PHYS 612, MID-TERM 1

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1. Hermitian Operator and Unitary Operator

- Hermitian: $H^\dagger = H$
- Unitary: $U^\dagger U = I$

1.1. Hermitian Operator.

- $\langle\alpha|H|\alpha\rangle$ is real
- Eigenvalues of H are real

$$H|\psi\rangle = h|\psi\rangle$$
$$\langle\psi|H|\psi\rangle = h\langle\psi|\psi\rangle$$

- Eigenvectors of H with distinct eigenvalues are orthogonal
- One can always construct an orthonormal basis out of eigenstates of H
- Each physical quantity is associated with a Hermitian operator, and can be written as $A = \sum_i a_i|i\rangle\langle i|$

1.2. Unitary Operator.

- One can always use a unitary operator to diagonalize a Hermitian operator
- We can always use a unitary transform to diagonalize $|i'\rangle = U|i\rangle$
- General unitary operator for 2-d QM space: $U(\delta,\theta,\hat{n}) = e^{i\delta}e^{i\theta\hat{n}\cdot\frac{\vec{\sigma}}{2}} = e^{i\delta}[\cos(\frac{\theta}{2}) + i\hat{n}\cdot\vec{\sigma}\sin(\frac{\theta}{2})]$

$$\begin{aligned}\exp\left(\frac{-i\vec{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right) =& \left[1 - \frac{(\vec{\sigma}\cdot\hat{\mathbf{n}})^2}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{(\vec{\sigma}\cdot\hat{\mathbf{n}})^4}{4!}\left(\frac{\phi}{2}\right)^4 - \cdots\right] \\ &- i\left[(\vec{\sigma}\cdot\hat{\mathbf{n}})\frac{\phi}{2} - \frac{(\vec{\sigma}\cdot\hat{\mathbf{n}})^3}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right] \\ =& 1\cos\left(\frac{\phi}{2}\right) - i\vec{\sigma}\cdot\hat{\mathbf{n}}\sin\left(\frac{\phi}{2}\right)\end{aligned}$$

- If u is the eigenvalue of a unitary operator, we have $|u|^2 = u^*u = 1$
- $U^\dagger e^B U = e^{U^\dagger BU}$ and $(e^B)^\dagger = e^{B^\dagger}$
- If H is a Hermitian operator, then e^{iH} is unitary
- Any unitary operator U can be written as e^{iH}, where H is a Hermitian operator

1.3. Schmidt orthogonalization.

2. Bra, Ket and Operators

2.1. Basic.

- $\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle$
- $\langle\alpha|\alpha\rangle$ is real
- $\langle\alpha|\alpha\rangle \geq 0$
- Given a set of **orthonormal** basis, an operator can be written as $A = \sum A_{ij}|i\rangle\langle j|$
- $\langle A\rangle = \langle\psi|A|\psi\rangle$ does not depend on basis
- $\psi(x) = \langle x|\psi\rangle$ and $\phi(p) = \langle p|\phi\rangle$

2.2. Different kinds of operators.

- Projection operator $\rightarrow$ measurement
- Hermitian operator $\rightarrow$ physical quantity
- Unitary operator $\rightarrow$ transform of basis / operator

2.3. Commutator.

- Jacob Identity: $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$
- compatable(can be measured at the same time) means $[A,B] = 0$
- If $[A,B] \neq 0$, we have $\sigma_A^2\sigma_B^2 \geqslant \frac{1}{4}|\langle[A,B]\rangle|^2$

$$\sigma_A^2 = \langle(\hat{A} - \langle\hat{A}\rangle)\Psi|(\hat{A} - \langle\hat{A}\rangle)\Psi\rangle = \langle f|f\rangle$$

$$\sigma_B^2 = \langle(\hat{B} - \langle\hat{B}\rangle)\Psi|(\hat{B} - \langle\hat{B}\rangle)\Psi\rangle = \langle g|g\rangle$$

$$\sigma_A^2\sigma_B^2 = \langle f|f\rangle\langle g|g\rangle$$

$$\langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$$

$$|\langle f|g\rangle|^2 = \left(\frac{\langle f|g\rangle + \langle g|f\rangle}{2}\right)^2 + \left(\frac{\langle f|g\rangle - \langle g|f\rangle}{2i}\right)^2 \geq \left(\frac{\langle f|g\rangle - \langle g|f\rangle}{2i}\right)^2$$

