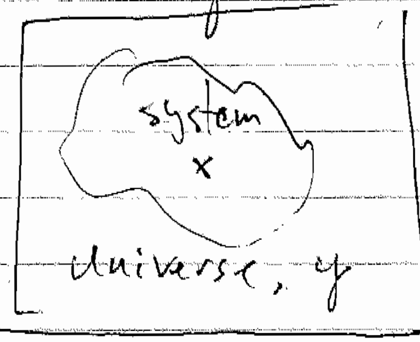
Lecture #12

Quantum Statistics - Density Matricies

$$\Psi(x,y) = \sum_i c_i(y)\,\phi_i(x)$$



One has access to only part of the system, or some systematic source of randomness.

ϕ_i = complete set of states on x

define $\phi_i(x) = \langle x|\phi_i\rangle$; $\theta_i(y) = \langle y|\theta_i\rangle$ complete set of states on y.

$$|\Psi\rangle = \sum_{ij} c_{ij}|\phi_i\rangle|\theta_j\rangle$$

$$\Rightarrow \Psi(x,y) = \sum_{ij} c_{ij}\langle x|\phi_i\rangle\langle y|\theta_j\rangle \Rightarrow c_i(y) = \sum_j c_{ij}\langle y|\theta_j\rangle$$

Let A act only on the system $\{|\phi_i\rangle\}$, not θ's

$$\hat{A}\left[|a\rangle_s|b\rangle_{bath}\right] = \left[\hat{A}|a\rangle_s\right]|b\rangle_{bath}$$

$\hat{A}$ is $\sum_{i,i'} A_{ii'}|\phi_i\rangle\langle\phi_{i'}|$ or, insert complete set of θ states to act on both

$$\hat{A} = \sum_{i,i',j} A_{ii'}|\phi_i\rangle|\theta_j\rangle\langle\theta_j|\langle\phi_{i'}|$$

$$\langle A\rangle = \langle\Psi|A|\Psi\rangle = \sum_{\substack{ij\\i'j'}} c_{ij}^{*}c_{i'j'}\langle\theta_j|\langle\phi_i|\hat{A}|\phi_{i'}\rangle|\theta_{j'}\rangle$$

$$\langle A \rangle = \sum_{\substack{i,j \\ i',j'}} c_{ij}\, c^{*}_{i'j'}\, A_{i,i'}\, \delta_{j,j'}$$

$$= \sum_{\substack{i,i' \\ j}} c_{ij}\, c^{*}_{i',j}\, A_{i,i'} \quad ; \; A_{i,i'} = \langle \phi_i | \hat{A} | \phi_{i'} \rangle$$

$$= \sum_{i,i'} \left(\rho^{*}_{i,i'} \right) A_{i,i'}$$

(1) where $\rho^{*}_{i,i'} = \sum_j c_{ij}\, c^{*}_{i',j} = \sum_j c^{*}_{i',j}\, c_{i,j}$

$\rho^{*}_{i,i'}$ = Density Matrix $= \mathrm{Tr}_{\text{bath}}\, |\Psi\rangle\langle\Psi|$

define $\rho_{i',i} = \langle \phi_{i'} | \rho | \phi_i \rangle$, ρ operates on system only.

$$\therefore \langle A \rangle = \sum_{i i'} \langle \phi_{i'} | \rho | \phi_i \rangle \langle \phi_i | A | \phi_{i'} \rangle$$

$$= \sum_{i'} \langle \phi_{i'} | \rho A | \phi_{i'} \rangle \quad \text{(completeness)}$$

$$= \mathrm{Tr}\,[\rho A]$$

Properties of ρ: $(\rho^{*})^{T} = \rho$ (Hermitian)
from (1)

Diagonalize $\rho = \sum_i w_i |i\rangle\langle i|$; w_i are real.

Let $\hat{A} = 1 \Rightarrow 1 = \mathrm{Tr}\,\rho = \langle\psi|\psi\rangle$

$\therefore \sum_i w_i = 1$

Let $\hat{A} = |i'\rangle\langle i'| \Rightarrow \mathrm{Tr}\,\rho|i'\rangle\langle i'|$

Tr in ~~ee~~ eigenbasis $\{|i\rangle\}$

$= \sum_i \langle i|\rho|i'\rangle\langle i'|i\rangle = \langle i'|\rho|i'\rangle = w_{i'}$

$= \cancel{\sum |\langle\Psi|i'\rangle|^2 \langle\Psi\rangle = \sum_{i,j} c_j \langle\theta_j|\theta_j\rangle}$

$\therefore w_{i'} = \langle\Psi|i'\rangle\langle i'|\Psi\rangle = \sum_j \langle\Psi|i'\rangle|\theta_j\rangle\langle\theta_j|\langle i'|\Psi\rangle$

