口试讲稿

评分标准：

- 选题与思路 5分
- 内容充实、完整性 5分
- 数学方法应用（适当、清晰、准确）10分
- 难度与创新性 5分

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Chapter 7: Quantum Mechanics

1. Uncertainty principle
2. Representation
3. Quantum dynamics
4. Approximate methods

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Quantum conditions

Commutation relations:

$$[X,Y]\stackrel{?}{=}[Y,X]$$

Classical-quantum mechanical correspondence:

Poisson bracket:

$$\{u,v\}=\sum_r\left(\frac{\partial u}{\partial q_r}\frac{\partial v}{\partial p_r}-\frac{\partial u}{\partial p_r}\frac{\partial v}{\partial q_r}\right)$$

Canonical coordinates and momenta

1. Bilinear

$$[aX+bY,Z]=a[X,Z]+b[Y,Z]$$
$$[Z,aX+bY]=a[Z,X]+b[Z,Y]$$

2. Multiplication

$$[X,YZ]=[X,Y]Z+Y[X,Z]$$

$$\longrightarrow [X,c]=0$$

3. Skew symmetric

$$[X,Y]=-[Y,X] \longrightarrow [X,X]=0$$

4. Jacobi identity

$$[[X,Y],Z]+[[Y,Z],X]+[[Z,X],Y]=0$$

Example:

$$\{x_i,p_j\}=\delta_{ij} \qquad \{\ ,\ \}\to\frac{1}{i\hbar}[\ ,\ ] \qquad [x_i,p_j]=i\hbar\delta_{ij} \qquad [x_i,x_j]=0,\ [p_i,p_j]=0$$

Lie algebra

Definition:

V is n-dimensional vector space on number field R

$$\forall X, Y \in V, \text{the Lie product } [X,Y] \in V$$

1. Bilinear

$$[aX + bY, Z] = a[X,Z] + b[Y,Z]$$
$$[Z, aX + bY] = a[Z,X] + b[Z,Y]$$

2. Skew symmetric

$$[X,Y] = -[Y,X]$$

3. Jacobi identity

$$[[X,Y],Z] + [[Y,Z],X] + [[Z,X],Y] = 0$$

A vector space V with a bilinear skew-symmetric operation $V \times V \to V$ **, which satisfies the Jacobi identity.**

Example:

The set of n x n matrices becomes a Lie algebra if we define the commutator by [A,B]=AB-BA.

Uncertainty principle

Variance (mean square deviation):

$$\Delta A = A - \langle A \rangle$$

$$\left\langle (\Delta A)^2 \right\rangle = \left\langle \left(A - \langle A \rangle\right)^2 \right\rangle = \left\langle A^2 \right\rangle - \langle A \rangle^2$$

Schwarz inequality:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq \left| \langle \alpha | \beta \rangle \right|^2$$

$$|\alpha\rangle = \Delta A | \;\rangle$$

$$|\beta\rangle = \Delta B | \;\rangle$$

Uncertainty relation:

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \frac{1}{4} \left| \langle [A, B] \rangle \right|^2$$

$$\langle \alpha | \beta \rangle = \frac{1}{2} \left[\langle \alpha | \beta \rangle + \langle \beta | \alpha \rangle + \langle \alpha | \beta \rangle - \langle \beta | \alpha \rangle \right]$$

$$\left| \langle \alpha | \beta \rangle \right|^2 \geq \frac{1}{4} \left| \langle \alpha | \beta \rangle - \langle \beta | \alpha \rangle \right|^2 = \frac{1}{4} \left| \langle AB - BA \rangle \right|^2$$

The other way:

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \left| \langle \Delta A \Delta B \rangle \right|^2$$

$$\Delta A \Delta B = \frac{1}{2} [\Delta A, \Delta B] + \frac{1}{2} \{\Delta A, \Delta B\}$$

