Preview : Born of Quantum Mechanics

Bohr's model : hydrogen atom nuclear model

$\Downarrow$ explain

hydrogen spectral series : Balmer - Series : $H_{\alpha,\beta,\gamma,\delta}$

energy level formula : $E_n = -\frac{\mu}{2\hbar^2 n^2}\left(\frac{e}{4\pi\varepsilon_0}\right)^2$

Heisenberg : realize the ignorance of the light intencity of the spectral series

matrix mechanics : Heisenberg . Born

Quantum Physics 理论描述中只应出现实验上观测物理量

Ritz associative law : $\begin{cases} \nu(m_1, n_2) = \nu(m_1, n_1) + \nu(n_1, n_2) \\ \nu(m, n) = -\nu(n, m) \end{cases}$

abandon the concept of particle's coordinates

indensity of spectral lines are observable

position vector : (constrained on x axis) Fourier expansion.

$$x(n,t) = \sum_{\alpha=-\infty}^{+\infty} a(n,\alpha)\exp[-i\omega(n)\alpha t]$$

$$nh = \int_0^{2\pi/\omega} \mu \dot{x}^2\, dt \Rightarrow h = 2\pi\mu \sum_{\alpha=-\infty}^{+\infty} \alpha \frac{d}{dn}\left[\alpha\omega(n)\,|a(n,\alpha)|^2\right]$$

consider the electric dipole radiation in classic electrodynamite

$$P = \frac{\omega^2 e^2 |x(n,t)|^2}{12\pi\varepsilon_0 c^3}$$

$x(n,t) = \sum_{m=-\infty}^{+\infty} x_{nm}$ $x_{nm} \propto E_n, E_m$ 间跃迁概率幅

Heisenberg quantization condition :

$$h = 4\pi\mu \sum_{\alpha=0}^{+\infty} \left\{ |a(n,n+\alpha)|^2 \omega(n,n+\alpha) + |a(n,n-\alpha)|^2 \omega(n,n-\alpha) \right\}$$

$$x(n,t) = \sum_{m=-\infty}^{+\infty} x_{nm} \left(:= a(n,m) \exp[-i\omega(n,m)t] \right) \qquad X = [x_{nm}]$$

$$X^2 = \left[\sum_{l=-\infty}^{+\infty} x_{nl} x_{lm} \right]$$

in matrix mechanics, the coordinates $x(n,t)$ has been turned into a matrix

$$X = [x_{mn}]$$
$$\Downarrow$$
$E_n \sim E_m$ 自发跃迁概率幅

$x_{nn} = 0$ cannot transit between the same energy level

property : $[x_{nm}]^* = x_{mn}$ $\quad X$: 厄米矩阵

力学算符 $\longrightarrow$ 厄米矩阵

$$\dot{x}_{nm} = \frac{1}{i\hbar} \sum_{l=-\infty}^{+\infty} [x_{nl} h_{lm} - h_{nl} x_{lm}] \qquad (h_{nm} := E_n \delta_{nm})$$

$H = [h_{nm}]$: 体系 Hamilton 矩阵

$$\dot{X} = \frac{1}{i\hbar}(XH - HX)$$

矩阵间对易子 $[A, B] = AB - BA$

Heisenberg Dynamic Equation $\quad \dot{X} = \frac{1}{i\hbar}[X, H]$, $\dot{P} = \frac{1}{i\hbar}[P, H]$

conservative system : $\quad H = \frac{P^2}{2\mu} + V(X)$

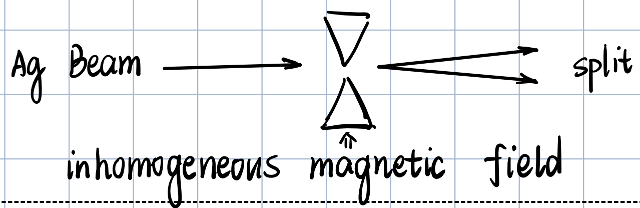
$\Omega := [X, P]$

$\dot{\Omega} = [\dot{X}, P] + [X, \dot{P}] = 0$, $\Omega_{nm} = i\hbar\delta_{nm}$

量子力学基本对易关系: $[X, P] = i\hbar I$

Quantum System State & Observable

Stern - Gerlach Experiment



classical electrodynamic interpret : 基态银原子磁矩 $\mu = \frac{gqL}{2mc}$ $\vec{F} = \vec{e}_3 \mu_3 \frac{\partial B(z)}{\partial z}$

旧量子论 : $L_3 = 0, \pm\hbar, \cdots$ 奇数条 ★ 带状连续分布

Outcome : two splits ⇒ conclude : 内禀角动量 — 自旋角动量

△ Explanation :

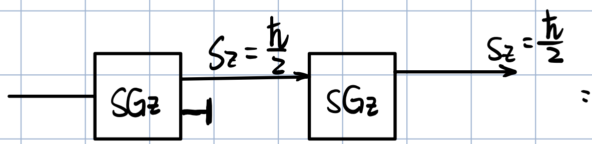
$|\cdots\rangle$ ket (右矢)

$|\pm n\rangle \rightarrow S_n = \pm\frac{\hbar}{2}$ 自旋态

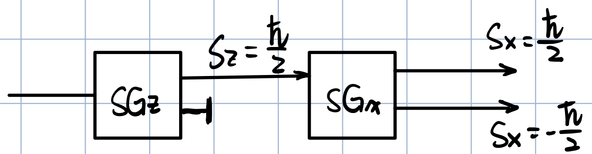
自旋态互斥 : $\langle +n|-n\rangle = \langle -n|+n\rangle = 0$

$|+n\rangle, |-n\rangle$ 二维线性空间单位矢量 $\langle +n|+n\rangle = \langle -n|-n\rangle = 1$

银原子状态表示为 : $|\psi\rangle = p_+|+z\rangle + p_-|-z\rangle$: $p_+ = p_- = 0.5$

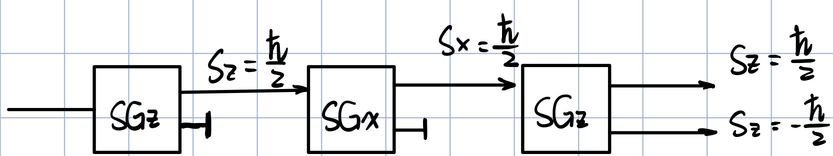


: prove that $\langle n+|n-\rangle = 0$

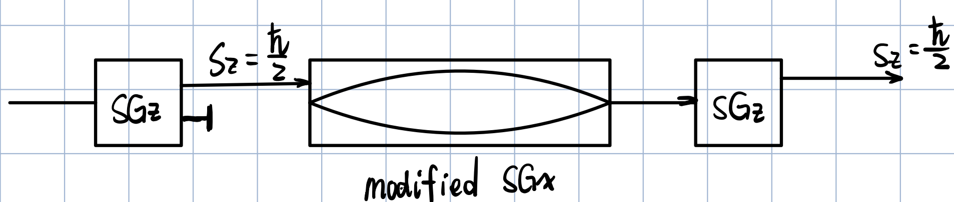


contain : $|+z\rangle = \frac{1}{2}[|+x\rangle + |-x\rangle]$

$|-z\rangle = \frac{1}{2}[|+x\rangle + |-x\rangle]$



$|+x\rangle = \frac{1}{2}[|+z\rangle + |-z\rangle]$



: 证伪思想

quantum mechanic's explanation : 态矢量不解释为概率

★ superposition state : $|\psi\rangle = C_+|+n\rangle + C_-|-n\rangle$

possibility of observation : $||\psi\rangle|^2$

probability of $S_z = \frac{\hbar}{2}$: $p_+ = |C_+|^2$

Quantum States.

