Phys. 528 Lecture 10

Quantum Statistics

In quantum stat. mech., the mean value of an observable is a double average, both quantum and statistical. Suppose we have an ensemble of $\mathcal{N}$ quantum systems, with quantum states

$$|\psi^k(t)\rangle, \quad k = 1, 2, \ldots, \mathcal{N}.$$

Then

$$\langle \hat{Q}(t) \rangle = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \langle \psi^k(t) | \hat{Q} | \psi^k(t) \rangle$$

$$= \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \langle \hat{Q} \rangle|_k$$

To describe both the quantum and statistical state of a system, we introduce the <u>density matrix</u>

$$\hat{\rho}(t) = \frac{1}{N} \sum_{k=1}^{N} |\psi^k(t)\rangle\langle\psi^k(t)|$$

1) <u>Properties of the density matrix</u>:

i) $\hat{\rho}^\dagger = \hat{\rho}$

ii) $Tr\{\hat{\rho}\} = 1$

Proof: $Tr\{\hat{\rho}\} = \frac{1}{N} \sum_{k=1}^{N} \sum_{n} \langle n|\psi^k\rangle\langle\psi^k|n\rangle$

$$= \frac{1}{N} \sum_{k=1}^{N} \langle\psi^k|\psi^k\rangle = 1 \checkmark$$

iii) $P(u) = \langle u|\hat{\rho}|u\rangle$

Proof:

$$\langle u|\hat{\rho}|u\rangle = \frac{1}{N} \sum_{k=1}^{N} \langle u|\psi^k\rangle\langle\psi^k|u\rangle$$

$$= \frac{1}{N} \sum_{k=1}^{N} |\langle u|\psi^k\rangle|^2 = \frac{1}{N} \sum_{k=1}^{N} P_k(u)$$

iv) $\langle \hat{Q}(t) \rangle = \mathrm{Tr}\{ \hat{\rho}(t)\, \hat{Q} \}$

Proof: $\mathrm{Tr}\{ \hat{\rho}(t)\, \hat{Q} \} = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \sum_{n} \langle n | \psi^k(t) \rangle \langle \psi^k(t) | \hat{Q} | n \rangle$

$$= \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \sum_{n} \langle \psi^k(t) | \hat{Q} | n \rangle \langle n | \psi^k(t) \rangle$$

$$= \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \langle \psi^k(t) | \hat{Q} | \psi^k(t) \rangle \quad \checkmark$$

v) $i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] \equiv \hat{H}\hat{\rho} - \hat{\rho}\hat{H}$

Proof: $i\hbar \frac{d\hat{\rho}}{dt} = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \Big\{ \Big(i\hbar \frac{d}{dt} |\psi^k(t)\rangle \Big) \langle \psi^k(t)|$

$$+ |\psi^k(t)\rangle\, i\hbar \frac{d}{dt} \langle \psi^k(t)| \Big\}$$

$$i\hbar \frac{d}{dt} |\psi^k(t)\rangle = \hat{H}\, |\psi^k(t)\rangle$$

$$-i\hbar \frac{d}{dt} \langle \psi^k(t)| = \langle \psi^k(t)|\, \hat{H}$$

$$i\hbar \frac{d\hat{\rho}}{dt} = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \{ \hat{H} |\psi^k(t)\rangle\langle\psi^k(t)| - |\psi^k(t)\rangle\langle\psi^k(t)| \hat{H} \}$$

$$= \hat{H}\hat{\rho} - \hat{\rho}\hat{H} = [\hat{H}, \hat{\rho}]$$

Note: this eq has the opposite sign of the usual Heisenberg eq of motion for an operator!

2) <u>Alternative expression</u>

We can also write $\hat{\rho}$ as

$$\hat{\rho} = \sum_j P_j |\psi_j\rangle\langle\psi_j| ,$$

where the states $|\psi_j\rangle, |\psi_{j'}\rangle$ need not be orthogonal.

$$Tr\{\hat{\rho}\} = \sum_j P_j \sum_n \langle n|\psi_j\rangle\langle\psi_j|n\rangle = \sum_j P_j \sum_n \langle\psi_j|n\rangle\langle n|\psi_j\rangle$$

$$= \sum_j P_j \langle\psi_j|\psi_j\rangle = \sum_j P_j = 1$$

Eigenbasis Because $\hat{\rho}^{+} = \hat{\rho}$,

$\exists$ an orthonormal basis in which $\hat{\rho}$ is diagonal

$$\hat{\rho} = \sum_i w_i |i\rangle\langle i| , \qquad \langle i|j\rangle = \delta_{ij}$$

