但此时 $\hat{a}|n_0\rangle = \sqrt{n_0}|n_0-1\rangle$ → 与①矛盾.

$\Longrightarrow$ $n_0=0$, 即 n 为非负整数.

最后: $\hat{a}|\hat{n}_0+1\rangle = \sqrt{n_0+1}\,|n_0\rangle$

$$\hat{H}|n\rangle = \underbrace{(n+\tfrac{1}{2})\hbar\omega}_{E_n}|n\rangle$$

$E_n = (n+\frac{1}{2})\hbar\omega \quad n=0,1,2\cdots$ 能量量子化.

且 $E_0 = \frac{1}{2}\hbar\omega > 0$

注: 究其本源, $E_0=\frac{1}{2}\hbar\omega$ 来自于 $[x,p]=i\hbar$. $E_0=\frac{1}{2}\hbar\omega$ 被称为真空能, 来自于量子涨落.

$|0\rangle \longrightarrow$ 真空态.

定义了 $|0\rangle$ 之后, 反复用 $\hat{a}^+$ 作用.

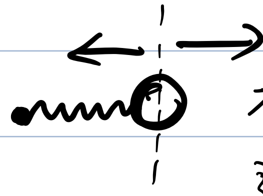
$$|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$$

考察 $\hat{x}|n\rangle$ 而 $\hat{x} \propto (\hat{a}+\hat{a}^+)$

$$\Longrightarrow \hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$

同理:

$$\hat{p}|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n}|n-1\rangle - \sqrt{n+1}\,|n+1\rangle\right)$$

$\Longrightarrow \langle n|\hat{x}|n\rangle = 0$ (类比于  在平衡位置附近振动)

$\langle n|\hat{p}|n\rangle = 0$

$\Rightarrow \langle n|\hat{x}^2|n\rangle \sim \Delta x$ 最后可得出 $\Delta x \Delta p = (n+\frac{1}{2})\hbar$.

$\langle n|\hat{p}^2|n\rangle \sim \Delta p$.

b. $|n\rangle$态的波函数.

$$|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$$，即重点是求 $|0\rangle$.

考察 $\langle x|\hat{a}|0\rangle = 0 \quad (\hat{a}|0\rangle = 0)$

$$\Longrightarrow \sqrt{\frac{m\omega}{2\hbar}}\langle x|\hat{x} + \frac{i}{m\omega}\hat{p}|0\rangle = 0$$

$$\xrightarrow[\hat{p}\to -i\hbar\frac{\partial}{\partial x}]{\hat{x}\to x} \left(x + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\varphi_0(x) = 0 \qquad \varphi_0(x) = \langle x|0\rangle$$

$$\Longrightarrow \varphi_0(x) = \frac{1}{\pi^{\frac{1}{4}}\sqrt{x_0}}e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}$$ 其中 $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$ → 特征长度.

注：上式中

$$\langle x|\hat{p}|0\rangle = \int dx'\langle x|\hat{p}|x'\rangle\langle x'|0\rangle \quad \left(\int dx'|x'\rangle\langle x'| = I\right)$$

$$= \int dx'\left[-i\hbar\frac{\partial}{\partial x}\delta(x-x')\right]\langle x'|0\rangle$$

$$= -i\hbar\frac{\partial}{\partial x}\langle x|0\rangle$$

于是 $\langle x|1\rangle = \langle x|a^+|0\rangle$

$$= \frac{1}{\sqrt{2}x_0}\left(x - x_0^2\frac{\partial}{\partial x}\right)\varphi_0(x)$$

...

$$\langle x|n\rangle = \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}}\left(\frac{1}{x_0^{n+\frac{1}{2}}}\right)\left(x - x_0^2\frac{\partial}{\partial x}\right)^n e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}$$

厄米多项式

c. 相干态 (coherent state)

$\hat{a}$的本征态 (虽然 $\hat{a}$ 不是厄米的)