Example:

$$[x, p] = i\hbar \qquad \Delta x \Delta p \geq \frac{\hbar}{2}$$

Wave function

Position space

$$x|x'\rangle = x'|x'\rangle$$

$$\langle x''|x'\rangle = \delta(x''-x')$$

Representation:

$$|\alpha\rangle = \int dx' |x'\rangle\langle x'|\alpha\rangle$$

$$\langle\alpha|\alpha\rangle = \int dx' \langle\alpha|x'\rangle\langle x'|\alpha\rangle = \int dx' |\langle x'|\alpha\rangle|^2$$

Wave function in position space

$$\psi_\alpha(x') = \langle x'|\alpha\rangle$$

$$\langle\beta|A|\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle\langle x'|A|x''\rangle\langle x''|\alpha\rangle$$
$$= \int dx' \int dx'' \psi_\beta^*(x')\langle x'|A|x''\rangle\psi_\alpha(x'')$$

Example:

$$A = f(x)$$

$$\langle\beta|f(x)|\alpha\rangle = \int dx' \psi_\beta^*(x') f(x')\psi_\alpha(x')$$

Eigenfunction expansion:

$$|\alpha\rangle = \sum_{\alpha'} |\alpha'\rangle\langle\alpha'|\alpha\rangle$$

$$\langle x'|\alpha\rangle = \sum_{\alpha'} \langle x'|\alpha'\rangle\langle\alpha'|\alpha\rangle = \sum_{\alpha'} u_{\alpha'}(x')c_{\alpha'}$$

Momentum operator

Translational operator:

$$\mathrm{T}(\Delta x'\hat{\mathbf{x}}) = \lim_{N\to\infty}\left(1-\frac{ip_x\Delta x'}{N\hbar}\right)^N = \exp\left(-\frac{ip_x\Delta x'}{\hbar}\right)$$

Momentum operator:

$$\left(1-\frac{ip_x\Delta x'}{\hbar}\right)|\alpha\rangle = \int dx' T(\Delta x')|x'\rangle\langle x'|\alpha\rangle = \int dx'|x'+\Delta x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx'|x'\rangle\langle x'-\Delta x'|\alpha\rangle = \int dx'|x'\rangle\left(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

$$p|\alpha\rangle = \int dx'|x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

Properties:

$$\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \qquad \langle x'|p|x''\rangle = \left(-i\hbar\frac{\partial}{\partial x'}\right)\delta(x'-x'')$$

Matrix element

$$\langle\beta|p|\alpha\rangle = \int dx'\langle\beta|x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right) = \int dx'\psi_\beta^*(x')\left(-i\hbar\frac{\partial}{\partial x'}\right)\psi_\alpha(x')$$

Representation

Transformation function:

$$\langle x'|p|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle = p'\langle x'|p'\rangle$$

$$\Rightarrow \langle x'|p'\rangle = N\exp\left(\frac{ip'x'}{\hbar}\right)$$

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ip'x'}{\hbar}\right)$$

$$\langle x'|x''\rangle = \int dp'\langle x'|p'\rangle\langle p'|x''\rangle = |N|^2\int dp'\exp\left[\frac{ip'(x'-x'')}{\hbar}\right]$$

$$= |N|^2 2\pi\hbar\delta(x'-x'') \Rightarrow N = \frac{1}{\sqrt{2\pi\hbar}}$$

Dual space transformation:

$$\langle x'|\alpha\rangle = \int dp'\langle x'|p'\rangle\langle p'|\alpha\rangle$$

$$\langle p'|\alpha\rangle = \int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle$$

$$\psi_\alpha(x') = \frac{1}{\sqrt{2\pi\hbar}}\int dp'\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p')$$

$$\phi_\alpha(p') = \frac{1}{\sqrt{2\pi\hbar}}\int dx'\exp\left(-\frac{ip'x'}{\hbar}\right)\psi_\alpha(x')$$

Gaussian wave packet

$$\langle x'|\alpha\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{d}}\right)\exp\left(-\frac{x'^2}{2d^2}+ikx'\right)$$

$$\langle x\rangle = ?, \langle p\rangle = ?, \langle x^2\rangle = ?, \langle p^2\rangle = ?$$

