Title: Quantum Theory - Lecture 220914

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Collection: Quantum Theory (2022-2023)

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Lecture-5 (14-September,2022)

Our learning goals:

- Questions & doubts
- Heisenberg picture
  - Comparison
  - Equation of motion
- Introduction to density operators
  - Defining (with examples)
  - Properties
  - Pure & mixed states
  - Examples
  - Generic density matrix for a two level system

$$\underbrace{-\frac{\hbar^2}{2m}\nabla_1^2\psi - \frac{1}{r_1}\psi}_{H} = E\psi \quad \checkmark$$

$$H_1\psi + H_2\psi + \frac{ze\psi}{|r_1 - r_2|} = E\psi$$

V

H

$$H_1 \psi + H_2 \psi + \frac{Z e \psi}{|r_1 - r_2|} = E \psi \qquad -4 \text{ au}$$

$$H_1\psi + H_2\psi + \frac{ze\psi}{|r_1 - r_2|} = E\psi$$

$$\langle r| \; |\psi\rangle \langle \; | \; | \; \rangle \langle \; | \; | \; \rangle$$

-4 au

first -2.75

-2.9077

13' $\rightarrow 2.90372433$

Cohen Tanojji

Bramsden & Jochain $\rightarrow$ QM /

$$H_1\psi + H_2\psi + \frac{ze\psi}{|r_1 - r_2|} = E\psi$$

$\langle n| \; | \rangle \langle \; | \; | \; \rangle \langle \; | \; | \; \rangle$

-4 au

$\Downarrow$

first $\quad -2.75$

-2.9077

13' $\quad \rightarrow 2.90372433$

Cohen Tanojji

Bransden & Jochain → QM / AP.

Convergence of Dyson Series

$$i\hbar \frac{dU}{dt} = HU$$

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$$U = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt' \int_0^t dt'' \ldots \int_0^t dt^n \; H(t') H(t'') \ldots H(t^n) + \ldots$$

$$e^{iHt/\hbar} = \sum_{n=0}^{\infty} \int \left(\frac{i}{\hbar}\right) H(t')\, dt'$$

Convergence of

$$i\hbar \frac{dU}{dt} = H U$$

$$U = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt' \int_0^t dt'' \cdots \int_0^t dt^n \, H(t') H(t'') \cdots H(t^n) + \cdots$$

$$e^{\int \frac{i}{\hbar} H(t') dt'} = \sum_{n=0}^{\infty} \left[\int_0^t \left(\frac{i}{\hbar}\right) H(t') \, dt'\right]^n \frac{1}{n!} \qquad e^A =$$

$$U = 1 + \sum_{n=1} \frac{1}{n!} \left(\frac{\;}{\hbar} \right) \int_0 \int_0 \int_0$$

$$e^{\int \frac{i}{\hbar} H(t') dt'} = \sum_{n=0}^{\infty} \left[\int_0^t \left(\frac{i}{\hbar} \right) H(t')\, dt' \right]^n \frac{1}{n!} \qquad e^A =$$

$$U = 1 + \left(\frac{-i}{\hbar} \right) \int_0^t dt' H(t') + \underbrace{\left(\frac{-i}{\hbar} \right)^2 \int_0^t dt' \int_0^{t'} dt'' H(t') H(t'')}_{} + \cdots$$

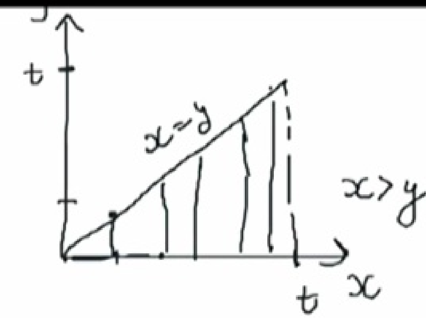
consi

consider

$$J_1 = \int_0^t dt' \int_0^{t'} dt'' \, H(t') \, H(t'') \qquad t' \to x \qquad t'' \to y$$

$$= \int_0^t dx \int_0^x dy \, H(x) \, H(y) \qquad \underline{\underline{x > y}}$$

$x \mid y$

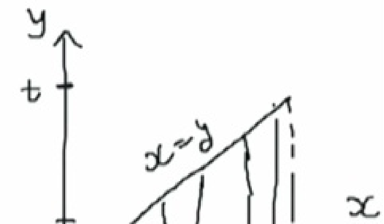


$$J_2 = \int_0^t dx$$

$$\checkmark\, U = 1 + \sum_{n=1}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_0^t dt' \int_0^t dt'' \cdots \int_0 dt^n \, H(t')H(t'') \cdots H(t^n) + \cdots$$

$$e^{\int \frac{i}{\hbar} H(t')dt'} = \sum_{n=0}^{\infty}\left[\int_0^t \left(\frac{i}{\hbar}\right) H(t')\,dt'\right]^n \frac{1}{n!} \qquad e^A =$$

$$\checkmark\, U = 1 + \left(-\frac{i}{\hbar}\right)\int_0^t dt' H(t') + \underbrace{\left(-\frac{i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' H(t')H(t'')}_{} + \cdots$$