Quantum Mechanics Protulate 1

quantum state vector

体系由 Hilbert 空间 $\mathcal{H}$ 中矢量 $|\psi\rangle$ 描述

$\mathbb{C}^n$ 上定义内积的线性空间

△ for non-zero $c \in \mathbb{C}^n$, $c|\psi\rangle \sim |\psi\rangle$

Quantum Mechanics Protulate 2

$|\alpha\rangle, |\beta\rangle \in \mathcal{H} \Rightarrow c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \in \mathcal{H}$.

possible quantum state

★ 态叠加原理 ⇒ satisfy linear equation

* Inner product in $\mathcal{H}$: $\langle\psi|\varphi\rangle$

$$\begin{cases} \langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^* \\ \langle\psi|\varphi\rangle = 0 \Rightarrow \text{orthogonal} \\ \langle\psi|\psi\rangle \geq 0 \\ \sqrt{\langle\psi|\psi\rangle} : \text{norm of } |\psi\rangle \end{cases}$$

normalization:

$$|\Psi\rangle = \left[\frac{1}{\sqrt{\langle\psi|\psi\rangle}}\right]|\psi\rangle$$

normalization constant

Dual Hilbert Space

For each $|\psi\rangle \in \mathcal{H}$, linear mappin $\langle\psi| : |\varphi\rangle \longmapsto \langle\psi|\varphi\rangle \in \mathbb{C}$

Dirac 左矢

$\langle\psi| \in \tilde{\mathcal{H}}$: Dual Hilbert Space ★ $\langle\psi|$ is not a state vector

$\mathcal{H}$ & $\tilde{\mathcal{H}}$: Dual Correspondence

Hermitian Conjugate (厄米共轭) : symbol $\dagger$

$$|\psi\rangle^\dagger = \langle\psi| , \quad \langle\psi|^\dagger = |\psi\rangle , \quad c^\dagger = c^*$$

$$(c_1|\psi_1\rangle + c_2|\psi_2\rangle)^\dagger = c_1^*\langle\psi_1| + c_2^*\langle\psi_2|$$

$$(A_1 A_2 \cdots A_N)^\dagger = A_N^\dagger \cdots A_1^\dagger$$

any combination of ket & bra

linear Operator (算符) $\hat{A} : |\psi\rangle \to \hat{A}|\psi\rangle = \underline{|\varphi\rangle \in \mathcal{H}}$ *

$$\hat{A}(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1(\hat{A}|\psi_1\rangle) + c_2(\hat{A}|\psi_2\rangle)$$

Special Cases $\hat{I}$: $\hat{I}|\psi\rangle = |\psi\rangle$ unit operator

* NOTE $\hat{A}\hat{B} \neq \hat{B}\hat{A}$ (common situation)

if $\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{I}$, then $\hat{A}^{-1} = \hat{B}$

operator commutator $[\hat{A}, \hat{B}]|\psi\rangle = \hat{A}\hat{B}|\psi\rangle - \hat{B}\hat{A}|\psi\rangle$

* quantum state vector evolve as $|\psi(t)\rangle = e^{-it\hat{H}/\hbar}|\psi(0)\rangle$ (without observor)

$\hat{H}$: Hamilton Operator $\Rightarrow$ $e^{-it\hat{H}/\hbar}$ is the function of $\hat{H}$, Linear Operator

[as Taylor's Expansion : $e^{-it\hat{H}/\hbar} = \sum_{n=0}^{\infty} \frac{(-it/\hbar)^n}{n!}\hat{H}^n$]

Hermition Conjugate Operator $\hat{A}^{\dagger}$ defined in $\tilde{\mathcal{H}}$

Defination : $\hat{A}|\psi\rangle = |\varphi\rangle \Rightarrow \langle\psi|\hat{A}^{\dagger} = \langle\varphi|$

* Linear Operator can be constructed linear combination of outer product :

$\hat{A} = \sum_{ij} c_{ij}|i\rangle\langle j|$

$\hat{A}^{\dagger} = \sum_{ij} c_{ij}^{*}(|i\rangle\langle j|)^{\dagger} = \sum_{ij} c_{ij}^{*}|j\rangle\langle i| \Rightarrow \langle\alpha|\hat{A}^{\dagger}|\beta\rangle := \langle\beta|\hat{A}|\alpha\rangle^{*}$

eg. $|a\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$ $|b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$ $\Rightarrow$ $\langle a| = \frac{1}{\sqrt{2}}(1\ \ -i)$ $\langle b| = \frac{1}{\sqrt{2}}(1, -1)$

inner product : $\langle a|b\rangle = \frac{1}{2}(1+i)$ $\langle b|a\rangle = \frac{1}{2}(1-i)$

outer product : $|a\rangle\langle b| = \frac{1}{2}\begin{pmatrix}1 & -1\\ i & -i\end{pmatrix}$ $|b\rangle\langle a| = \frac{1}{2}\begin{pmatrix}1 & -i\\ -1 & i\end{pmatrix}$

Hermitian Operator

Def. $\hat{X}^{\dagger} = \hat{X}$, $\langle\psi|\hat{X}|\varphi\rangle = \langle\varphi|\hat{X}|\psi\rangle^{*}$

Hermitian matrix diagonal elements are real $\langle\psi|\hat{X}|\psi\rangle = \langle\psi|\hat{X}|\psi\rangle^{*}$

Operator's eigenvectors & eigenvalues

* For specific $|\alpha_i\rangle \in \mathcal{H}$ $(i = 1, 2, \cdots, N)$. s.t.

eigenvalue eigenvector

$\boxed{\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle}$ $\leftarrow$ eigenvalue equation

* eigenvalues $\xrightarrow{\text{consist}}$ spectrum

* when eigenvectors aren't unique : $\hat{A}|\alpha_{i a}\rangle = a_i |\alpha_{i a}\rangle$: $a = 1, 2, \cdots f$

$\Rightarrow$ the spectrum is degenrate (Degeneracy $D(a_i) = f$)

★ Important Properties $\begin{cases} \text{Hermitian Operator's eigenvalues are real} \\ \text{Hermitian Operator's eigenvectors belonged to distinctive eigenvalues are orthogonal} \end{cases}$

Elimination of Degeneracy

For any $\hat{A}$ which $\hat{A}|a_{i\alpha}\rangle = a_i|a_{i\alpha}\rangle$, a linear Operator $\hat{B}$ which enables $[\hat{A}, \hat{B}] = 0$, s.t.

$$\hat{B}|a_{i\alpha}\rangle = b_\alpha |a_{i\alpha}\rangle$$

for any $|a_{i\alpha}\rangle$, it has the corresponding $\{a_i, b_\alpha\}$ $\Rightarrow$ elimination of degeneracy

$$\langle a_{i\alpha} | a_{j\beta}\rangle = C_{i\alpha}\delta_{ij}\delta_{\alpha\beta}$$

normalization ($C_{i\alpha} = 1$)

Quantum Mechanics Protulate3:

$\mathcal{H}$ 中 Linear Hermitian Operator $\longrightarrow$ 力学量 (Observable)

