_\nu \, \delta(V - V_\nu)$$

discard equiprobability

Can still recover a thermodynamics, as long as

$$\omega_{\nu+\nu'} = \omega_\nu \, \omega_{\nu'}$$

Generalized ensembles

Other extensive quantities that are conserved in jammed (blocked) states?

$$\hat{\Sigma} = \sum_{\substack{\text{contacts} \\ \{c\}}} \vec{r}_c \otimes \vec{f}_c$$

Has dimensions of energy

For a system in force & torque balance Σ^{a} is "conserved"

Follows from
$$\partial_i \Sigma_{ij} = 0 \quad \left\{ \begin{array}{l} \text{no} \\ \text{external} \\ \text{forces} \end{array} \right.$$

Will discuss this in much more detail but let's try to understand this type of an ensemble by looking at a simpler system.