2.4. Pauli Matrix.

$$\sigma_x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = -i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow| = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- $[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$
- $\{\sigma_j, \sigma_k\} = 2\delta_{jk}I$
- General Hermitian matrix $H = h_1 I + \vec{h}\cdot\vec{\sigma}$, with $Det[H] = h_1^2 - \vec{h}^2$ and $Tr[H] = 2h_1$
- Eigenvalues λ of H satisfy $\lambda^2 - \lambda Tr[H] + Det[H] = 0$, $\lambda = h_1 \pm |\vec{h}|$

- Operator $\hat{h} \cdot \vec{\sigma}$ has eigenvalues ± 1, and is commute with H
- Operator $\sigma^{x-y}(\phi) = \cos(\phi)\sigma_x + \sin(\phi)\sigma_y$ satisfies $[\frac{\sigma_z}{2}, \sigma^{x-y}(\phi)] = -i\frac{\partial}{\partial \phi}\sigma^{x-y}(\phi)$
- $e^{i\theta\frac{\sigma_z}{2}}\sigma^{x-y}(\phi)e^{-i\theta\frac{\sigma_z}{2}} = \sigma^{x-y}(\phi + \theta)$
- $(\hat{n} \cdot \vec{\sigma})^2 = I$
- $e^{i\theta(\hat{n}\cdot\vec{\sigma})} = \cos\theta I + i\sin\theta(\hat{n} \cdot \vec{\sigma})$
- $\mathrm{Tr}[\sigma_i\sigma_j] = 2\delta_{ij}$

3. Entanglement and Tensor Product

- Entangled state cannot be written as a tensor product
- Not entangled state / a tensor product can be considered as two isolated quantum systems
- Definition of the tensor product

$$\sigma_x^{(1)} \otimes I^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

3.1. **Density matrix.**

- Reduced density matrix: $\rho_\psi^{(1)} = \mathrm{Tr}_2[\rho_\psi]$
- For any operator $O^{(1)}$ and any state $|\psi\rangle$, $\mathrm{Tr}[\rho_\psi O^{(1)} \otimes I^{(2)}] = \mathrm{Tr}_1[\rho_\psi^{(1)} O^{(1)}]$
- $\mathrm{Tr}_1[\rho_\psi^{(1)}] = 1$
- Projection operator on a pure state has one eigenvalue 1 and all others are 0
- ψ is a pure state if $\mathrm{Tr}[\rho_\psi^2] = 1$
- $S = -\mathrm{Tr}[\rho\log(\rho)]$, pure state will have $S = 0$

4. About Momentum

4.1. **Basic.**

- Start from the assumption $\langle x|p\rangle = \text{const } e^{ip\cdot x}$
- With $\langle p'|p''\rangle = \delta(p' - p'')$, we have $\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ip\cdot x}$
- $\hat{p}$ is the generator of infinitesimal transition $e^{i\hat{p}x_0}|x'\rangle = |x' - x_0\rangle$
- $[\hat{x}, \hat{p}] = i$
- $\hat{p}|x\rangle = i\frac{\partial}{\partial x}|x\rangle$ and $\langle x|\hat{p} = -i\frac{\partial}{\partial x}\langle x|$
- $\hat{x}|p\rangle = -i\frac{\partial}{\partial p}|p\rangle$ and $\langle p|\hat{x} = i\frac{\partial}{\partial p}\langle p|$

4.2. **Quantum Dynamics.**

- U is an unitary operator satisfies $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$, then $i\dot{\hat{U}}\hat{U}^\dagger = \hat{H}$ is a Hermitian operator

$$\frac{d}{dt}\left(\hat{U}(t)\hat{U}^\dagger(t)\right) = \frac{d}{dt}\hat{I} = 0$$

- $i\dot{\hat{U}}(t) = \hat{H}\hat{U}(t)$, where H is Hamiltonian, then we got $\hat{H}|\psi(t)\rangle = i\frac{\partial}{\partial t}|\psi(t)\rangle$ and $\hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)}$
- When $\hat{H}(t)$ depends on time, $U(t,t_0) = \mathrm{T}[\exp(-i\int_{t_0}^{t}\hat{H}(t')dt')]$
- $\frac{1}{n!}T\left[\left(-\mathrm{i}\int_{t_0}^{t} dt'\widehat{H}\left(t'\right)\right)^n\right] = (-i)^n\int_{t_0}^{t} dt^1\int_{t_0}^{t^1} dt^2\cdots\int_{t_0}^{t^{n-1}} dt^n\widehat{H}\left(t^1\right)\widehat{H}\left(t^2\right)\ldots\widehat{H}\left(t^n\right)$