$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \qquad (\alpha \in \mathbb{C})$

$\langle\alpha|\hat{a}^+ = \langle\alpha|\alpha^* \qquad$ 注 $\hat{a}^+|\alpha\rangle \neq \alpha^*|\alpha\rangle$

i) 相干态"$|\alpha\rangle$"与Fock态"$|n\rangle$"的关系

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

$$|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$$

$$\langle n|\alpha\rangle = \frac{1}{\sqrt{n!}}\langle 0|\hat{a}^n|\alpha\rangle$$

$$= \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle$$

设 $\langle\alpha|\alpha\rangle = 1$

$$\Rightarrow \sum_n \langle\alpha|n\rangle\langle n|\alpha\rangle = 1$$

$$\Rightarrow \sum_n \frac{1}{n!}|\alpha|^{2n}\,|\langle 0|\alpha\rangle|^2 = 1$$

$$\Rightarrow e^{|\alpha|^2}|\langle 0|\alpha\rangle|^2 = 1$$

规定$\langle 0|\alpha\rangle$取实数

$$\langle 0|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}$$

$$\Rightarrow |\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$= e^{-\frac{1}{2}|\alpha|^2}\sum_n \frac{\alpha^n}{\sqrt{n!}}\frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$$

$$= e^{-\frac{1}{2}|\alpha|^2}\sum_n \frac{(\alpha\hat{a}^+)^n}{n!}|0\rangle$$

$$= e^{-\frac{1}{2}|\alpha|^2+\alpha\hat{a}^+}|0\rangle$$

验证归一化

$$\langle\alpha|\alpha\rangle = e^{-|\alpha|^2}\sum_{nm}\frac{\alpha^n(\alpha^*)^m}{\sqrt{n!\,m!}}\langle m|n\rangle$$

$$= e^{-|\alpha|^2}\sum_n \frac{|\alpha|^{2n}}{n!} = 1$$

iii) 正交，完备性？

① $$\langle\alpha|\beta\rangle = \sum_{mn} \frac{(\alpha^*)^m \beta^n}{\sqrt{m!\,n!}} \langle m|n\rangle\, e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2}$$

$$= \sum_n \frac{(\alpha^*\beta)^n}{n!} e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2}$$

$$= e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2-\alpha^*\beta} \neq 0 \Rightarrow \text{无正交性.}$$

② $\int d^2\alpha\, |\alpha\rangle\langle\alpha|$ （复平面上积分）

$$= \int d^2\alpha\, e^{-|\alpha|^2} \sum_{mn} \frac{\alpha^n (\alpha^*)^m}{\sqrt{m!\,n!}} |n\rangle\langle m|$$

令 $\alpha = \rho e^{i\varphi}$ $\rho \in \mathbb{R}$.

$$= \int \rho\, d\rho\, d\varphi\, e^{-\rho^2} \sum_{mn} \frac{\rho^{n+m}}{\sqrt{m!\,n!}} e^{i\varphi(n-m)} |n\rangle\langle m|$$

利用 $\int_0^{2\pi} d\varphi\, e^{i\varphi(m-n)} = 2\pi\delta_{mn}$

$$= 2\pi \int \rho\, d\rho\, e^{-\rho^2} \sum_n \frac{\rho^{2n}}{n!} |n\rangle\langle n|$$

令 $\rho^2 = t$

$$= \pi \int dt\, e^{-t} \sum \frac{t^n}{n!} |n\rangle\langle n|$$

$$= \sum_n \frac{\pi}{n!} \int_0^{+\infty} dt\, e^{-t} t^n |n\rangle\langle n|$$ $\int_0^{\infty} dt\, e^{-t} t^n = n!$

$$= \pi \sum_n |n\rangle\langle n| = \pi \hat{I}$$

$\Rightarrow \int d^2\alpha\, |\alpha\rangle\langle\alpha| = \pi \longrightarrow$ 超完备.

