Lecture 24

Information entropy

density operator ⟶ stat. mech.

For completely random ensemble (in any representation)

$$\rho = \frac{1}{N}\begin{pmatrix} 1 & & & & \hat{0} \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \\ \hat{0} & & & & & 1 \end{pmatrix}$$

[N # of elements in the Hilbert space]

equally populated states

For a pure ensemble

$$\rho = \begin{pmatrix} 0 & & & & & \hat{0} \\ & 0 & & & & \\ & & 0 & & & \\ & & & 1 & & \\ & & & & 0 & \\ \hat{0} & & & & & 0 \end{pmatrix}$$

Define a quantity

$$S = -\,\mathrm{tr}(\hat{\rho}\ln\hat{\rho})$$

In the basis in which $\hat{\rho}$ is diagonal

$$S = -\sum_k \rho_{kk} \ln \rho_{kk}$$

$0 \leq \rho_{kk} \leq 1 \Rightarrow S \geq 0$

For completely random ensemble

$$S = -\sum_{k=1}^{N} \frac{1}{N} \ln\left(\frac{1}{N}\right) = \ln N$$

For a pure ensemble

$S = 0$ [def. $0 \log 0 = 0$]

S can be regarded as a measure of disorder (entropy)

• A pure ensemble is an ensemble with a maximum amount of order: all members characterized by same state

- A completely random ensemble (all states are equally likely) has maximum disorder (entropy).

$\ln N$ is maximum value with constraint $\mathrm{Tr}\,\rho = 1$

__Ensemble in thermal equilibrium__

Assumption: maximize S subject to the constraint that the ensemble average of the Hamiltonian has a fixed value

in equilibrium

$$\frac{\partial \rho}{\partial t} = 0 \Rightarrow [\hat{H}, \hat{\rho}] = 0$$

use energy eigensolutions

maximize S $\delta S = 0$

internal energy of the system U

$$U = tr(\rho H)$$

and $tr\,\rho = 1$

$$\delta S - \beta \delta Tr(\rho H) - \gamma \delta tr \rho = 0$$

$$-\sum_k \left[\delta_{kk}(\ln \rho_{kk} + 1) - \beta \delta \rho_{kk} E_k - \gamma \delta \rho_{kk}\right] = 0$$

for an arbitrary variation it is possible only if

$$\rho_{kk} = e^{(-\beta E_k - \gamma - 1)}$$

We know that $\sum_k \rho_{kk} = 1$

$$\Downarrow$$

$$\rho_{kk} = \frac{e^{-\beta E_k}}{\sum_l^N e^{-\beta E_l}}$$ canonical ensemble