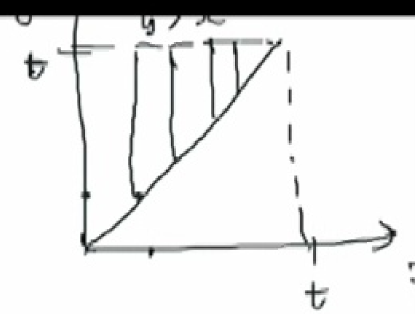


consider

$$I = \int^t dt' \int^{t'} dt'' H(t')\, H(t'') \qquad t' \to x$$

$$J_2 = \int_0^t dx \int_x^t dy \; H(y)\, H(x) \qquad y > x$$

x	y
$0-1$	$1-t$
time order $0-2$	$2-t$



$$J_2 = J_1 \qquad T[H(x)\, H(y)] \quad x>y$$

$$2J = \int_0^t dx \left[\int_0^x dy\, [H(x)\, H(y)] + \int_x^t dy\, \underbrace{T[H(x)\, H(y)]}_{H(y)\, H(x)} \right]$$

$$H(y)\, H(x)$$

$$y > x$$

$$J = \frac{1}{2!} \int_0^t dx \int_0^t dy \int H(x)\, H(y) =$$

$$T[H(x)\, H(y)]$$

$$= H(y)\, H(x)$$

State kets

Operators

$t = t_0 =$ $|\alpha(t_0)\rangle_H$

$A^H(t_0) = A^{(S)}(t_0)$

$t = t$ $|\alpha(t)\rangle_H = |\alpha(t_0)\rangle_H =$

$A^H(t) = U^\dagger(t, t_0)\, A^{(S)}\, U(t, t_0)$

$|\alpha(t_0)\rangle_S \Rightarrow U\, |\alpha(t)\rangle_S$

$$\boxed{|\alpha(t)\rangle_H = U^\dagger(t, t_0)\, |\alpha(t)\rangle_S}$$

$$- \frac{-iH}{\hbar} U |\alpha\rangle$$

[redacted]

$$\frac{dA^H(t)}{dt} = \frac{i}{\hbar}\left[H^H A^H(t) - A^H(t) H^H\right]$$

$$\boxed{\frac{dA^{(H)}(t)}{dt} = \frac{i}{\hbar}\left[H , A^H\right]}$$

$$\rho = |\alpha\rangle\langle\alpha|$$

$$\rho_{\uparrow} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix}$$

$$|\uparrow\rangle\langle\uparrow| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$|\alpha\rangle \rightarrow$ State Kets

$$|\alpha\rangle = \sum_n C_n |n\rangle$$

$$|\uparrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \checkmark \qquad |\downarrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\langle \uparrow | \rho | \uparrow \rangle = 1$$

$$\langle \downarrow | \rho | \downarrow \rangle = 0$$

$N\ e^-s$ $\qquad$ $N_\uparrow$ are in $\uparrow$

$N_\downarrow$ are in $\downarrow$

$$W_\uparrow = \frac{N_\uparrow}{N_\uparrow + N_\downarrow} \qquad W_\downarrow = \frac{N_\downarrow}{N_\uparrow + N_\downarrow}$$

N e s $\quad N_\uparrow$ ...

$N_\downarrow$ are in $\downarrow$

$$\rho = \underbrace{|\alpha\rangle\langle\alpha|}$$

$$W_\uparrow = \frac{N_\uparrow}{N_\uparrow + N_\downarrow} = \frac{1}{2} \checkmark \qquad W_\downarrow = \frac{N_\downarrow}{N_\uparrow + N_\downarrow} = \frac{1}{2} \checkmark$$

unpolarized $\quad$ no. of up $\uparrow$ $=$ no. of down $\downarrow$

$\qquad\qquad N_\uparrow \qquad\qquad N_\downarrow$

$$\rho = \sum_\alpha |\alpha\rangle W_\alpha \langle\alpha| \qquad \sum W_\alpha = 1$$

$$= W_\uparrow |\uparrow\rangle\langle\uparrow| + W_\downarrow |\downarrow\rangle\langle\downarrow| \qquad W_\uparrow + W_\downarrow = 1$$

$$\rho = \frac{1}{2}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \Rightarrow \text{mixture.}$$

$$\rho = \frac{1}{2}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \Rightarrow \text{mixture / mixed state.}$$