iv) 不确定关系

定义广义位置/动量算符

$$\hat{x}_1 = \frac{1}{2}(\hat{a} + \hat{a}^+)$$

$$\hat{x}_2 = \frac{1}{2i}(\hat{a} - \hat{a}^+)$$

$$\begin{aligned}
&\langle\alpha|\hat{x}_1|\alpha\rangle \\
&= \langle\alpha|\tfrac{1}{2}(\hat{a}+\hat{a}^+)|\alpha\rangle \\
&= \tfrac{1}{2}\langle\alpha|(\hat{a}|\alpha\rangle) + \tfrac{1}{2}(\langle\alpha|\hat{a}^+)|\alpha\rangle \\
&= \tfrac{1}{2}(\alpha+\alpha^*) = Re(\alpha)
\end{aligned}$$

$$\langle\alpha|\hat{x}_2|\alpha\rangle = \frac{1}{2i}(\alpha-\alpha^*) = Im(\alpha)$$

$$\Rightarrow \langle\alpha|\hat{x}_1^2|\alpha\rangle = \langle\alpha|\tfrac{1}{4}(\hat{a}^2+(\hat{a}^+)^2+\underbrace{\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}}_{=2\hat{a}^+\hat{a}+1})|\alpha\rangle$$
$$= \tfrac{1}{4}(\alpha^2+(\alpha^*)^2+2|\alpha|^2+1)$$

$$\langle\alpha|\hat{x}_2^2|\alpha\rangle = \langle\alpha|-\tfrac{1}{4}(\hat{a}^2+(\hat{a}^+)^2-\hat{a}\hat{a}^+-\hat{a}^+\hat{a}|\alpha\rangle$$
$$= -\tfrac{1}{4}(\alpha^2+(\alpha^*)^2-2|\alpha|^2-1)$$

$$\Rightarrow \langle\hat{x}_1^2\rangle_\alpha = \tfrac{1}{4}[(\alpha+\alpha^*)^2+1] = Re^2(\alpha)+\tfrac{1}{4}$$
$$\langle\hat{x}_2^2\rangle_\alpha = -\tfrac{1}{4}[(\alpha-\alpha^*)^2-1] = Im^2(\alpha)+\tfrac{1}{4}$$

$$\Rightarrow \Delta x_1 = \sqrt{\langle\hat{x}_1^2\rangle_\alpha-(\langle\hat{x}_1\rangle)^2} = \tfrac{1}{2}$$
$$\Delta x_2 = \sqrt{\langle\hat{x}_2^2\rangle_\alpha-(\langle\hat{x}_2\rangle)^2} = \tfrac{1}{2}$$

$\Rightarrow \Delta x_1 \Delta x_2 = \frac{1}{4} \longrightarrow$ 最小不确定度，且与α无关

而 $|\alpha\rangle = e^{\alpha\hat{a}^+}|0\rangle$

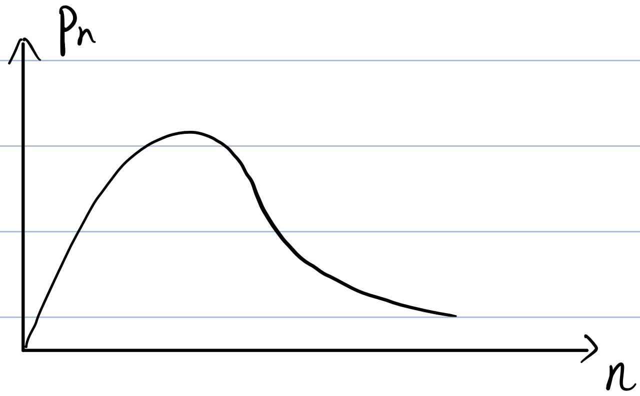
↳ 将不确定度移除

v) 粒子数 $(\hat{N})$

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$\langle\alpha|\hat{N}|\alpha\rangle = \langle\alpha|\hat{a}^+\hat{a}|\alpha\rangle = |\alpha|^2 \triangleq \bar{n}$$

$$P_n = |\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2}\frac{|\alpha|^{2n}}{n!} = e^{-\bar{n}}\frac{\bar{n}^n}{n!}$$ ~ 泊松分布



vi) 三维谐振子.