5. Heisenberg Picture

- $\hat{A}^H(t) = U(t)^\dagger\hat{A}^S U(t)$
- $\dot{A}^H(t) = i[H, A^H(t)]$
- When $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, $\dot{\hat{x}} = i[\hat{H},\hat{x}^H] = \frac{\hat{p}^H}{m}$ and $\dot{\hat{p}}^H = -V'(\hat{x}^H)$

5.1. An example of spin $\frac{1}{2}$ particle.

We put an electron in a magnetic field, then the Hamiltonian is $H = -\vec{\mu}\cdot\vec{B}$ and $\vec{\mu} = -g\mu_B\vec{s} = -g\mu_B\frac{\vec{\sigma}}{2}$, in which $\mu_B = \frac{e}{2m_e}$.

Let $\vec{B} = B_0\hat{z}$, we have $H = \frac{1}{2}g\mu_B B_0\hat{\sigma_z} = \frac{1}{2}\omega\hat{\sigma_z}$. So, $U(t) = \exp(-i\omega t\frac{\hat{\sigma}_z}{2})$, and we have

$$\begin{pmatrix} \hat{s}_x^H(t) \\ \hat{s}_y^H(t) \\ \hat{s}_z^H(t) \end{pmatrix} = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) & 0 \\ -\sin(\omega t) & \cos(\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{s}_x^H(0) \\ \hat{s}_y^H(0) \\ \hat{s}_z^H(0) \end{pmatrix}$$

5.2. Simple 1-d Harmonic Oscillator.

We have the Hamiltonian $H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2$. Replace with $\tilde{x} = \sqrt{m\omega}x$ and $\tilde{p} = \frac{p}{\sqrt{m\omega}}$, it keeps $[\tilde{x},\tilde{p}] = i$. Now, $H = \frac{\omega}{2}(\tilde{p}^2 + \tilde{x}^2)$.

With Heisenberg equations of motion, we have $\dot{\tilde{x}}^H = i[\hat{H},\hat{x}^H] = \omega\hat{p}^H$ and $\dot{\hat{p}}^H = -\omega\hat{x}^H$.

The solutions are

$$\tilde{x}^H(t) = \cos(\omega t)\tilde{x}^H(0) + \sin(\omega t)\tilde{p}^H(0)$$
$$\hat{p}^H(t) = -\sin(\omega t)\tilde{x}^H(0) + \cos(\omega t)\hat{p}^H(0)$$

which is same as the classical solutions.

Also, there is another way by changing variables

$$\hat{a} = \frac{1}{\sqrt{2}}(\tilde{x} + i\tilde{p})$$
$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\tilde{x} - i\tilde{p})$$

Then we have $\hat{a}^H(t) = e^{i\omega t}\hat{a}^H(0)$ and $(\hat{a}^\dagger)^H(t) = e^{-i\omega t}(\hat{a}^\dagger)^H(0)$.

- $[\hat{a},\hat{a}^\dagger] = 1$
- $\hat{N} = \hat{a}^\dagger\hat{a} = \frac{1}{2}(\tilde{x}^2 + \tilde{p}^2) - \frac{i}{2}[\tilde{p},\tilde{x}]$, so $\hat{H} = (\hat{N} + \frac{1}{2})\omega$
- $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ (Here n can only be the integer)
- Partition function $Z(\beta) = \sum_n e^{-\beta E_n}$, $\mathrm{Tr}[U(-i\beta)] = \mathrm{Tr}[e^{-\beta H}] = Z(\beta)$

5.3. About the derivative of Dirac delta function.

5.3.1. *Definition.*

$$\delta'(x) = \lim_{h\to 0}\frac{\delta(x+h)-\delta(x)}{h}$$

5.3.2. *Properties.*

$$\delta'(-x) = -\delta'(x)$$

$$x\delta'(x) = -\delta(x)$$

$$\int_{-\infty}^{\infty}\delta'(x)\varphi(x)dx = -\int_{-\infty}^{\infty}\delta(x)\varphi'(x)dx = -\varphi'(x)|_{x=0}$$

$$\int_{-\infty}^{\infty}\delta'(x-x')\varphi(x')dx' = \int_{-\infty}^{\infty}\delta(x-x')\varphi'(x')dx' = \varphi'(x)$$