3) Pure and mixed states

A pure state $|\psi\rangle$ has

$$\hat{\rho} = |\psi\rangle\langle\psi| .$$

$$\langle \hat{Q} \rangle = Tr\{\hat{\rho}\hat{Q}\} = \langle\psi|\hat{Q}|\psi\rangle ;$$

no statistical averaging. For a pure state,

$$\hat{\rho}^2 = \hat{\rho} .$$

Proof: $\hat{\rho}^2 = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{1}\langle\psi| = |\psi\rangle\langle\psi|$ ✓

As an example of a <u>mixed state</u>, consider

$$\hat{\rho} = P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2|$$

$$\langle\hat{Q}\rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{Q}\} = P_1 \langle\psi_1|\hat{Q}|\psi_1\rangle + P_2 \langle\psi_2|\hat{Q}|\psi_2\rangle$$

This is different than a <u>superposition of states</u>

$$|\psi\rangle = \sqrt{P_1}\, e^{i\theta_1} |\psi_1\rangle + \sqrt{P_2}\, e^{i\theta_2} |\psi_2\rangle$$

$$\begin{aligned}\langle\hat{Q}\rangle = \langle\psi|\hat{Q}|\psi\rangle = {} & P_1 \langle\psi_1|\hat{Q}|\psi_1\rangle + P_2 \langle\psi_2|\hat{Q}|\psi_2\rangle \\ & + \sqrt{P_1 P_2}\, e^{i(\theta_1-\theta_2)} \langle\psi_2|\hat{Q}|\psi_1\rangle \\ & + \sqrt{P_1 P_2}\, e^{i(\theta_2-\theta_1)} \langle\psi_1|\hat{Q}|\psi_2\rangle\end{aligned}$$

$$\begin{aligned}\hat{\rho}' = |\psi\rangle\langle\psi| = {} & P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2| \\ & + \sqrt{P_1 P_2}\, e^{i(\theta_1-\theta_2)} |\psi_1\rangle\langle\psi_2| \\ & + \sqrt{P_1 P_2}\, e^{i(\theta_2-\theta_1)} |\psi_2\rangle\langle\psi_1|\end{aligned}$$

Matrix representation

$$\rho_{nm} = \langle n | \hat{\rho} | m \rangle, \quad \langle n | m \rangle = \delta_{nm}$$

For the example $\hat{\rho} = P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2|$,

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix}$$

For the example $\hat{\rho}' = |\psi\rangle\langle\psi|$,

$$\hat{\rho}' = \begin{pmatrix} P_1 & \sqrt{P_1 P_2}\, e^{i(\theta_1 - \theta_2)} \\ \sqrt{P_1 P_2}\, e^{i(\theta_2 - \theta_1)} & P_2 \end{pmatrix}$$

4) Entropy

In the eigenbasis,

$$S = -k_B \sum_{\mu} P(\mu) \ln P(\mu)$$

$$= -k_B \langle \ln P(\mu) \rangle$$

$$S = -k_B \, \mathrm{Tr} \{ \hat{\rho} \ln \hat{\rho} \}$$

For a pure state,

$$S = 0.$$

Phys. 528 Lecture 11

Quantum Statistics (cont.)

1) Statistical ensembles

To describe a stationary (steady state) ensemble with $\dot{\hat{\rho}}=0$, we require $\hat{\rho}$ to be a function of a constant of the motion. e.g.,

$$\hat{\rho} = \hat{\rho}(\hat{A}) \quad , \quad [\hat{A}, \hat{H}] = 0$$

Then $[\hat{\rho}, \hat{H}] = 0$ so $\dot{\hat{\rho}} = 0$.

This implies that the density matrix describing a system in a steady state (even a nonequilibrium steady state) must be <u>diagonal</u> in the <u>energy</u> basis.

2) microcanonical ensemble

For equilibrium systems, typically $\hat{\rho} = \hat{\rho}(\hat{H})$. In the energy basis, the microcanonical ensemble is described by the density matrix

$$\rho_{nm} = \begin{cases} \frac{1}{\Omega}\delta_{nm}, & E - \frac{\Delta}{2} \le \mathcal{E}_n \le E + \frac{\Delta}{2} \\ 0, & \text{otherwise} \end{cases}$$

with $\mathrm{Tr}\,\hat{\rho} = 1$.