力学量算符特征向量构成 $\mathcal{H}$ 的一组正交基

测量时以一定概率得到 Hermitian Operator 的某本征值

★ $\hat{A}^\dagger = \hat{A}$, $\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle \longrightarrow |\psi\rangle = \sum_i C_i|\alpha_i\rangle \in \mathcal{H}$

complete base

For Hermitian Operator $\hat{B} = \hat{B}^\dagger$, if its eigenvectors can't make up as complete bases for $\mathcal{H}$, then $\hat{B}$ isn't an observable.

$$|\psi\rangle = \sum_i C_i|\alpha_i\rangle \rightarrow \langle\psi|\psi\rangle = \sum_i |C_i|^2 = 1$$

★ For mechanical quantities, the observation will cause the collapse of quantum state, the state vector would transit to the eigenvector of the operator with the prob. of $|C_i|^2$

$$|\psi\rangle = \sum_i c_i|\alpha_i\rangle \xrightarrow{|c_i|^2} |\alpha_i\rangle$$

★ the outcome of the measurement for mechanical quantities will be the eigenvalue a_i at the prob. $|c_i|^2$ [ensemble]★

$$|\psi\rangle = \sum_i c_i|\alpha_i\rangle = \sum_i \langle\alpha_i|\psi\rangle|\alpha_i\rangle = \left[\sum_i|\alpha_i\rangle\langle\alpha_i|\right]|\psi\rangle$$

$$\Downarrow$$

$$\sum_i |\alpha_i\rangle\langle\alpha_i| = \hat{1}$$

力学量算符本征矢量系完备性公式

Projection Operator 投影算符

$$|\psi\rangle \xrightarrow{|\langle\alpha_i|\psi\rangle|^2} |\alpha_i\rangle$$

$\langle\alpha_i|\psi\rangle = c_i$: prob. amplitude

projection form $\hat{\Lambda}_i : |\psi\rangle \rightsquigarrow |\alpha_i\rangle \approx \hat{\Lambda}_i|\psi\rangle$

projection operator $\Lambda_i = |\alpha_i\rangle\langle\alpha_i|$

properties :

* Hermitian Operator $\hat{\Lambda}_i = \hat{\Lambda}_i^+$
* $\hat{\Lambda}_i^2 = \hat{\Lambda}_i$ → eigenvalue $\omega_1 = 1$, $|\omega_1\rangle = |a_i\rangle$
  $\omega_2 = 0$, $|\omega_2\rangle = |a_j\rangle$ $(j \neq i)$
  thus $\hat{\Lambda}_i$ is observable $(\Lambda_i)_{mn} = \langle a_m|\Lambda_i|a_n\rangle$
* $[\hat{A}, \hat{\Lambda}_i] = 0$
* $tr(\hat{\Lambda}_i) = 1$
* $\sum_i \hat{\Lambda}_i = \hat{1}$

Pure State & Density Operator (Matrix)

pure state : quantum system described by a specific state vector

pure state's density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$

properties :

* Hermitian, $\hat{\rho}^+ = \rho$
* $\hat{\rho}$ is projection operator of pure state $|\psi\rangle$ $(\hat{\rho}^2 = \hat{\rho})$
  eigenvalues : $\rho_1 = 1$, $\rho_2 = 0$
* $tr(\hat{\rho}^2) = 1$ (actually the property difference between pure & mixed state)

Expectation value of Observable (力学量平均值)

$$\hat{A}|a_i\rangle = a_i|a_i\rangle \,,\quad \langle a_i|a_j\rangle = \delta_{ij} \,,\quad \sum_i |a_i\rangle\langle a_i| = \hat{I}$$

random collapse process: $|\psi\rangle \xrightarrow{|\langle a_i|\psi\rangle|^2} |a_i\rangle$

The expectation of $\hat{A}$ (essemble average value): $\langle A\rangle_\psi = \sum_i a_i |\langle a_i|\psi\rangle|^2$

also $\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$

also $\langle A\rangle_\psi = tr(\hat{\rho}\cdot\hat{A}) = tr(\hat{A}\cdot\hat{\rho})$

Representation & Uncertainty Principle

Representation & Wave function

Suppose observable $\hat{F}$: $\hat{F}|f_i\rangle = f_i|f_i\rangle$, $\sum_i |f_i\rangle\langle f_i| = \hat{I}$

$\hat{F}$ representation in Quantum System : Select $|f_i\rangle$ as basis of $\mathcal{H}$

$$|\psi\rangle = \hat{I}|\psi\rangle = \left[\sum_i |f_i\rangle\langle f_i|\right]|\psi\rangle = \sum_i \langle f_i|\psi\rangle |f_i\rangle$$

* coordinate for $|\psi\rangle$ along $|f_i\rangle$

* wave function in Representation $\hat{F}$

Observable Matrix

Observable's description :

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left[\sum_i |f_i\rangle\langle f_i|\right]\hat{A}\left[\sum_j |f_j\rangle\langle f_j|\right] = \sum_{ij} \underbrace{\langle f_i|\hat{A}|f_j\rangle}_{\parallel\triangle \; A_{ij}} |f_i\rangle\langle f_j|$$

Properties : $\hat{A} = (A_{ij})$: Hermitian (Observable Matrix)

F_{ij} is Real diagonal matrix in $\hat{F}$ representation

$\hat{A}|\psi\rangle = |\phi\rangle \sim \sum_j A_{ij}\psi_i = \phi_i$

For dual vector : $\langle\phi| = \langle\psi|\hat{B} \sim \phi_i^* = \sum_j \psi_j^* B_{ji}$

row matrix

Representation Transformation

Diversity of Representation : Observables $\begin{cases} \hat{F} : \{|f_i\rangle\} \\ \hat{G} : \{|g_i\rangle\} \end{cases}$

Transformation : $\{|f_i\rangle\} \to \{|g_i\rangle\}$
$\{|g_i\rangle\} \to \{|f_i\rangle\}$

Linear Operator $\hat{u} = \sum_i |g_i\rangle\langle f_i|$ $\quad (\hat{u}|f_i\rangle = |g_i\rangle)$

Inverse Linear Operator $\hat{u}^{-1} = \sum_i |f_i\rangle\langle g_i|$ $\quad (\hat{u}^{-1}|g_i\rangle = |f_i\rangle)$ $\quad (\hat{u}\hat{u}^{-1} = \hat{I})$

$\hat{u}^{-1} = \hat{u}^+$: Unitary Operator

☆ representation transformation is done by unitary operator.

△ $u_{ij}^{(F)} = \langle f_i|\hat{u}|f_j\rangle = \langle f_i|g_j\rangle$, $u_{ij}^{(G)} = \langle g_i|f_j\rangle$

* Wave function transformation :

$$\boxed{\begin{aligned}\psi_i^{(F)} &= \langle f_i|\psi\rangle \\ \psi_i^{(G)} &= \langle g_i|\psi\rangle\end{aligned}}$$

$$\psi_i^{(F)} = \sum_j \langle f_i|g_j\rangle\langle g_j|\psi\rangle = \sum_j u_{ij}^{(G)\dagger}\psi_j^{(G)}$$

$$\psi_i^{(G)} = \sum_j \langle g_i|f_j\rangle\langle f_j|\psi\rangle = \sum_j u_{ij}^{(F)\dagger}\psi_j^{(F)}$$

☆ $\psi^{(G)} = u^{\dagger(F)}\psi^{(F)}$, $\psi^{(F)} = u^{\dagger(G)}\psi^{(G)}$

* Observable transformation :

$$A^{(G)} = u^{\dagger(F)}A^{(F)}u^{(F)} , \quad A^{(F)} = u^{\dagger(G)}A^{(G)}u^{(G)}$$

Compatible observable operators

Defination : any quantum state : $[\hat{A},\hat{B}]|\psi\rangle = 0$ compatible

property : Compatible observable operators have common complete eigenstates set.

