lecture - 7 Quantum Mechanics - I Oct. 12, 2009 (6)

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More on the density operator,

* any Hermitian, non-negative define, with unit trace operator can be viewed as a density operator.

* Assume R has all three features –

$$R|n\rangle = r_n|n\rangle \quad , \quad r_n : \text{eigenvalue}, \ |n\rangle : \text{eigenstate of } R$$

Since R is Hermitian, r_n is real.

$$\langle n|R|n\rangle = r_n \geq 0 \quad \text{because it's nonnegative definite}$$

Also, the unit trace says $\sum_n r_n = 1$.

$\Rightarrow$ r_n can be interpreted as probabilities.

R can be expanded in terms of its projection operators and eigenvalues

$$R = \sum_n r_n |n\rangle\langle n|$$

$\Rightarrow$ This is ~~exactly~~ exactly the same definition of ρ in the discrete case.

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* An arbitrary ρ can be represented in terms of an orthonormal set of pure states; BUT in the general form $|\psi_i\rangle$ need not to be orthogonal at all!!

$$\rho = \sum_i f_i |\psi_i\rangle\langle\psi_i|$$

* $tr(\rho^2) \leq 1$, with equality iff ρ represents a pure state

$$tr(\rho^2) = \sum_k \langle k| \left(\sum_n f_n |n\rangle\langle n|\right)\left(\sum_m f_m |m\rangle\langle m|\right)|k\rangle$$

$$= \sum_k \langle k| \left(\sum_n f_n^2 |n\rangle\langle n|\right)|k\rangle = \sum_n f_n^2 \leq 1$$

only pure state can be 1.

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☆ Another test is that $\rho^2 = \rho$ iff pure state

By pure state, $\rho = |n\rangle\langle n|$ (no sum)

$$\rho^2 = (|n\rangle\langle n|)(|n\rangle\langle n|) = |n\rangle\langle n| = \rho$$

☆ Or by checking the entropy. —

In statistical mechanics, $S = -k_B \sum_i p_i \ln p_i$

So, in QM,

k_B : Boltzmann const

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

$$= -k_B \sum_k \langle k| \left(\sum_m p_m |m\rangle\langle m|\right)\left(\sum_n \ln(p_n) |n\rangle\langle n|\right)|k\rangle$$

$$= -k_B \sum_k \langle k| \left(\sum_n p_n \ln(p_n) |n\rangle\langle n|\right)|k\rangle$$

$$= -k_B \sum_i p_i \ln p_i$$

For a pure state $p_0 = 1$, and no other $\Rightarrow$ $\underline{S = 0}$

for a mixed state $\underline{S > 0}$

☆ An interesting case, if we maximize S with constraint $\mathrm{tr}\rho = 1$ with a fixed expected energy $\mathrm{tr}(\rho H)$ (see next page)

$\Rightarrow$ We obtain the density operator for a system at thermal equilibrium at a given temperature.

$$\boxed{\rho = \frac{1}{Z} e^{-\beta H}}$$; $\beta = \frac{1}{k_B T}$, Z : the partition function

$$\boxed{Z(\beta) = \mathrm{tr}\left(e^{-\beta H}\right)}$$

such that $\mathrm{tr}(\rho) = 1$

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maximize S

$$\delta S = -k_B \sum_i \delta f_i (\ln f_i + 1) = 0$$

fixed H, $\mathrm{tr}\rho = 1$

$$\delta(H) = \sum_i \delta f_i \varepsilon_i = 0$$

$$\delta(\mathrm{tr}\rho) = \sum_i \delta f_i = 0$$

Therefore $k_B(1 + \ln f_i) + \alpha \varepsilon_i + \gamma = 0$, α, γ : Lagrange multipliers.

$$\Rightarrow \quad f_i = \exp\left(-\frac{\alpha \varepsilon_i + \gamma}{k_B} - 1\right)$$

① Since one requires the argument to be dimensionless $\alpha = \frac{\pm 1}{T}$
such that $[k_B T] = [\varepsilon]$

② The sign must be $(+)$, so the energy of system will be bounded.

③ normalization fixes the rest.

$$\Rightarrow \quad \rho = \frac{1}{Z} e^{-\beta H} \quad , \quad \beta = \frac{1}{k_B T}$$

☆ The physics of the above ρ is that of a system which has been prepared by allowing it to equilibrate with a heat bath at temperature T. then detach from the heat bath and be delivered to a measurement.

e.g. silver atoms ⟺ hot wall
⇘
silver atoms ⟶ leave the oven, no more interaction.
do not all have the same energy, but a distribution of energy.

All information is contained in the density operator.

☆ If $H|n\rangle = E_n|n\rangle$

$$\rho = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n| \quad , \quad Z(\beta) = \sum_n e^{-\beta E_n}$$

The partition function is essentially important in statistical Mechanics.

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The difference between

☆ density operator $\Longleftrightarrow$ coherent superposition
(incoherent superposition)

$$|\psi\rangle = \sum_n c_n |n\rangle$$

c_n: are presumed known.

☆ If you like, you can imagine a ket vector that represents the state of a system at a given T, but the c_n are only known in a statistical sense.

$$c_n = a_n e^{i\theta_n}$$

then, according to the Boltzmann distribution,

$$\langle a_n^2 \rangle = \frac{e^{-\beta E_n}}{Z}, \quad \text{and} \quad \theta_n \in [0, 2\pi] \quad \text{totally random}$$

So $$|\psi\rangle\langle\psi| = \sum_{nm} c_n c_m^* |n\rangle\langle m| = \sum_{n,m} a_n a_m e^{i(\theta_n - \theta_m)} |n\rangle\langle m|$$

Due to the random phase,

$$\langle e^{i(\theta_n - \theta_m)} \rangle_{phase} = \delta_{nm},$$

if $n \neq m$ $\langle e^{i\theta_n} \rangle = \langle e^{i\theta_m} \rangle = 0$

therefore

$$\langle |\psi\rangle\langle\psi| \rangle_{phase} = \sum_n a_n^2 |n\rangle\langle n|,$$ and we recover the canonical density operator.

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Now we can revise the postulates of QM to incorporate the density operator.

① Every physical system is associated with a Hilbert space $\mathcal{E}$

② Every state of a physical system is associated with a density operator ρ acting on $\mathcal{E}$. (And ρ is Hermitian, nonnegative definite operator of unit trace, $tr\rho = 1$)

③ Every measurement which can be carried out on the system corresponds to a complete Hermitian operator A,

④ The possible outcomes are the eigenvalues of A
(discrete : $a_1, a_2 \cdots$ or continuous $a(\nu)$)

⑤ The average value of measurement A is $tr(\rho A)$

discrete : $\text{Prob}(A = a_n) = tr(\rho \mathbb{P}_n)$

$\mathbb{P}_n$ is the projection operator onto the eigenspace $\mathcal{E}_n$ corresponding to eigenvalue a_n.

continuous : $\text{Prob}(a_0 \leq A \leq a_1) = tr(\rho \mathbb{P}_I)$, $I = [a_0, a_1]$

⑥ After measuring a eigenvalue $\begin{cases} a_n, & \rho \Rightarrow \dfrac{\mathbb{P}_n \rho \mathbb{P}_n}{tr(\rho \mathbb{P}_n)} \\ I & \Rightarrow \dfrac{\mathbb{P}_I \rho \mathbb{P}_I}{tr(\rho \mathbb{P}_I)} \end{cases}$