3) Canonical ensemble

$$\rho_{nm} = C e^{-\beta E_n} \delta_{nm}$$

$$C = \frac{1}{Z_N(\beta)}$$

$$\hat{\rho} = \sum_n |n\rangle \frac{e^{-\beta E_n}}{Z_N(\beta)} \langle n|$$

$$= \frac{e^{-\beta \hat{H}}}{Z_N(\beta)} \sum_n |n\rangle\langle n|$$

$$= \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}}, \quad Z_N(\beta) = \mathrm{Tr}\{e^{-\beta H}\}$$

$$E = \langle \hat{H} \rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{H}\} = \frac{\mathrm{Tr}\{\hat{H}\, e^{-\beta \hat{H}}\}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}}$$

$$= -\frac{\partial \ln \mathrm{Tr}\{e^{-\beta \hat{H}}\}}{\partial \beta}$$

4) <u>Grand canonical ensemble</u>

$$\hat{\rho} = \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{\mathrm{Tr}\{e^{-\beta(\hat{H}-\mu)\hat{N}}\}}, \quad [\hat{H}, \hat{N}] = 0$$

$$\rho_{nm} = \langle n | \hat{\rho} | m \rangle = \frac{e^{-\beta(E_n - \mu N_n)}}{\mathcal{Z}} \delta_{nm}$$

$$\mathcal{Z} = \mathrm{Tr}\left\{ e^{-\beta(\hat{H} - \mu \hat{N})} \right\}$$

5) Examples

i) Two-level system

$$\hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

A mixed state

$$\hat{\rho} = \begin{pmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{pmatrix}$$

e.g., canonical ensemble with $\rho_i = \dfrac{e^{-\beta E_i}}{Z}$

is stationary $\dot{\rho}_{nm} = 0$.

A pure state

$\hat{\rho} = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \dfrac{|1\rangle + e^{i\theta}|2\rangle}{\sqrt{2}}$

has $\hat{\rho}(0) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}e^{-i\theta} \\ \frac{1}{2}e^{i\theta} & \frac{1}{2} \end{pmatrix}$

and $\hat{\rho}(t) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}e^{-i(\theta-\omega t)} \\ \frac{1}{2}e^{i(\theta-\omega t)} & \frac{1}{2} \end{pmatrix}$,

where $\omega = \dfrac{E_2 - E_1}{\hbar}$.

The observable

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

has $\langle\sigma_x\rangle = \mathrm{Tr}\{\rho\sigma_x\} = \mathrm{Tr}\left\{\begin{pmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right\}$

$= \mathrm{Tr}\left\{\begin{pmatrix} 0 & \rho_1 \\ \rho_2 & 0 \end{pmatrix}\right\} = 0$ in the mixed state.

But $\langle \sigma_x(t) \rangle = \mathrm{Tr}\{ \rho(t)\, \sigma_x \}$

$$= \mathrm{Tr}\left\{ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} e^{i(\omega t - \theta)} \\ \frac{1}{2} e^{i(\theta - \omega t)} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}$$

$$= \mathrm{Tr}\left\{ \begin{pmatrix} \frac{1}{2} e^{i(\omega t - \theta)} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} e^{i(\theta - \omega t)} \end{pmatrix} \right\}$$

$$= \cos(\omega t - \theta)$$ in the pure state

$$\omega = \frac{E_2 - E_1}{\hbar} = \text{Rabi frequency}$$

Ex. ii) <u>Particle in a box</u> $V = L^3$

$$\hat{H} = \frac{\vec{p}^{\,2}}{2m} \qquad \psi_{\vec{k}} = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$$\hat{H}\psi_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}\psi_{\vec{k}} \quad , \quad E = \frac{\hbar^2 \vec{k}^2}{2m}$$