$$\hat{H} = \sum_i \left(\hat{P}_i^2/2m + \frac{1}{2}m\omega^2\hat{r}_i^2\right) \quad i = x, y, z$$

分析方法：分不同方向，成为一维问题

$$\Rightarrow \hat{H} = \left(\hat{N}_x + \hat{N}_y + \hat{N}_z + \frac{3}{2}\right)\hbar\omega$$

本征态： $|n_x, n_y, n_z\rangle$

eg: $|1.0\ 0\rangle$

$|0\ 1\ 0\rangle$ (简并)

$|0\ 0\ 1\rangle$

$\Big\}$ $E = \frac{5}{2}\hbar\omega$，但是3个不同态

第四章 表象与表象变换

1.表象为量子态的表示方式

类比: 坐标系 ⟶ 表象

坐标 ⟶ 量子态的表示

$|\psi\rangle = \sum_n C_n |\psi_n\rangle$ $\{|\psi_n\rangle\}$: 基矢 $\{C_n\}$: 展开系数

$|\psi\rangle = \int d^3r\ \psi(r)|r\rangle$

核心问题: $\begin{cases} \text{如何确定表象?} \\ \text{量子态在不同表象下表示之间的关系} \end{cases}$

2. 如何确定一组基、

用力学量算符的本征态 → 数学上应用厄米算符的性质

→ 物理上可以对应可观测量.

用本征值作为标定基组中不同态的量子数.

a. $\hat{A}$ 为力学量算符 $\hat{A} = \hat{A}^+$ $\hat{A}|\psi_n\rangle = A_n|\psi_n\rangle$

如 $\hat{A}$ 的本征态均非简并, 则它们构成一组正交归一完备的基, 任意态均可用该基展开.

$|\psi\rangle = \sum_n C_n |\psi_n\rangle$

b. $\hat{A}$的本征态有简并

$$A_1、A_2\cdots\cdots \underbrace{A_m\cdots A_m}_{S个}\cdots\cdots A_n$$

$$|\psi_1\rangle、|\psi_2\rangle\cdots \underbrace{|\psi_{m1}\rangle\cdots|\psi_{ms}\rangle}_{S个}\cdots\ |\psi_n\rangle$$

$|\psi_{m\alpha}\rangle,\ \alpha=1,2\ldots S.$

简并子空间的讨论

i) $\hat{A}|\psi_{m\alpha}\rangle=A_m|\psi_{m\alpha}\rangle,\ \alpha=1,2\ldots S.$

ii) 构造两两正交的$|\psi_{m\alpha}\rangle$ （施密特正交化）

① 找到任一$|\psi_{m1}\rangle$态

② 构造与$|\psi_{m1}\rangle$正交且满足$\hat{A}|\psi_{m2}\rangle=A_m|\psi_{m2}\rangle$的$|\psi_{m2}\rangle$态

③ 构造与$\{|\psi_{m1}\rangle,|\psi_{m2}\rangle\}$均正交，且满足$\hat{A}|\psi_{m3}\rangle=A_m|\psi_{m3}\rangle$的$|\psi_{m3}\rangle$态

⋮

直到找不到为止，得到S个两两正交的本征值为A_m的本征态

iii) 所有$\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle$构成简并子空间，S为简并子空间的维度.

性质：

i) $\hat{A}\left(\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle\right)=A_m\left(\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle\right)$

ii) 子空间内任意态与本征值不为A_m的本征态正交.

$$\langle\psi_n|\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle=0\quad(n\neq m)$$

iii) 简并子空间内任意态均可以表示为$|\psi_{m\alpha}\rangle$的线性叠加.

iv) 所有$\hat{A}$的本征值为A_m的本征态均属于该子空间.