$\{|a_i,b_i\rangle \mid i=1,2,3,\cdots\}$: $\hat{A}|a_i,b_i\rangle = a_i|a_i,b_i\rangle$, $\hat{B}|a_i,b_i\rangle = b_i|a_i,b_i\rangle$

$$\sum_i |a_i,b_i\rangle\langle a_i,b_i| = \hat{I}$$

the measurement & collapsing process

$|\psi\rangle \xrightarrow{|\langle a_i|\psi\rangle|^2} |a_i\rangle$: the measurement of $\hat{A}$

$|a_i\rangle \xrightarrow{|\langle a_i,b_i|a_i\rangle|^2} |a_i,b_i\rangle$: the measurement of $\hat{B}$

re-described $|a_i\rangle$ by their common complete eigenstates set $\{|a_i,b_i\rangle\}$

Complete Set of Compatible Observables (CSCO) 力学量完全集

$$[\hat{A},\hat{B}] = [\hat{B},\hat{C}] = [\hat{C},\hat{A}] = 0 \rightarrow \begin{cases}\hat{A}|a_i,b_i,c_i\rangle = a_i|a_i,b_i,c_i\rangle \\ \hat{B}|a_i,b_i,c_i\rangle = b_i|a_i,b_i,c_i\rangle \\ \hat{C}|a_i,b_i,c_i\rangle = c_i|a_i,b_i,c_i\rangle\end{cases}$$

☆ If correspondency formed. $(a_i,b_i,c_i) \rightarrow |a_i,b_i,c_i\rangle$, $\{\hat{A},\hat{B},\hat{C}\}$ consist CSCO

(一一对应)

Incompatible Observables

$[\hat{A},\hat{B}] \neq 0$, their commutator has the form of $[\hat{A},\hat{B}] = i\hat{C}$, $\hat{C} = \hat{C}^{\dagger}$

Uncertainty Principle

★ Incompatible observables usually don't have certain measurement values at the same time

Deviation Operator : $\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$ → Uncertainty Value $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$

For incompatible observables $[\hat{A}, \hat{B}] = i\hat{C}$

$[\Delta\hat{A}, \Delta\hat{B}] = i\hat{C}$, $(\Delta\hat{A})^\dagger = \Delta\hat{A}$, $(\Delta\hat{B})^\dagger = \Delta\hat{B}$

For any real number ξ. $|\eta\rangle := [\xi(\Delta\hat{A}) - i(\Delta\hat{B})]|\psi\rangle \in \mathcal{H}$ $(|\psi\rangle \in \mathcal{H})$

$$||\eta\rangle|^2 = \langle\eta|\eta\rangle = \langle\psi|[\xi^2(\Delta\hat{A})^2 + (\Delta\hat{B})^2 + \xi\hat{C}]|\psi\rangle$$
$$= \xi^2(\Delta A)^2 + (\Delta B)^2 + \xi\langle\hat{C}\rangle \geq 0$$

★ → $(\Delta A)^2(\Delta B)^2 \geq \frac{\langle C\rangle^2}{4}$ → $(\Delta A)(\Delta B) \geq \frac{1}{2}\langle\hat{C}\rangle$ uncertainty principle

Position Representation & Momentum Representation

Position Operator

Def (1D). $\hat{x}|x\rangle = x|x\rangle$ → eigenstates for position operator

properties: * $\hat{x} = \hat{x}^\dagger$. $-\infty < x < +\infty$ (anywhere along x-axis)

* $\langle x'|x\rangle = 0$, if $x' \neq x$

* $\int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| = \hat{I}$ → $|\psi\rangle = \int_{-\infty}^{+\infty} dx\, |x\rangle \langle x|\psi\rangle$

continuous spectrum

$\langle x|\psi\rangle \to \psi(x)$ wavefunction in position representation

* $\langle x|x'\rangle = \delta(x-x')$: $|x\rangle$ cannot be normalized.

Probability Distribution for Position

$\psi(x)$ is called prob. amplitude for position

Def. Prob. density $\rho(x) = |\psi(x)|^2 \xrightarrow{\text{distribution along } x} \rho(x)dx = |\psi(x)|^2 dx$

* $\int_{-\infty}^{+\infty} dx\, |\psi(x)|^2 = \langle\psi| \left[\int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| \right] |\psi\rangle = \langle\psi|\psi\rangle = 1$ ★ normalization condition

Inner product in PR:

wavefunction

$$\langle\alpha|\beta\rangle = \int_{-\infty}^{+\infty} \langle\alpha|x\rangle\langle x|\beta\rangle\, dx = \int_{-\infty}^{+\infty} [\alpha(x)]^* \beta(x)\, dx$$

$$\langle\alpha|\hat{A}|\beta\rangle = \langle\alpha| \left[\int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| \right] \hat{A} \left[\int_{-\infty}^{+\infty} dy\, |y\rangle\langle y| \right] |\beta\rangle$$

$$= \iint_{-\infty}^{+\infty} dx\,dy\, \langle\alpha|x\rangle\langle x|\hat{A}|y\rangle\langle y|\beta\rangle = \iint_{-\infty}^{+\infty} dx\,dy\, [\alpha(x)]^* A_{xy}\, \beta(x)$$

matrix element

★ Equivalent Operator in Wavefunction system: $\hat{A}\langle x|\psi\rangle = \langle x|\hat{A}|\psi\rangle$

$\hat{A}\langle x|y\rangle = \langle x|\hat{A}|y\rangle \Rightarrow \hat{A}\delta(x-y) = A_{xy}$

operate on wave-func. operate on statevector

eg. $\hat{x}\delta(x-y) = \langle x|\hat{x}|y\rangle = x\langle x|y\rangle = x\delta(x-y) \Rightarrow \hat{x} = x$

(作用在波函数上特征值相同)

3D Position Operator

Def. $\hat{\vec{r}}\,|\vec{r}\rangle = \vec{r}\,|\vec{r}\rangle$, where $\hat{\vec{r}} = \sum_i \hat{x}_i \vec{e}_i$ → CSCO: $\{\hat{x}_1, \hat{x}_2, \hat{x}_3\}$

assumption: $[x_i, x_j] = 0$ $|\vec{r}\rangle = |x_1, x_2, x_3\rangle$ ($\hat{x}_i |\vec{r}\rangle = x_i |\vec{r}\rangle$)

properties: * $\hat{\vec{r}} = \hat{\vec{r}}^\dagger$, $\langle \vec{r} | \vec{r}' \rangle = \delta^{(3)}(\vec{r} - \vec{r}')$

* $\int d^3x\, |\vec{r}\rangle\langle\vec{r}| = \hat{I}$

* $|\psi\rangle = \int d^3x\, |\vec{r}\rangle \langle \vec{r} | \psi\rangle$ → $\psi(\vec{r})$: wavefunc.