Verify uncertainty relation

$$\langle p'|\alpha\rangle = ?$$

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Propagator

Time evolution operator:

$$|\alpha,t_0;t\rangle = U(t,t_0)|\alpha,t_0\rangle$$

$$\langle\alpha,t_0;t|\alpha,t_0;t\rangle = \langle\alpha,t_0|\alpha,t_0\rangle \Rightarrow U^{+}(t,t_0)U(t,t_0)=1$$

$$U(t_2,t_0)=U(t_2,t_1)U(t_1,t_0) \qquad (t_2>t_1>t_0)$$

Infinitesimal time evolution operator:

$$U(t_0+dt,t_0)=1-\frac{iHdt}{\hbar}$$

Schrodinger equation:

$$U(t+dt,t_0)=U(t+dt,t)U(t,t_0)=\left(1-\frac{iHdt}{\hbar}\right)U(t,t_0)$$

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)=HU(t,t_0)$$

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t\rangle = H|\alpha,t_0;t\rangle$$

What's the solution? $U(t,t_0)=?$

I. H time independent

$$U(t,t_0)=\exp\left[\frac{-iH(t-t_0)}{\hbar}\right]$$

II. H time dependent, and commute at different t

$$U(t,t_0)=\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}dt'H(t')\right]$$

III. H time dependent, but NOT commute at different t

$$U(t,t_0)=1+\sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\ldots\int_{t_0}^{t_{n-1}}dt_nH(t_1)H(t_2)\ldots H(t_n)$$

Heisenberg picture

Unitary transformation:

$$|\alpha\rangle \to U|\alpha\rangle \qquad\qquad \langle\beta|\alpha\rangle \to \langle\beta|U^{\dagger}U|\alpha\rangle = \langle\beta|\alpha\rangle$$

$$\langle\beta|X|\alpha\rangle \to \left(\langle\beta|U^{\dagger}\right)X\left(U|\alpha\rangle\right) = \langle\beta|U^{\dagger}XU|\alpha\rangle \qquad\qquad X \to U^{\dagger}XU$$

Example: $\mathrm{T}(dx') = 1 - \frac{ip \cdot dx'}{\hbar}$

Schrodinger's picture:

$$|\alpha\rangle \to \left(1 - \frac{ip \cdot dx'}{\hbar}\right)|\alpha\rangle, x \to x$$

Heisenberg's picture:

$$|\alpha\rangle \to |\alpha\rangle, x \to \left(1 + \frac{ip \cdot dx'}{\hbar}\right)x\left(1 - \frac{ip \cdot dx'}{\hbar}\right)$$

The physics: $\langle x\rangle \to \langle x\rangle + \langle dx'\rangle$?

Infinitesimal time evolution operator:

$$U(t, t_0 = 0) \equiv U(t, t_0 = 0) = \exp\left[\frac{-iHt}{\hbar}\right] \qquad\qquad A^{(H)}(t) \equiv U^{\dagger}(t)A^{(S)}U(t)$$

Heisenberg equation:

$$\frac{dA^{(H)}(t)}{dt} = \frac{\partial U^{\dagger}(t)}{\partial t}A^{(S)}U(t) + U^{\dagger}(t)A^{(S)}\frac{\partial U(t)}{\partial t}$$

$$= -\frac{1}{i\hbar}U^{\dagger}(t)HU(t)U^{\dagger}(t)A^{(S)}U(t) + \frac{1}{i\hbar}U^{\dagger}(t)A^{(S)}U(t)U^{\dagger}(t)HU(t) = \frac{1}{i\hbar}\left[A^{(H)}, H^{(H)}\right]$$

Equation of motion

Schrodinger:

$$i\hbar\frac{\partial}{\partial t}\left|\alpha,t_0;t\right\rangle = H\left|\alpha,t_0;t\right\rangle$$