$w_i' = \sum_j |\langle\Psi|i'\rangle|\theta_j\rangle|^2 \geq 0$

Therefore $\sum_i w_i = 1$; $w_i \geq 0$

Reformulate Quantum Mechanics:

Any system described by a density matrix ρ, where $\rho = \sum_i w_i |i\rangle\langle i|$

(a) set $|i\rangle$ is a complete orthonormal set of vectors
(b) $w_i \geq 0$; (c) $\sum_j w_j = 1$; (d) Given an operator A, expectation $\langle A\rangle = \mathrm{Tr}\,\rho A$

Notice $\langle A \rangle = \sum_i \langle i' | \rho A | i' \rangle = \sum_i w_i' \langle i' | A | i' \rangle$

Interpretation, w_i = probability ~~for~~ system to be in state i;

If $w_j = 1$, $w_j' = 0$, then ρ is <u>pure</u>
otherwise, ρ is <u>mixed</u>

Simple test $\text{Tr}\,\rho^2 = \text{Tr}\,\rho$ if ρ is pure

If a system has a position representation,

$$\rho(x, x') = \langle x | \rho | x' \rangle = \sum_i w_i \langle x' | i \rangle \langle i | x \rangle$$

$$= \sum_i w_i \, i(x') \, i(x)$$

$$\langle A \rangle = \int dx \, \langle x | \rho A | x \rangle = \int dx\, dx' \rho(x, x') A(x', x)$$

Time evolution : $|i(t)\rangle = e^{-iHt} |i(0)\rangle$

H operates on system variables

$$\therefore \rho(t) = \sum_i w_i \, e^{-iHt} |i\rangle\langle i| e^{+iHt}$$

$$= e^{-iHt} \rho(0) \, e^{+iHt}$$

$\Rightarrow \frac{d\rho}{dt} = -i [H, \rho]$ Schrodinger's eq. for DMs

Notice $\mathrm{Tr}\,\dot{\rho} = \frac{d}{dt}\mathrm{Tr}\,\rho = \frac{d}{dt}1 = 0$

$$\mathrm{Tr}\,\rho^n = \mathrm{Tr}\left(e^{-iHt}\rho e^{+iHt}\right)^n$$

$$= \mathrm{Tr}\left[e^{-iHt}\rho \underbrace{e^{+iHt}\, e^{-iHt}}_{1} \rho \underbrace{e^{+iHt} \cdots e^{-iHt}}_{1} \rho \underbrace{e^{-iHt}}_{1}\right]$$

$$= \mathrm{Tr}\left[e^{-iHt}\rho^n e^{+iHt}\right]; \text{ but } \mathrm{Tr}\,AB = \mathrm{Tr}\,BA$$

$= \mathrm{Tr}\,\rho^n \Rightarrow$ indep. of time.

$\Rightarrow \mathrm{Tr}\,f(\rho)$ is indep. of time.

Define von Neumann entropy $S = -\sum_j W_j \ln W_j$

as analogue of Shannon entropy for DM's

$S := -\mathrm{Tr}[\rho \ln \rho]$ is a measure of purity.

$S = 0$ for pure state; if $W_i = \frac{1}{N}$, $i = 1, \dots, N$

unchanged by unitaries ~~keep~~ it

$S = -\sum_{j=1}^{N} \frac{1}{N} \ln \frac{1}{N} = \ln N$ for fully mixed state.

- cannot increase in time without measurements or interactions

Density Matrix in Stat. Mech.

Recall, probability in canonical ensemble of being in state j is

$$P(j) = \frac{e^{-\beta E_j}}{\sum_j e^{-\beta E_j}} = \frac{e^{-\beta E_j}}{Z}$$

Therefore the DM is $\rho = \sum_j w_j |\phi_j\rangle\langle\phi_j|$

$$w_j = e^{-\beta E_j}/Z \Rightarrow \rho(x,x') = \sum_j \frac{1}{Z} e^{-\beta E_j} \langle x|\phi_j\rangle\langle\phi_j|x'\rangle$$

$$\rho = e^{-\beta \hat{H}} / \mathrm{Tr}\, e^{-\beta H} \quad ; \quad U = \mathrm{Tr}\, \rho H$$

~~F = U - TS~~ Consider the unnormalized version

$\tilde{\rho} = e^{-\beta H}$, Notice this solves the differential equation $\frac{\partial}{\partial\beta}\tilde{\rho} = -H\tilde{\rho}$

with the initial condition $\rho(0) = 1$

very similar to $i\frac{\partial}{\partial t}\psi = H\psi$ or $\frac{\partial \psi}{\partial t} = (-iH\psi)$

identify $\psi \leftrightarrow \rho$, $\beta \leftrightarrow it$