Spatial Translation for Arbitrary Quantum State

$\vec{r} \to \vec{r} + d\vec{r}$, $\hat{\vec{r}}\,|\vec{r}\rangle = \vec{r}\,|\vec{r}\rangle \to \hat{\vec{r}}\,|\vec{r} + d\vec{r}\rangle = (\vec{r} + d\vec{r})\,|\vec{r} + d\vec{r}\rangle$

$\hat{\mathcal{T}}(d\vec{r})$: $|\vec{r} + d\vec{r}\rangle = \hat{\mathcal{T}}\,|\vec{r}\rangle$

⇑

Translation Operator in infinitesimal space

$$|\psi\rangle_{tr} = \hat{\mathcal{T}}(d\vec{r})\,|\psi\rangle = \int d^3x\, [\hat{\mathcal{T}}(d\vec{r})\,|\vec{r}\rangle]\,\psi(\vec{r}) = \int d^3x\, |\vec{r} + d\vec{r}\rangle\, \psi(\vec{r})$$

properties * unitary operator $[\hat{\mathcal{T}}]^\dagger \hat{\mathcal{T}} = \hat{\mathcal{T}}\,[\hat{\mathcal{T}}]^\dagger = \hat{I}$

* $\langle\psi|\psi\rangle_{tr} = \langle\psi|[\hat{\mathcal{T}}]^\dagger\hat{\mathcal{T}}|\psi\rangle = \langle\psi|\psi\rangle$

* $\hat{\mathcal{T}}(d\vec{r}')\,\hat{\mathcal{T}}(d\vec{r}) = \hat{\mathcal{T}}(d\vec{r})\,\hat{\mathcal{T}}(d\vec{r}') = \hat{\mathcal{T}}(d\vec{r} + d\vec{r}')$

* $\lim_{d\vec{r} \to 0} \hat{\mathcal{T}}(d\vec{r}) = \hat{I}$

* $[\hat{\mathcal{T}}(d\vec{r})]^{-1} = [\hat{\mathcal{T}}(d\vec{r})]^\dagger = \hat{\mathcal{T}}(-d\vec{r})$ (平移变换群，阿贝尔云正))

★ in infinitesimal space, the spacial translation can be described as

$$\hat{\mathcal{T}}(d\vec{r}) \approx \hat{I} - \frac{i}{\hbar}\, d\vec{r} \cdot \hat{\vec{p}}$$

⇓ Hermitian

$\hat{\vec{p}} = \hat{\vec{p}}^\dagger$ → 平移变换群生成元，物理诠释为动量算符（Noether 定理）

physically $\hat{\vec{p}} = \sum_i \hat{p}_i \vec{e}_i$ $[\hat{p}_i, \hat{p}_j] = 0$, $\int d^3p\, |\vec{p}\rangle\langle\vec{p}| = \hat{I}$

$|\vec{p}\rangle = |p_1, p_2, p_3\rangle$ (CSCO $\{\hat{p}_1, \hat{p}_2, \hat{p}_3\}$) , $\hat{p}_i |\vec{p}\rangle = p_i |\vec{p}\rangle$

$\langle \vec{p} | \vec{p}' \rangle = \delta^{(3)}(\vec{p} - \vec{p}')$

Equivalent Operator $\hat{p} = p$; $\hat{p}\,\psi_p(p) = p\,\psi_p(p)$ ← $\langle p|\psi\rangle$

Specially: Considering $\begin{cases} \hat{\vec{r}}\,\hat{\mathcal{T}}(d\vec{r})|\vec{r}'\rangle = \hat{\vec{r}}|\vec{r}'+d\vec{r}\rangle = (\vec{r}'+d\vec{r})|\vec{r}'+d\vec{r}\rangle \\ \hat{\mathcal{T}}(d\vec{r})\,\hat{\vec{r}}\,|\vec{r}\rangle = \vec{r}\,|\vec{r}+d\vec{r}\rangle \end{cases}$

$$\rightarrow [\hat{\vec{r}}, \underbrace{\hat{\mathcal{T}}(d\vec{r})}_{\hat{I}-\frac{i}{\hbar}d\vec{r}\cdot\hat{\vec{p}}}]|\vec{r}\rangle = d\vec{r}\,|\vec{r}+d\vec{r}\rangle \approx d\vec{r}\,|\vec{r}\rangle$$

$$\rightarrow [\hat{\vec{r}}, d\vec{r}\cdot\hat{\vec{p}}] = i\hbar\, d\vec{r} \quad \rightarrow [\hat{x}_i, dx_i \cdot \hat{p}_i] = i\hbar\, dx_i$$

★ commuting relationship: $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$

For any finate spatial translation $\vec{a}$, divide it into $\sum_N \frac{\vec{a}}{N}$, while $N\rightarrow\infty$, each translation is infinatesimal $\hat{\mathcal{T}}(\frac{\vec{a}}{N}) \approx \hat{I} - \frac{i}{\hbar}\frac{\vec{a}}{N}\cdot\hat{\vec{p}}$

$$\hat{\mathcal{T}}(\vec{a}) = \lim_{N\rightarrow\infty}[\hat{I} - \frac{i}{\hbar}\frac{\vec{a}}{N}\cdot\hat{\vec{p}}]^N = \exp(-i\vec{a}\cdot\frac{\hat{\vec{p}}}{\hbar})$$

Momentum Operator in PR

* Matrix Element: $\langle\vec{r}|\hat{\vec{p}}|\vec{r}'\rangle$

$$\langle\vec{r}|\hat{\vec{p}}|\psi\rangle = -i\hbar\nabla\psi(\vec{r}) \;/\; \langle\vec{r}|\hat{\vec{p}}|\vec{r}'\rangle = -i\hbar\nabla\delta^{(3)}(\vec{r}-\vec{r}')$$

Equivalent Operator $\hat{\vec{p}}\psi(\vec{r}) = \langle\vec{r}|\hat{\vec{p}}|\psi\rangle = -i\hbar\nabla\psi(\vec{r}) \rightsquigarrow \hat{\vec{p}} = -i\hbar\nabla$

Eigenstates of Momentum Operator in PR

1D case: $\hat{P}_x\langle x|p\rangle = \langle x|\hat{p}_x|p\rangle = p\langle x|p\rangle \rightarrow -i\hbar\frac{d}{dx}\phi_p(x) = p\phi_p(x)$

Seeming eigenstate wavefunction: $\phi_p(x) = N\exp(ipx/\hbar)$

Hermitian: $\hat{p}_x = \hat{p}_x^{\dagger}$, $\langle\varphi|\hat{p}_x|\psi\rangle = \langle\psi|\hat{p}_x^{\dagger}|\varphi\rangle^*$

$$\int_a^b dx\,\varphi^*(x)\frac{d}{dx}\psi(x) \begin{cases} = -\int_a^b dx\,\psi(x)\frac{d}{dx}\varphi^*(x) \\ = [\varphi^*(x)\psi(x)]\Big|_a^b - \int_a^b dx\,\psi(x)\frac{d}{dx}\varphi^*(x) \end{cases}$$

whether $\hat{p}_x \,/\, \hat{P}_x = -i\hbar\frac{d}{dx}$ is Hermitian depends on boundary condition satisfaction

$$\varphi^*(x)\psi(x)\Big|_a^b = 0$$

situation 1: $\psi(x)|_a = \psi(x)|_b = 0$. $\varphi^*(x)\psi(x)|_a^b = 0$

No such $\phi_p(x)$ meets the condition → momentum operator is not observable

situation 2: any wave function: $\Psi(x)|_{x=a} = e^{i\theta}\Psi(x)|_{x=b}$. $\theta \in \mathbb{R}$

$\varphi^*(x)\psi(x)|_a^b = 0 \Rightarrow$ Hermitian

$\phi_p(x) = N\exp(ipx/\hbar) \Rightarrow p_n = [\frac{2\pi n-\theta}{b-a}]\hbar \qquad n \in \mathbb{Z}$