Heisenberg equation:

$$\frac{dA^{(H)}(t)}{dt}=\frac{1}{i\hbar}\left[A^{(H)},H^{(H)}\right]$$

$$\left[x_i,F(\mathbf{p})\right]=i\hbar\frac{\partial F}{\partial p_i},\qquad \left[p_i,G(\mathbf{x})\right]=-i\hbar\frac{\partial G}{\partial x_i}$$

Example:

A free particle of mass *m*

$$H=\frac{\mathbf{p}^2}{2m}=\frac{p_x^2+p_y^2+p_z^2}{2m}$$

$$\frac{dp_i}{dt}=\frac{1}{i\hbar}\left[p_i,H\right]=0$$

$$\frac{dx_i}{dt}=\frac{1}{i\hbar}\left[x_i,H\right]=\frac{1}{i\hbar}\frac{1}{2m}i\hbar\frac{\partial}{\partial p_i}\left(\sum_{j=1}^{3}p_j^2\right)=\frac{p_i}{m}=\frac{p_i(0)}{m}$$

$$\left[x_i(t),x_i(0)\right]=?$$

$$\left\langle(\Delta x_i)^2\right\rangle_{\mathrm{t}}\left\langle(\Delta x_i)^2\right\rangle_{\mathrm{t=0}}\geq ?$$

A particle of mass *m* under a potential *V*(**x**)

$$H=\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})$$

$$\frac{dp_i}{dt}=\frac{1}{i\hbar}\left[p_i,H\right]=-\frac{\partial}{\partial x_i}V(\mathbf{x})$$

$$\frac{dx_i}{dt}=\frac{1}{i\hbar}\left[x_i,H\right]=\frac{p_i}{m}$$

$$\frac{d^2x_i}{dt^2}=\frac{1}{i\hbar}\left[\frac{dx_i}{dt},H\right]=\frac{1}{i\hbar}\left[\frac{p_i}{m},H\right]=\frac{1}{m}\frac{dp_i}{dt}$$

$$m\frac{d^2\mathbf{x}}{dt^2}=\frac{d\mathbf{p}}{dt}=-\nabla V(\mathbf{x})$$

Ehrenfest theorem

$$m\frac{d^2}{dt^2}\langle\mathbf{x}\rangle=\frac{d\langle\mathbf{p}\rangle}{dt}=-\langle\nabla V(\mathbf{x})\rangle$$

Examples

Harmonic oscillator:

$$H=\frac{\mathbf{p}^2}{2m}+V(\mathbf{x}) \qquad V(x)=\frac{1}{2}m\omega^2x^2$$

$$m\frac{d^2x}{dt^2}=\frac{dp}{dt}=-\nabla V(x)=-m\omega^2x \longrightarrow \begin{aligned} x(t)&=x(0)\cos\omega t+\frac{p(0)}{m\omega}\sin\omega t\\ p(t)&=-m\omega x(0)\sin\omega t+p(0)\cos\omega t\end{aligned}$$

The other way:

$$x(t)=\exp\left(\frac{iHdt}{\hbar}\right)x(0)\exp\left(-\frac{iHdt}{\hbar}\right)$$

$$=x(0)+\left(\frac{it}{\hbar}\right)[H,x(0)]+\frac{1}{2!}\left(\frac{it}{\hbar}\right)^2[H,[H,x(0)]]+\ldots$$

Baker-Hausdoff lemma

$$[H,x(0)]=\frac{-i\hbar p(0)}{m}, \qquad [H,p(0)]=i\hbar m\omega^2x(0)$$

$$x(t)=\exp\left(\frac{iHdt}{\hbar}\right)x(0)\exp\left(-\frac{iHdt}{\hbar}\right)$$

$$=x(0)+\frac{p(0)}{m}t-\frac{1}{2!}\omega^2t^2x(0)-\frac{1}{3!}\frac{\omega^2t^3p(0)}{m}\ldots=x(0)\cos\omega t+\frac{p(0)}{m\omega}\sin\omega t$$