5.4. **Schrodinger Equation in 3-D coordinate space.**

- Strat from $\hat{H}|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle$, we can get $\langle\vec{x}|\frac{\hat{\vec{p}}\cdot\hat{\vec{p}}}{2m} + V(\hat{\vec{x}})|\psi\rangle = (\frac{-\nabla^2}{2m} + V(\vec{x}))\psi(\vec{x},t) = i\langle\vec{x}|\frac{\partial}{\partial t}\psi\rangle = i\frac{\partial}{\partial t}\psi(\vec{x},t)$

5.4.1. *Propagator and Green's function.*
Basically, we want to get $\psi(\vec{x}',t)$ with $\psi(\vec{x},t_0)$. As we know, $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$.

$\psi(\vec{x},t) = \langle\vec{x}|\psi(t)\rangle = \int d^3\vec{x}'\langle\vec{x}|U(t,t_0)|\vec{x}'\rangle\langle\vec{x}'|\psi(t_0)\rangle = \int d^3\vec{x}' K(\vec{x},t;\vec{x}',t_0)\psi(\vec{x}',t_0)$, in which K is a propagator.

$(-\frac{\nabla^2}{2m}+V(\vec{x})-i\frac{\partial}{\partial t})\psi(\vec{x},t) = \hat{O}\psi(\vec{x},t) = 0$, we have $\hat{O}K(\vec{x},t;\vec{x}',t_0) = -i\delta^3(\vec{x}-\vec{x}')\delta(t-t_0)$. We call K is the Green's function of $\hat{O}$.

5.5. **Gauge Potentials and Electronicmagnetics.**

Hamiltonian for charged particle in Electronicmagnetic field is $H = \frac{(\vec{p}-q\vec{A})^2}{2m} + q\phi$.

- $\vec{B} = \vec{\nabla}\times\vec{A}$ and $\vec{E} = -\vec{\nabla}\phi - \frac{\partial\vec{A}}{\partial t}$
- Here canonical momentum $\vec{p}$ is not equal to $m\vec{v}$ and does not corresponding to "mechanical momentum", but this is the the only way to write a Hamiltonian formalism in terms of local object.

5.5.1. *Gauge transform.*

- $\vec{A}(\vec{x},t) \to \vec{A}'(\vec{x},t) = \vec{A}(\vec{x},t) + \vec{\nabla}\Lambda(\vec{x},t)$
- $\phi(\vec{x},t) \to \phi'(\vec{x},t) = \phi(\vec{x},t) - \frac{\partial\Lambda(\vec{x},t)}{\partial t}$
- The transform leave $\vec{E}$, $\vec{B}$ and all physical things the same.
- This corresponding to an unitary transformation that leave all matrix elements of $\vec{x}$ unchanged but can alter $\vec{p}$, which is not physical and cannot be measured unless $\vec{A}$ is specified.
- The expression is $U = \exp(-iq\Lambda(\hat{\vec{x}}))$. Obviously, $U^\dagger f(\hat{\vec{x}})U = f(\hat{\vec{x}})$, $U^\dagger\hat{\vec{p}}U = \hat{\vec{p}} - q\vec{\nabla}\Lambda$.
- $U^\dagger(\hat{\vec{p}} - q\vec{A}(\hat{\vec{x}}))U = \hat{\vec{p}} - q\vec{A}'(\hat{\vec{x}})$

An example: $\vec{B} = B_0\hat{n_z}$, $\vec{A} = xB_0\hat{n_y}$.

Schrodinger Equation: $\frac{1}{2m}(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial z^2} + (i\frac{\partial}{\partial y} - xqB_0)^2)\psi = E\psi$

Consdiering there is no dependence on y and z apart from derivatives, we assume $\psi = e^{iP_z z} \cdot e^{iP_y y} \cdot f(x)$, where P_z and P_y are numbers.

Introduce $\omega_0 = \frac{qB_0}{m}$, we have $[-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_0^2(x - \frac{P_y}{m\omega_0})^2 + \frac{P_z^2}{2m}]f(x) = Ef(x)$.

The first two terms are Harmonic Oscillator, so $E = \frac{P_z^2}{2m} + \omega_0(n + \frac{1}{2})$. (Each set of wave functions with the same value of n is called a Landau level)

6. Homework Tricks

6.1. **Problem Set 2, Q3.** 2-D Hermitian matrix can be decomposed into the linear combination of I, σ_x, σ_y and σ_z.