⇑

quantization

$\phi_n(x) = N\exp\{i[\frac{2\pi n-\theta}{b-a}]x\}$, $n \in \mathbb{N}$

normalization : $\int_a^b \phi_m^*(x)\phi_n(x) = \delta_{mn} \Rightarrow N = \sqrt{\frac{1}{b-a}}$ momentum operator is observable

situation 3: $-\infty < x < +\infty$, any wave func. $\Psi(x)|_{x\to\pm\infty} = 0$

$\varphi^*(x)\psi(x)|_{-\infty}^{+\infty} = 0 \Rightarrow$ Hermitian

$\phi_p(x)|_{x\to\pm\infty} \sim \lim_{L\to+\infty}[\cos(pL/\hbar) \pm i\sin(pL/\hbar)]$

$L \to +\infty$, $\phi_p(x) \to 0$

continuous spectrum : $-\infty < p < +\infty$, $p \neq 0$

$$\delta(x-x') = \langle x|x'\rangle = \int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\langle p|x'\rangle = |N|^2\int_{-\infty}^{+\infty} dp \exp[ip(x-x')/\hbar]$$

$$= |N|^2 \cdot 2\pi\hbar\,\delta(x-x')$$

★ momentum operator is observable, eigenstates :

$$\{\frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar), -\infty < p < +\infty, p \neq 0\}$$

completeness : $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} c(p)\, e^{(ipx/\hbar)}\, dp$

Scattering Situation : $\psi(x)|_{x\to\pm\infty} = A\exp(ikx) + B\exp(-ikx)$, $k > 0$

eigenstates : $\phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar)$ is complete

$\int_{-\infty}^{+\infty} dx\, \phi_p^*(x)\phi_{p'}(x) = \delta(p-p')$

3D case : condition
$$\begin{cases} \psi(\vec{r})\big|_{|\vec{r}|\to\infty} = 0 & \text{Bound State Boundary} \\ \psi(\vec{r})\big|_{|\vec{r}|\to\infty} = A\exp(i\vec{k}\cdot\vec{r}) + B\exp(-i\vec{k}\cdot\vec{r}) & \text{Scattering Boundary} \end{cases}$$

$$\phi_p(\vec{r}) = \langle \vec{r} | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp(i\vec{p}\cdot\vec{r}/\hbar)$$

Normalization Condition : $\int d^3x\, \phi_p^*(\vec{r})\, \phi_{p'}^*(\vec{r}) = \delta^{(3)}(\vec{p}-\vec{p}')$

Completeness : $\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, C(\vec{p}) \exp(-i\vec{p}\cdot\vec{r}'/\hbar)$

Evolution of Quantum System

Time Evolution Operator

State vector evolement $|\psi(t_0)\rangle \longrightarrow |\psi(t)\rangle = \underset{\text{time evolution operator}}{\mathcal{U}(t,t_0)}|\psi(t_0)\rangle \quad (t>t_0)$

$\mathcal{U}(t,t_0)$ properties $\begin{cases} * \text{ unitary operator } [\mathcal{U}(t,t_0)]^\dagger\,\mathcal{U}(t,t_0) = \hat{I} \\ * \ \mathcal{U}(t_2,t_0) = \mathcal{U}(t_2,t_1)\,\mathcal{U}(t_1,t_0) \text{ 半群关系} \end{cases}$

for infinitesimal time

$$\begin{cases} \frac{\partial}{\partial t}|\psi(t)\rangle = \lim\limits_{t\to 0}\frac{\mathcal{U}(t)-I}{t}|\psi(0)\rangle \\ i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle = H(t)\,\mathcal{U}(t)|\psi(0)\rangle \end{cases}$$

$$\text{def. } H(t) = i\hbar\lim_{t\to 0}\mathcal{U}^\dagger(t)\frac{\mathcal{U}(t)-I}{t}$$

* Show $H(t)$ is the Hamiltonian Operator (Dirac)

In Heisenberg Picture

$A(t) = \mathcal{U}^\dagger(t)\,A\,\mathcal{U}(t) \Rightarrow i\hbar\frac{\partial}{\partial t}A(t) = [A(t), H(t)]$ $[A(t) = x(t)/p(t)]$

☆与经典运动方程对应 ⇒ $H(t)$: Hamiltonian

☆ Dirac 正则量子化：经典对应

$F(P,X) = \sum\limits_{nm} C_{nm}P^nX^m \rightarrow F(p,x) = \sum\limits_{nm} C_{nm}p^nx^m$

$[X,P]=0 \qquad [x,p]=i\hbar$

$\boxed{\{\,,\,\} \rightarrow \frac{[\,,\,]}{i\hbar} \quad \text{(poisson 括号)}}$

$\Downarrow$

$\dot{A} = \{A,H\} \rightarrow \dot{A} = \frac{1}{i\hbar}[A,H]$

thus $\mathcal{U}(t+dt,t) = I - \frac{i}{\hbar}dt\,H(t)$

$$\mathcal{U}(t+dt,t_0) = \mathcal{U}(t+dt,t)\,\mathcal{U}(t,t_0) = \left[I - \frac{i}{\hbar}dt\,H\right]\mathcal{U}(t,t_0)$$

$dt\to 0$: $i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) = H\,\mathcal{U}(t,t_0) \xrightarrow[\text{operate on } |\psi(t_0)\rangle]{} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$

* when $H(t) = H$, then

$$\mathcal{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]$$

Stationary States

Def. eigenstate of specific energy : $\hat{H}|E\rangle = E|E\rangle$

* Superposition State $|\psi\rangle = c_1|E_1\rangle + c_2|E_2\rangle$ $(E_1 \neq E_2)$ is not Stationary State

QM assumption : $\hat{H}$ is observable

- E are real, $\{|E\rangle\}$ are complete base for $\mathcal{H}$
- while in bound state, the spectrum is discrete

Time evolution operator in form of stationary states :

$$\hat{\mathcal{U}}(t,t_0) = \exp[-i\hat{H}(t-t_0)/\hbar]$$

complete sets

$$= \exp[-i\hat{H}(t-t_0)/\hbar]\sum_n |E_n\rangle\langle E_n|$$

$$= \sum_n \exp[-iE_n(t-t_0)/\hbar]|E_n\rangle\langle E_n|$$

hence

$$|E_n(t)\rangle = \hat{\mathcal{U}}(t,t_0)|E_n\rangle = \left[\sum_m \exp(-iE_m(t-t_0)/\hbar)|E_m\rangle\langle E_m|\right]|E_n\rangle$$

$$= \sum_m \exp(-iE_m(t-t_0)/\hbar)|E_m\rangle\delta_{mn}$$

$$= \exp(-iE_n(t-t_0)/\hbar)|E_n\rangle$$

★ Obviously $|E_n(t)\rangle$ is still the eigenstate of eigenvalue E_n with an unrelated coefficient $\exp[-iE_n(t-t_0)/\hbar]$

* For superposition State $|\psi(t_0)\rangle = \sum_n C_n|E_n\rangle$

$$|\psi(t)\rangle = \hat{\mathcal{U}}(t,t_0)|\psi(t_0)\rangle = \sum_n C_n\exp(-iE_n(t-t_0)/\hbar)|E_n\rangle$$

* $|\psi(t)\rangle / |\psi(t_0)\rangle$ aren't equivalent

Schrödinger Equation

Wavefunction in Position Representation $\langle\vec{r}|\psi(t)\rangle = \psi(\vec{r},t)$,

* Equivalent Hamiltonian Operator $\hat{\mathcal{H}}$: $i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \hat{\mathcal{H}}\psi(\vec{r},t)$