但由于 $|\psi_{mi}\rangle$ 选取的任意性，我们无法唯一确定一组基。

解决方法：

找到一个合适的力学量算符 $\hat{B}$，满足 $[\hat{A},\hat{B}]=0$．由 $\hat{B}$ 在简并子空间内的非简并态唯一确定一组 $\{|\psi_{m\alpha}\rangle\}$．

$$\begin{cases}\hat{A}|\psi_{m\alpha}\rangle = A_m|\psi_{m\alpha}\rangle \\ \hat{B}|\psi_{m\alpha}\rangle = B_{m\alpha}|\psi_{m\alpha}\rangle\end{cases}$$

$$|\psi_{m\alpha}\rangle \Longrightarrow |A_m, B_{m\alpha}\rangle$$

此时，每一个本征态均可以由 $\hat{A}$，$\hat{B}$ 的本征值的组合唯一标定

定理：如 $[\hat{A},\hat{B}]=0$，则 $\hat{A}$，$\hat{B}$ 有共同本征态．

证：i) 如 $[\hat{A},\hat{B}]=0$，则对于 $\hat{A}$ 的非简并本征态亦为 $\hat{B}$ 的本征态

$$\hat{B}\hat{A}|\psi_n\rangle = A_n(\hat{B}|\psi_n\rangle) = \hat{A}(\hat{B}|\psi_n\rangle)$$

$$\Longrightarrow \hat{B}|\psi_n\rangle = B_n|\psi_n\rangle.$$

等价的 $\langle\psi_n|[\hat{A},\hat{B}]|\psi_k\rangle=0$

$$\Longrightarrow \langle\psi_n|\hat{A}\hat{B}-\hat{B}\hat{A}|\psi_k\rangle=0$$

$$\Longrightarrow (A_n-A_k)\langle\psi_n|\hat{B}|\psi_k\rangle=0$$

$$\Longrightarrow \langle\psi_n|\hat{B}|\psi_k\rangle = B_n\delta_{nk}.$$

$$\hat{B}|\psi_n\rangle = \sum_k|\psi_k\rangle\langle\psi_k|\hat{B}|\psi_n\rangle = B_n|\psi_n\rangle$$

ii) 简并子空间．

$$\hat{A}(\hat{B}|\psi_{m\alpha}\rangle) = \hat{B}\hat{A}|\psi_{m\alpha}\rangle = A_m(\hat{B}|\psi_{m\alpha}\rangle)$$

则 $\hat{B}|\psi_{m\alpha}\rangle$ 也在简并子空间中．

$$\Rightarrow \hat{B}|\psi_{m\alpha}\rangle = \sum_{\alpha'} B_{\alpha'\alpha}|\psi_{m\alpha'}\rangle$$

由 $\{|\psi_{m\alpha}\rangle\}$ 的正交性.

$$\langle\psi_{m\beta}|\hat{B}|\psi_{m\alpha}\rangle$$

$$= \sum_{\alpha'} B_{\alpha'\alpha}\langle\psi_{m\beta}|\psi_{m\alpha'}\rangle$$

$$= B_{\alpha\beta}.$$

$$\Rightarrow B_{\alpha'\alpha} = \langle\psi_{m\alpha'}|\hat{B}|\psi_{m\alpha}\rangle$$

构造 $\hat{B}$ 的本征态.