P.B.C.s: $\psi(x+L,y,z) = \psi(x,y+L,z)$
$= \psi(x,y,z+L) = \psi(x,y,z)$

$$\Rightarrow \quad k_i = \frac{2\pi n_i}{L}, \qquad \vec{k} = \frac{2\pi \vec{n}}{L}$$

$$\langle \vec{r}| e^{-\beta \hat{H}} |\vec{r}'\rangle = \sum_{\vec{k}} \langle \vec{r}|\vec{k}\rangle e^{-\beta E_{\vec{k}}} \langle \vec{k}|\vec{r}'\rangle$$

$$\langle \vec{r}|\vec{k}\rangle = \psi_{\vec{k}}(\vec{r}), \qquad \langle \vec{k}|\vec{r}'\rangle = \psi^{*}_{\vec{k}}(\vec{r}')$$

$$\langle \vec{r}| e^{-\beta \hat{H}} |\vec{r}'\rangle = \frac{1}{V}\sum_{\vec{k}} e^{-\beta \frac{\hbar^2 k^2}{2m} + i\vec{k}\cdot(\vec{r}-\vec{r}')}$$

$$\approx \int \frac{d^3k}{(2\pi)^3} e^{-\beta\frac{\hbar^2 k^2}{2m} + i\vec{k}\cdot(\vec{r}-\vec{r}')}$$

$$= \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} e^{-\frac{m|\vec{r}-\vec{r}'|^2}{2\beta\hbar^2}}$$

$$Z_1 = \mathrm{Tr}\{e^{-\beta\hat{H}}\} = \int d^3r \, \langle \vec{r}| e^{-\beta\hat{H}} |\vec{r}\rangle$$

$$= V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}$$

$$\langle \vec{r} \,|\, \hat{\rho} \,|\, \vec{r}\,' \rangle = \frac{1}{V} e^{-\frac{m|\vec{r}-\vec{r}\,'|^2}{2\beta\hbar^2}}$$

$$E = \langle \hat{H} \rangle = -\frac{\partial \ln Z_1}{\partial \beta} = \frac{3}{2\beta} = \frac{3}{2} k_B T$$

iii) Harmonic oscillator

$$\hat{H} = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots, \infty$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{H_n(\xi)}{(2^n n!)^{1/2}} e^{-\frac{1}{2}\xi^2}$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$\langle x | e^{-\beta\hat{H}} | x' \rangle = \sum_{n=0}^{\infty} e^{-\beta E_n} \psi_n(x) \psi_n^*(x')$$

$$= \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)}}$$

$$\times \exp\left\{ -\frac{m\omega}{4\hbar}\left[(x+x')^2 \tanh\left(\frac{\beta\hbar\omega}{2}\right) + (x-x')^2 \coth\left(\frac{\beta\hbar\omega}{2}\right) \right] \right\}$$

$$\mathrm{Tr}\left\{e^{-\beta\hat{H}}\right\} = \int_{-\infty}^{\infty} dx\ \langle x|e^{-\beta\hat{H}}|x\rangle$$

$$= \sum_{n=0}^{\infty} \langle n|e^{-\beta\hat{H}}|n\rangle = \frac{e^{-\beta\frac{\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}}$$

$$= \frac{1}{2\sinh\left(\beta\frac{\hbar\omega}{2}\right)}$$

$$\langle x|\hat{\rho}|x\rangle = \rho(x,x) = \left[\frac{m\omega\tanh\left(\beta\frac{\hbar\omega}{2}\right)}{\pi\hbar}\right]^{1/2}$$

$$\times \exp\left\{-\frac{m\omega x^2}{\hbar}\tanh\left(\beta\frac{\hbar\omega}{2}\right)\right\}$$

$$\langle x^2\rangle = \frac{\hbar}{2m\omega\tanh\beta\frac{\hbar\omega}{2}}$$

$$= \begin{cases} \dfrac{\hbar}{2m\omega}, & \dfrac{k_BT}{\hbar\omega} \to 0 \\[2ex] \dfrac{k_BT}{m\omega^2}, & \dfrac{k_BT}{\hbar\omega} \to \infty \end{cases}$$

$$\langle V \rangle = \frac{m\omega^2}{2} \langle x^2 \rangle = \frac{\hbar\omega}{4 \tanh \beta\frac{\hbar\omega}{2}}$$

$$E = -\frac{\partial \ln \mathrm{Tr}\{e^{-\beta \hat{H}}\}}{\partial \beta} = \frac{\partial}{\partial \beta} \ln \sinh \beta\frac{\hbar\omega}{2}$$

$$= \frac{\hbar\omega}{2} \frac{1}{\tanh \beta\frac{\hbar\omega}{2}} = 2\langle V \rangle$$

Cf. virial theorem.