★ Schrödinger Equation

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(\hat{\vec{r}}) \Rightarrow \hat{\mathcal{H}} = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t)$$

Law of Conservation of Probability

Physical meaning of $\psi(\vec{r},t)$: $\rho(\vec{r},t) = |\psi(\vec{r},t)|^2$

Schrödinger Equation

$\Downarrow$ conjugate

$\star$ $\psi^*(\vec{r},t)$ is not a wavefunc.

$$-i\hbar\frac{\partial}{\partial t}\psi^*(\vec{r},t) = -\frac{\hbar^2}{2\mu}\nabla^2\psi^*(\vec{r},t) + V(\vec{r})\psi^*(\vec{r},t)$$

$$\rightarrow \quad i\hbar\frac{\partial}{\partial t}\rho(\vec{r},t) = i\hbar\frac{\partial}{\partial t}|\psi(\vec{r},t)|^2$$

$$= \psi^*(\vec{r},t)\left[i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)\right] + \left[i\hbar\frac{\partial}{\partial t}\psi^*(\vec{r},t)\right]\psi(\vec{r},t)$$

$$= -\frac{\hbar^2}{2\mu}\nabla\cdot\underline{\left[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\nabla\psi^*(\vec{r},t)\right]}$$

Def. $\vec{J}(\vec{r},t) = \frac{\hbar}{2i\mu}\left[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\nabla\psi^*(\vec{r},t)\right]$

$\frac{\partial}{\partial t}\rho(\vec{r},t) + \nabla\cdot\vec{J}(\vec{r},t) = 0$ Law of conservation of prob.

Stationary State Schrödinger Equation in Position Representation

$$\hat{\mathcal{H}}\langle r|\psi\rangle := \langle r|\hat{H}|\psi\rangle \ , \ \forall\ |\psi\rangle \in \mathcal{H}$$

$$\hat{\mathcal{H}}\psi_E(\vec{r}) = E\psi_E(\vec{r})$$ $\rightarrow$ stationary state

$\Rightarrow$ stationary state Schrödinger equation $\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi_E(r) = E\psi_E(r)$

Stationary state $\psi_E(\vec{r},t) = \psi_E(\vec{r})e^{-iEt/\hbar} \rightarrow \begin{cases}\rho_E(\vec{r},t) = \rho_E(\vec{r}) \\ \vec{J}_E(\vec{r},t) = \vec{J}_E(\vec{r})\end{cases} \rightarrow \nabla\cdot\vec{J}_E(\vec{r}) = 0$

The Evolution of Expectation of Observable

For $\hat{A} = \hat{A}(t)$ $\begin{cases}\langle\hat{A}\rangle_\psi = \langle\psi(t)|\hat{A}|\psi(t)\rangle \\ i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \xrightarrow{\text{conjugate}} -i\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}\end{cases}$

$$\rightarrow \frac{d}{dt}\langle\hat{A}\rangle_\psi = \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle_\psi + \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle_\psi$$

As for $\vec{r}$, $\vec{p}$: $\left\langle\frac{\partial\vec{r}}{\partial t}\right\rangle = \left\langle\frac{\partial\vec{p}}{\partial t}\right\rangle = 0$

set $\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + V(\hat{\vec{r}})$, $V(\vec{r}) = \sum_{m,n,l=0}^{\infty} V_{mnl}\hat{x}_1^m\hat{x}_2^n\hat{x}_3^l$

$[A, BC] = B[A,C] + [A,B]C$

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} \Rightarrow \begin{cases} [\hat{x}_i, \hat{H}] = [\hat{x}_i, \frac{\hat{p}_i\hat{p}_i}{2\mu}] = i\hbar\frac{\hat{p}_i}{\mu} \\ [\hat{p}_i, \hat{H}] = -i\hbar\frac{\partial V(\vec{r})}{\partial x_i}, \quad (i = 1,2,3) \end{cases} \xrightarrow{3D} \begin{cases} [\hat{\vec{r}}, \hat{H}] = i\hbar\frac{\hat{\vec{p}}}{\mu} \\ [\hat{\vec{p}}, \hat{H}] = -i\hbar\nabla V(\vec{r}) \end{cases}$$

Ehrenfest Equation: $\frac{d}{dt}\langle\hat{\vec{r}}\rangle_\psi = \frac{\langle\hat{\vec{p}}\rangle_\psi}{\mu}$, $\frac{d}{dt}\langle\hat{\vec{p}}\rangle_\psi = -\langle\nabla V(\vec{r})\rangle_\psi$

Picture 绘景

① Schrödinger Picture:

$$\begin{cases} \text{State vector evolve } |\psi(t)\rangle_S = \hat{\mathcal{U}}(t,t_0)|\psi(t_0)\rangle_S \\ \text{Observable } \hat{A} \text{ \& complete bases } \{|f_i\rangle\} \text{ don't evolve } \quad \hat{A}_S(t) = \hat{A} \end{cases}$$

properties: * $\langle\psi(t)|\phi(t)\rangle_S = \langle\psi(t_0)|\phi(t_0)\rangle$

* $\langle\psi(t)|\hat{A}_S(t)|\phi(t)\rangle_S = \langle\psi(t_0)|[\hat{\mathcal{U}}(t,t_0)]^\dagger\hat{A}\hat{\mathcal{U}}(t,t_0)|\phi(t_0)\rangle$

② Heisenberg Picture:

$$\begin{cases} \text{State Vector doesn't evolve: } |\psi(t)\rangle_H \equiv |\psi(t_0)\rangle \\ \text{Observable evolve: } \quad \hat{A}_H(t) = [\hat{\mathcal{U}}(t,t_0)^\dagger]\hat{A}\hat{\mathcal{U}}(t,t_0) \end{cases}$$

properties: * $|\psi(t)\rangle_H = [\hat{\mathcal{U}}(t,t_0)]^\dagger|\psi(t)\rangle_S$ $\quad (|\psi(t)\rangle_S = \hat{\mathcal{U}}(t,t_0)|\psi(t)\rangle_H)$

* $\hat{A}_H(t) = [\hat{\mathcal{U}}(t,t_0)]^\dagger\hat{A}_S(t)\hat{\mathcal{U}}(t,t_0)$ $\quad \hat{\mathcal{U}}(t,t_0) = \exp[-i\hat{H}(t-t_0)/\hbar]$

* $|f_i\rangle_H = [\hat{\mathcal{U}}(t,t_0)]^\dagger|f_i\rangle_S$

In Sch-Picture, any observable $\hat{A}$ has the constant element:

$$\underline{A_{ij}^{(S)} = {}_S\langle f_i|\hat{A}|f_j\rangle_S}$$

(physically observable, doesn't depend on picture, that is, the prob. for translation from $|f_i\rangle$ to $|f_j\rangle$)

In Hei-Picture, observable $\hat{F}$ & its bases $\{|f_i\rangle_H\}$ evolve by time, however

$$A_{ij}^{(H)} = {}_H\langle f_i|\hat{A}|f_j\rangle_H = {}_S\langle f_i|\hat{A}|f_j\rangle = A_{ij}^{(S)}$$

★ A_{ij} doesn't depend on the chosen of picture

Heisingberg Equation of Motion

$\mathcal{U} = \exp(-i(t-t_0)\hat{H}/\hbar)$

$$\frac{d\hat{A}_{H(t)}}{dt} = \left[\frac{\partial \mathcal{U}(t)^\dagger}{\partial t}\right]\hat{A}_S\hat{\mathcal{U}} + \hat{\mathcal{U}}^\dagger\hat{A}_S\left[\frac{\partial \mathcal{U}}{\partial t}\right] \Rightarrow \frac{d\hat{A}_{H(t)}}{dt} = \frac{1}{i\hbar}[\hat{A}_{H(t)}, \hat{H}]$$