令 $|\varphi\rangle = \sum_{\alpha} C_\alpha|\psi_{m\alpha}\rangle$, 求 C_α 使其满足 $\hat{B}|\varphi\rangle = B|\varphi\rangle$.

$$\hat{B}|\varphi\rangle = \sum_{\alpha} C_\alpha \hat{B}|\psi_{m\alpha}\rangle$$

$$= \sum_{\alpha\alpha'} B_{\alpha'\alpha} C_\alpha |\psi_{m\alpha'}\rangle$$

$$B|\varphi\rangle = \sum_{\alpha} B C_\alpha |\psi_{m\alpha}\rangle$$

要求 $\hat{B}|\varphi\rangle = B|\varphi\rangle$

$$\Rightarrow \sum_{\alpha\alpha'} B_{\alpha'\alpha} C_\alpha |\psi_{m\alpha'}\rangle = \sum_{\alpha} B C_\alpha |\psi_{m\alpha}\rangle$$

用 $\langle\psi_{m\beta}|$ 作用

$$\Rightarrow \sum_{\alpha\beta} B_{\beta\alpha} C_\alpha = B C_\beta \longrightarrow \text{线性方程组.}$$

$$\begin{pmatrix} B_{11} & B_{12} & \cdots & \\ \vdots & \vdots & & \\ & & B_{\beta\alpha} & \cdots \\ & & \vdots & B_{ss} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ \vdots \end{pmatrix} = B \begin{pmatrix} C_1 \\ C_2 \\ \vdots \end{pmatrix}$$

$\swarrow$

矩阵的本征问题.

有S组解, 每组解给出一个 $B_m^{(\beta)}$ (本征值) 及一组 $\{C_\alpha^{(\beta)}\}$

$$|\varphi_{m\beta}\rangle = \sum_{\alpha} C_\alpha^{(\beta)}|\psi_{m\alpha}\rangle$$

$$\begin{cases} \hat{A}|\varphi_{m\beta}\rangle = A_m|\varphi_{m\beta}\rangle \\ \hat{B}|\varphi_{m\beta}\rangle = B_m^{(\beta)}|\varphi_{m\beta}\rangle \end{cases}$$ 即 $\hat{A}, \hat{B}$ 的共同本征态可求.

基于上述构造，如 $B_m^{(\beta)}$ 两两不相等（即 $\hat{B}$ 在 $\hat{A}$ 的简并子空间中非简并），则可以用 $\hat{A}$，$\hat{B}$ 的本征值 联合且唯一标定它们的共同本征态。

$$\{|\psi_1\rangle\ |\psi_2\rangle \cdots |\varphi_{m1}\rangle \cdots |\varphi_{ms}\rangle \cdots |\psi_n\rangle\}$$

$$\Downarrow$$

$$\{|A_1,B_1\rangle\ |A_2,B_2\rangle \cdots |A_m,B_m^{(1)}\rangle \cdots |A_m,B_m^{(s)}\rangle \cdots |A_n B_n\rangle\}.$$

如 $\hat{B}$ 在 $\hat{A}$ 的简并子空间内仍简并，则需要找到力学量 $\hat{C}$，则 $[\hat{A},\hat{C}]$，$[\hat{B},\hat{C}]=0$，并在 $\hat{B}$ 的残余简并子空间内求 $\hat{C}$ 的本征值问题，依此类推，直到找到一组彼此独立且两两对易的力学算符集合，它们的共同本征态可以由这些算符的本征值完全确定，则 $\{\hat{A},\hat{B},\hat{C}\cdots\}$ 构成一个力学量完备集，体系的任意态可写成 $|\psi\rangle=\sum_{\alpha,\beta,\gamma\cdots} C_{\alpha,\beta,\gamma\cdots}|\alpha,\beta,\gamma\cdots\rangle$ α,β,γ 为本征值，此时，力学量完全集确定了一个表象，共同本征态为表象的基。

利用矩阵表示 $\hat{A}$。

记 $A_{kk'}=\langle\psi_k|\hat{A}|\psi_{k'}\rangle$

当 $|\psi_k\rangle$ 为 $\hat{A}$ 的本征态时，

$$A_{kk'}=\langle\psi_k|\hat{A}|\psi_{k'}\rangle = A_{k'}\delta_{kk'}=A_k$$

即 A 为对角阵，假设 $\{A_k\}$ 中有一个简并子空间。

$$\hat{A}\rightarrow\begin{pmatrix} A_1 & & & & & & \\ & A_2 & & & & & \\ & & \ddots & & & & \\ & & & A_m & & & \\ & & & & A_m & & \\ & & & & & \ddots & \\ & & & & & & A_m \\ & & & & & & & A_s \end{pmatrix}$$

利用 $\hat{B}$ 的本征态，可将上面的简并空间解简并.