iii) Harmonic oscillator

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}}$$

$$Z = \mathrm{Tr}\{e^{-\beta \hat{H}}\} = \sum_{n=0}^{\infty} \langle n | e^{-\beta \hat{H}} | n \rangle$$

$$= e^{-\beta \frac{\hbar \omega}{2}} \sum_{n=0}^{\infty} e^{-\beta \hbar \omega n}$$

$$= \frac{e^{-\beta \hbar \omega / 2}}{1 - e^{-\beta \hbar \omega}}$$

$\langle x \rangle = ?$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^{+} \right)$$

$$\hat{p}_x = i \sqrt{\frac{\hbar m \omega}{2}} \left(a^{+} - a \right)$$

$$\langle x \rangle = \mathrm{Tr}\{ \hat{\rho}\, \hat{x} \} = \frac{1}{Z} \sum_{n} \langle n | e^{-\beta \hat{H}} \hat{x} | n \rangle$$

$$= \frac{1}{Z} \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + \frac{1}{2})} \underbrace{\langle n | a + a^{+} | n \rangle}_{\to 0}$$

$$= 0$$

$$\langle x^2 \rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{x}^2\}$$

$$= \frac{1}{Z}\frac{\hbar}{2m\omega}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})}\langle n|(a+a^\dagger)^2|n\rangle$$

$$\langle n|(a+a^\dagger)^2|n\rangle = \langle n|\underbrace{a^2}_{0}+\underbrace{(a^\dagger)^2}_{0}+aa^\dagger+a^\dagger a|n\rangle$$

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = \mathbb{1}$$

$$aa^\dagger = a^\dagger a + \mathbb{1}$$

$$\langle n|(a+a^\dagger)^2|n\rangle = \langle n|2a^\dagger a + \mathbb{1}|n\rangle = 2n+1$$

$$\langle x^2 \rangle = \frac{1}{Z}\frac{\hbar}{2m\omega}\sum_{n=0}^{\infty}(2n+1)\,e^{-\beta\hbar\omega(n+\frac{1}{2})}$$

$$= \frac{1}{Z}\frac{1}{m\omega^2}\left(-\frac{\partial Z}{\partial\beta}\right) = \frac{1}{m\omega^2}\left(-\frac{\partial \ln Z}{\partial\beta}\right)$$

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial\beta} = \hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right)$$

$$\langle x^2 \rangle = \frac{\hbar}{m\omega}\left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\right)$$

$$= \begin{cases} \dfrac{\hbar}{2m\omega}, & \dfrac{k_B T}{\hbar\omega} \to 0 \quad \text{(zero-pt. motion)} \\[2ex] \dfrac{k_B T}{m\omega^2}, & \dfrac{k_B T}{\hbar\omega} \to \infty \quad \text{(equipartition)} \end{cases}$$

Similarly,

$$\langle p_x \rangle = 0$$

$$\langle p_x^2 \rangle = m\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\right)$$

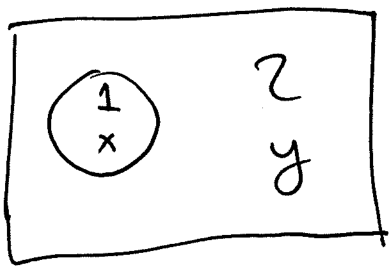
$$\left\langle \frac{m\omega^2 x^2}{2} \right\rangle = \left\langle \frac{p_x^2}{2m} \right\rangle = \frac{1}{2}\langle E \rangle$$

Virial theorem

Physics 528 Lecture 12

Quantum Statistics III

1) Reduced density matrix



Suppose a system can be divided into two parts 1 and 2, described by variables x and y, respectively. A pure state of the system is described by a wavefunction

$$\psi(x,y) = \langle x | \langle y | \psi \rangle .$$

Let $\{|\psi_n\rangle\}$ be a complete set of states in region 1, and $\{|\phi_k\rangle\}$ a complete set in region 2.

$$|\psi\rangle = \sum_{n,k} C_{nk} |\psi_n\rangle |\phi_k\rangle$$

Let $\hat{A}$ be an operator defined in $\mathcal{L}^2$ region 1:

$$\hat{A} = \sum_{n,n'} |\psi_n\rangle A_{nn'} \langle \psi_{n'}| \otimes \underbrace{\mathbb{1}_2}_{\sum_k |\phi_k\rangle\langle\phi_k|}$$

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle =$$

$$\sum_{n',k'} \sum_{n,k} c^*_{nk}\, C_{n'k'}\, A_{nn'}\, \delta_{kk'}$$

$$= \sum_{\substack{n,n' \\ k}} C_{n'k}\, C^*_{nk}\, A_{nn'}$$

$$= \mathrm{Tr}\{ \hat{\rho}_1 \hat{A} \}, \quad \text{where}$$

$$(\rho_1)_{n'n} = \sum_k C_{n'k}\, C^*_{nk}.$$

$\hat{\rho}_1$ is called the <u>reduced density matrix</u> for sub-system 1.