(Heisenberg Equation of Motion) / Same as Schrödinger Equ

For free particle:

$$\begin{cases} \dfrac{d\hat{p}}{dt} = \dfrac{1}{i\hbar}[\hat{p}, \hat{H}] = 0 \\ \dfrac{d\hat{x}}{dt} = \dfrac{1}{i\hbar}[\hat{x}, \hat{H}] = \dfrac{1}{i\hbar}[\hat{x}, \dfrac{\hat{p}^2}{2\mu}] = \dfrac{\hat{p}(0)}{\mu} \end{cases} \Rightarrow \hat{x}(t) = \hat{x}(0) + \frac{\hat{p}(0)}{\mu}t$$

Standard Quantum Limit

At time t $\quad \Delta x(t) = \sqrt{\Delta x^2(0) + \dfrac{\Delta p^2(0)t^2}{\mu^2}} \geq \sqrt{\Delta x^2(0) + \dfrac{\hbar^2 t^2}{4\mu^2\Delta x^2(0)}} \geq \sqrt{\dfrac{\hbar t}{\mu}}$ (standard quantum limit)

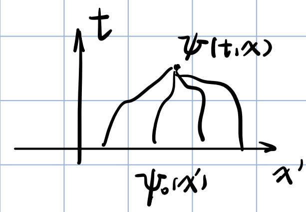
$$p = \mu \lim_{t\to 0}\frac{x(t) - x(0)}{t} \Rightarrow \Delta p = \frac{\mu}{t}\sqrt{(\Delta x_1)^2 + (\Delta x_2)^2 + (\Delta x_{add})^2}$$

★ 位置时间演化测量精度源于波包扩散

Propagator & Path Integral Formulation of QM

Propagator

Ferman hypothesis: $\psi(\vec{r},t)$ 为 t' 时在可能 $\vec{r}'$ 处 $\psi(\vec{r}',t')$ 的叠加



$$\star \quad \psi(\vec{r},t) = \int d^3x'\, G(\vec{r},\vec{r}',t,t')\,\psi(\vec{r}',t')$$

$\Downarrow$

Def. Propagator

Each path connecting $(\vec{r},t)$ & $(\vec{r}',t')$ contribute to propagator

$$G(\vec{r},t,\vec{r}',t) = A \sum_{\text{all path}} \exp\left[\frac{i}{\hbar} S(i,f)\right]$$

action between initial & final

In infinatesimal time interval, $t' = t-\varepsilon \;/\; \varepsilon \to 0^+$,

拉氏量平均值

$$G(\vec{r},t,\vec{r}',t) = A\exp\left[\frac{i}{\hbar}\int_{(\vec{r}',t')}^{(\vec{r},t)} L(\dot{\vec{r}},\vec{r})\,dt\right] \sim A\exp\left[\frac{i}{\hbar}\varepsilon L_{AVE}\right]$$

$$\downarrow \quad 1D: \; L_{AVE} \approx \frac{m}{2}\Big(\frac{\overbrace{x-x'}^{\eta}}{t-t'}\Big)^2 - V\left[\frac{x+x'}{2}\right] \approx \frac{m}{2}\frac{\eta^2}{\varepsilon^2} - V(x)$$

$$\xrightarrow{\text{Tay Expansion}} A\exp\left[\frac{im\eta^2}{2\hbar\varepsilon}\right]\left[1 - \frac{i}{\hbar}\varepsilon V(x) + O(\varepsilon^2)\right]$$

$$\psi(x) = A\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}\left[\psi(x,t) - \frac{i}{\hbar}\varepsilon V(x)\psi(x,t) - \varepsilon\frac{\partial\psi(x,t)}{\partial t} + \frac{i\hbar}{2m}\varepsilon\frac{\partial^2\psi(x,t)}{\partial x^2}\right]$$

$$\downarrow A = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}$$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$$

Schrödinger Equ

△ Propagator between spacial spot between infinatesimal time interval

$$G(x,t,x',t-\varepsilon) = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\exp\left\{\frac{i\varepsilon}{\hbar}\left[\frac{m}{2}\Big(\frac{x-x'}{\varepsilon}\Big)^2 - V(x)\right]\right\}$$

Physical Meaning of Propagator

$$\psi(x_b,t_b) = \int_{-\infty}^{+\infty} dx' G(x_b,t_b;x',t_a)\psi(x',t_a)$$

In Heisinberg picture

$$\langle x_b(t_b)|\psi\rangle = \int_{-\infty}^{+\infty} dx' G(x_b,t_b;x',t_a)\langle x'(t_a)|\psi\rangle$$

hence $\langle x_b(t_b)|x_a(t_a)\rangle = G(x_b,t_b,x_a,t_a)$

★ $G(x_b,t_b,x_a,t_a)$ is the prob. amplitude for $|x_a(t_a)\rangle$ (position operator's eigenstate at time t_a) to evolve to $|x_b(t_b)\rangle$ (position operator's eigenstate at time t_b)

any interval $\dfrac{t_b-t_a}{N} = \varepsilon$ $(N\to\infty,\ \varepsilon\to 0)$

$$\langle x_i(t_i)|x_{i-1}(t_{i-1})\rangle \approx \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\exp\left\{\frac{i\varepsilon}{\hbar}\left[\frac{m}{2}\left(\frac{x_i-x_{i-1}}{\varepsilon}\right)^2 - V(x_i)\right]\right\}$$

for t_i $(1\le i\le N-1)$ $\int_{-\infty}^{+\infty} dx_i(t_i)\,|x_i(t_i)\rangle\langle x_i(t_i)| = \hat{I}$

such $\langle x_b(t_b)|x_a(t_a)\rangle = \int_{-\infty}^{+\infty} dx_1 \langle x_b(t_b)|x_1(t_1)\rangle\langle x_1(t_1)|x_a(t_a)\rangle$

$$= \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \langle x_b(t_b)|x_2(t_2)\rangle\langle x_2(t_2)|x_1(t_1)\rangle\langle x_1(t_1)|x_a(t_a)\rangle$$

$$= \cdots = A^{N-1}\prod_{i=1}^{N-1}\int_{-\infty}^{+\infty} dx_i(t_i)\exp\left[\frac{i}{\hbar}S(a,b)\right]. \quad A = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}$$

propagator is described as

$$G(x_b,t_b;x_a,t_a) = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\varepsilon}\right]^{\frac{N-1}{2}}\prod_{i=1}^{N-1}\int_{-\infty}^{+\infty} dx_i(t_i)\exp\left[-\frac{i}{\hbar}S(a,b)\right]$$

△ In fact. propagator is the matrix element of time evolution operator

$$G(\vec{r},t,\vec{r}',t') := \langle\vec{r}|\hat{\mathcal{U}}(t,t')|\vec{r}'\rangle$$

assumption: $[\hat{A},\hat{H}]=0$, $\hat{A}|a_n\rangle = a_n|a_n\rangle$, $\hat{H}|a_n\rangle = E_n|a_n\rangle$

$$\Rightarrow \quad G(\vec{r},t,\vec{r}',t') = \sum_n \exp\left[-iE_n(t-t')/\hbar\right]\langle\vec{r}|a_n\rangle\langle a_n|\vec{r}'\rangle$$