例：一维运动.

$\{\hat{x}\}$ 与 $\{\hat{p}_x\}$ 都构成力学量完备集

$\{|x\rangle\}$ $\{|p_x\rangle\}$.

三维运动.

$\{\hat{x},\hat{y},\hat{z}\} \longrightarrow \{|\vec{r}\rangle\}$

$\{\hat{p}_x,\hat{p}_y,\hat{p}_z\} \longrightarrow \{|\vec{p}\rangle\}$

二维简谐振子.

$\{\hat{N}_x,\hat{N}_y\} \longrightarrow \{|n_x,n_y\rangle\}$

$\{\hat{H},\hat{N}_x\}$ $\hat{H}=(\hat{N}_x+\hat{N}_y+1)\hbar\omega$

$\hookrightarrow \{|E,n_x\rangle\}$

考虑 $\hat{H}$ 的简并，在 $|n_x,n_y\rangle$ 表象中

E.	$\hbar\omega$	$2\hbar\omega$
	$\|0,0\rangle$	$\|0,1\rangle$
		$\|1,0\rangle$

$\left.\begin{matrix}|0,1\rangle\\|1,0\rangle\end{matrix}\right\}$ 简并.

3、量子涨落，不确定关系及共同本征态.

期望值 $\langle A\rangle=\langle\psi|\hat{A}|\psi\rangle$ $\hat{A}$ 为厄米算符

涨落 $\Delta A=\sqrt{\overline{(\hat{A}-\bar{A})^2}}=\sqrt{\langle\psi|(\hat{A}-\bar{A})(\hat{A}-\bar{A})|\psi\rangle}$

当且仅当 $(\hat{A}-\bar{A})|\psi\rangle=0$ 时，$\Delta A=0$.

$\Longrightarrow \hat{A}|\psi\rangle=\bar{A}|\psi\rangle$ 即 $|\psi\rangle$ 为 $\hat{A}$ 的本征态.

而对任意的态 $|\psi\rangle$，$\Delta x \Delta p > 0$，即 $\hat{x}, \hat{p}$ 无共同本征态

不确定关系

对厄米算符 $\hat{A}, \hat{B}$，有 $\Delta A \Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$

证明：由 Schwartz 不等式

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2.$$

对任意 $|\psi\rangle$，令 $|\alpha\rangle = (\hat{A}-\bar{A})|\psi\rangle \quad |\beta\rangle = (\hat{B}-\bar{B})|\psi\rangle$

$\langle\alpha|\alpha\rangle = \Delta A^2 \quad \langle\beta|\beta\rangle = \Delta B^2$

$\langle\alpha|\beta\rangle = \langle\psi|(\hat{A}-\bar{A})(\hat{B}-\bar{B})|\psi\rangle$

$\Longrightarrow \Delta A^2 \Delta B^2 \geq |\langle(\hat{A}-\bar{A})(\hat{B}-\bar{B})\rangle|^2.$

$(\hat{A}-\bar{A})(\hat{B}-\bar{B}) = \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{2}\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}.$

$([\hat{A},\hat{B}])^\dagger = (\hat{A}\hat{B}-\hat{B}\hat{A})^\dagger = \hat{B}\hat{A}-\hat{A}\hat{B} = -[\hat{A},\hat{B}]$ (反厄米)

$(\{\hat{A}-\bar{A},\hat{B}-\bar{B}\})^\dagger = \{\hat{A}-\bar{A},\hat{B}-\bar{B}\}$ 厄米.