Clearly $\hat{\rho}_1$ is Hermitian.

$$\mathrm{Tr}\{\hat{\rho}_1\} = \sum_{n,k} |C_{nk}|^2 = 1$$

due to normalization of $|\Psi\rangle$.

Since $\hat{\rho}_1$ is Hermitian, it has an orthonormal set of eigenstates $|i\rangle$ with

$$\hat{\rho}_1 = \sum_i w_i |i\rangle\langle i| .$$

Let $\hat{A} = |j\rangle\langle j|$, where $|j\rangle$ is one of the eigenstates of $\hat{\rho}_1$.

$$w_j = \mathrm{Tr}\{\hat{\rho}_1 \hat{A}\} = \langle\Psi|\hat{A}|\Psi\rangle = |\langle j|\Psi\rangle|^2 \geq 0 .$$

Thus the eigenvalues of $\hat{\rho}_1$ satisfy

1) $w_i \geq 0$

2) $\sum_i w_i = 1$

Notice that

$$\langle \hat{Q} \rangle = \mathrm{Tr}\{\hat{\rho}_1 \hat{Q}\} = \sum_i \langle i | \hat{\rho}_1 \hat{Q} | i \rangle$$

$$= \sum_i w_i \langle i | \hat{Q} | i \rangle,$$

where $\hat{Q}$ is any operator acting only on region 1.

Thus $\hat{\rho}_1$ has all of the properties required for a density matrix.

In terms of the coordinates x of system 1,

$$\langle \hat{A} \rangle = \mathrm{Tr}\{\hat{\rho}_1 \hat{A}\} = \int dx \langle x | \hat{\rho}_1 \hat{A} | x \rangle$$

$$\langle \hat{A} \rangle = \int dx \int dx' \langle x | \hat{\rho}_1 | x' \rangle \langle x' | \hat{A} | x \rangle$$

$$= \int dx \int dx' \, \rho_1(x, x') \, A(x', x)$$

Moreover, in terms of $|\Psi\rangle$,

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \int dx \int dx' \int dy \, \Psi^*(x', y) \, A(x', x) \, \Psi(x, y)$$

Thus

$$\rho_1(x, x') = \int dy \, \Psi(x, y) \Psi^*(x', y).$$

$$= Tr_2 \{ \rho(x, y; x', y') \}$$

Notice that the reduced density matrix does not have the form required for a <u>pure state</u>. Pure states are thus not general enough to describe the state of a subsystem of a larger quantum system. The only known system that is not a part of a larger system is the universe as a whole.

It is unknown whether the universe as a whole is in a pure state.

Example Entangled (singlet) state of two spin-1/2 particles.

$$|\psi\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \quad \text{(a pure state)}$$

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + \frac{1}{2}|\downarrow\uparrow\rangle\langle\downarrow\uparrow| - \frac{1}{2}|\uparrow\downarrow\rangle\langle\downarrow\uparrow| - \frac{1}{2}|\downarrow\uparrow\rangle\langle\uparrow\downarrow|$$

$$\hat{\rho}_1 = \mathrm{Tr}_2\{\hat{\rho}\} = \langle 2\uparrow|\hat{\rho}|2\uparrow\rangle + \langle 2\downarrow|\hat{\rho}|2\downarrow\rangle$$

$$= \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \frac{1}{2}|\uparrow\rangle\langle\uparrow| \quad \text{(a mixed state!)}$$

$$S_1 = -k_B \,\mathrm{Tr}\{\hat{\rho}_1 \ln \hat{\rho}_1\} = k_B \ln 2$$

but $S = -k_B \,\mathrm{Tr}\{\hat{\rho} \ln \hat{\rho}\} = 0$

S_1 is sometimes refered to as
<u>entanglement entropy</u>.

<u>Discussion question</u>

Is it possible that the universe
as a whole is in a pure quantum
state, whose initial wave fuction
describes the big bang, but that
the microscopic degrees of freedom
of the observable universe are
now entangled with degrees of
freedom outside our light cone,
so that the entropy of the
observable universe is nothing
but entanglement entropy?