$|\alpha\rangle$ $\qquad$ $w_1 \underline{|\alpha_1\rangle} + w_2 |\alpha_2\rangle - - - .$

$|\alpha\rangle \qquad\qquad w_1|\underline{\alpha_1}\rangle \; + \; w_2|\alpha_2\rangle \; - - - .$

$|\alpha\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \rightarrow$ <u>Pure state</u>

$w_1|\alpha_1\rangle \qquad w_2|\alpha_2\rangle$

$|\alpha_1\rangle = \sum_n C_n|n\rangle \qquad |\alpha_2\rangle = \sum_{n'} C_{n'}|n'\rangle$

$\langle n|n'\rangle = \delta_{nn'}$

$$\mathrm{Tr}(\rho) = \sum_n \langle n|\rho|n\rangle$$

$$= \sum_{n,\alpha} \langle n|$$

1) Hermitian $\rho^\dagger = \sum_\alpha w_\alpha |\alpha\rangle\langle\alpha| ...$

2) if $|\alpha\rangle$ are normalized then trace$(\rho) = 1$

$$Tr(\rho) = \sum_n \langle n|\rho|n\rangle$$

$$= \sum_n \langle n| \sum_\alpha w_\alpha |\alpha\rangle\langle\alpha|n\rangle$$

$$\sum_n |c_n|^2 = 1$$

$$= \sum_{n,\alpha} w_\alpha \underbrace{\langle n|\alpha\rangle\langle\alpha|n\rangle}_{|c_n|^2}$$

$$= \underline{\underline{\sum_\alpha w_\alpha}} = 1$$

α $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\sum w_\alpha = 1$

$= \; W_\uparrow |\uparrow\rangle\langle\uparrow| + W_\downarrow |\downarrow\rangle\langle\downarrow| \qquad\qquad W_\uparrow + W_\downarrow = 1$

$$\rho = \frac{1}{2}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \Rightarrow \text{mixture / mixed state.}$$

$|\alpha\rangle \qquad\qquad w_1 |\alpha_1\rangle + w_2 |\alpha_2\rangle - - - .$

$|\alpha\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \rightarrow$ Pure State

$w_1 |\alpha_1\rangle \qquad w_2 |\alpha_2\rangle$

$\langle n|m\rangle = \delta_{nm} \Leftarrow |\alpha_1\rangle = \sum_n C_n |n\rangle \qquad |\alpha_2\rangle = \sum_{n'} C_{n'} |n'\rangle \qquad \langle n'|m'\rangle = \delta_{n'm'}$

$\langle n|n'\rangle \neq \delta_{nn'}$

3) Density

4) Trace of square of density matrix ≤ 1

$$Tr(\rho^2) = \sum_m \langle m | \rho \cdot \rho | m \rangle$$

$$= \sum_m$$

4) Trace of square of density matrix $= 1$

$$Tr(\rho^2) = \sum_{m} \langle m | \rho . \rho | m \rangle$$

$$= \sum_{\substack{m \\ \alpha \alpha'}} W_\alpha W_{\alpha'} \langle m | \alpha \rangle \underbrace{\langle \alpha | \alpha' \rangle}_{\text{othronormal.}} \langle \alpha' | m \rangle$$

$$\delta_{\alpha \alpha'}$$

$$= \sum_{m \alpha} |W_\alpha|^2 \langle m | \alpha \rangle \langle \alpha | m \rangle$$

$$= \sum_{m \alpha} 1$$

$$\mathrm{Tr}(\rho^2) = \sum_\alpha |W_\alpha|^2 \leq \left(\sum_\alpha W_\alpha\right)^2$$

$$\mathrm{Tr}(\rho^2) \leq \big(\underbrace{\mathrm{Tr}(\rho)}_{1}\big)^2$$

$$\mathrm{Tr}(\rho^2) \leq 1$$

Pure state T

$$\rho = \frac{1}{2}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} + \frac{1}{2}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \Rightarrow \text{mixture / mixed state.} \quad Tr(\rho^2)$$

$$\begin{bmatrix}1/2 & \\ & 1/2\end{bmatrix}\begin{bmatrix}1/2 & \\ & \end{bmatrix}$$

$|\alpha\rangle$ $\qquad w_1|\alpha_1'\rangle + w_2|\alpha_2'\rangle - - -$

$|\alpha\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \rightarrow$ Pure state

$w_1 |\alpha_1\rangle \qquad w_2 |\alpha_2\rangle$

$|\alpha_1\rangle = \sum c_n |n\rangle \qquad |\alpha_2\rangle = \sum_{n'} c_{n'} |n'\rangle \qquad \langle n'|m\rangle = \delta_{n'm}$

[redacted]

mixed state $\quad \mathrm{Tr}(\rho) < 1$

1) $\quad |\alpha\rangle$