则有

$\langle[\hat{A},\hat{B}]\rangle^* = \langle([\hat{A},\hat{B}])^*\rangle = -\langle[\hat{A},\hat{B}]\rangle$

即 $\langle[\hat{A},\hat{B}]\rangle$ 为纯虚数.

同理：$\langle\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle$ 为实数.

$\Longrightarrow \Delta A^2 \Delta B^2 \geq \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2 + \frac{1}{4}|\langle\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle|^2$

$\Longrightarrow \Delta A^2 \Delta B^2 \geq \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2$

4. 分离谱表象(矩阵表象)

假设我们已经建立一组基 $\{|\psi_n\rangle\}$ 且 $\sum_i |\psi_i\rangle\langle\psi_i| = \hat{I}$

则 $|\psi\rangle = \sum_i |\psi_i\rangle\langle\psi_i|\psi\rangle$

$\quad\quad = \sum_i c_i |\psi_i\rangle$

我们用 $\{c_i\}$ 或 $(c_1, c_2, \dots c_n)^T$ 表示 $|\psi\rangle$

相应的用 $\{c_i^*\}$ 或 $(c_1^*, c_2^* \dots c_n^*)$ 表示 $\langle\psi|$

若 $|\varphi\rangle = (a_1, a_2 \dots a_n)^T$

$|\psi\rangle = (c_1, c_2 \dots c_n)^T$

$$\Rightarrow \langle\varphi|\psi\rangle = (a_1^*, a_2^* \dots a_n^*)(c_1, c_2, \dots c_n)^T$$

$$= \sum_i a_i^* c_i$$

算符的表示

$$\hat{A}|\psi\rangle = |\varphi\rangle$$

$$\hat{A}|\psi\rangle = \sum_{ij} |\psi_i\rangle\langle\psi_i|\hat{A}|\psi_j\rangle\langle\psi_j|\psi\rangle$$

定义 $A_{ij} = \langle\psi_i|\hat{A}|\psi_j\rangle$

$$\hat{A}|\psi\rangle = \sum_{ij} A_{ij} c_j |\psi_i\rangle \quad \text{而} \ |\varphi\rangle = \sum_i a_i |\psi_i\rangle$$

$$\Rightarrow \sum_{ij} A_{ij} c_j |\psi_i\rangle = \sum_l a_l |\psi_l\rangle$$

用 $\langle\psi_k|$ 作用

$$\Rightarrow \sum_j A_{kj} c_j = a_k \Rightarrow \begin{pmatrix} & & \\ & A_{ij} & \\ & & \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

即算符在固定表象下与一个矩阵对应.

i) 算符不对易 $\Leftrightarrow$ 矩阵不对易.

ii) 力学算符的本征问题 $\Leftrightarrow$ 矩阵的本征问题.

性质:

i) 算符在其本征态为基的表象下为对角阵.

ii) 若一算符在某组基矢下为对角阵, 则该组基是该矩阵的本征态, 矩阵对角元为其本征值.

iii) 期望值.

$$\langle\psi|\hat{A}|\psi\rangle = \sum_{mn}\langle\psi|\psi_m\rangle\langle\psi_m|\hat{A}|\psi_n\rangle\langle\psi_n|\psi\rangle$$
$$= \sum_{mn} C_m^* A_{mn} C_n$$

iv) $$\hat{A} = \sum_{ij}|\psi_i\rangle\langle\psi_i|\hat{A}|\psi_j\rangle\langle\psi_j|$$
$$= \sum_{ij} A_{ij}|\psi_i\rangle\langle\psi_j|$$

例: 正交归一基组 $\{|1\rangle, |2\rangle\}$

$|1\rangle$ 的矩阵表示 $(1, 0)^T$

$|2\rangle$ 的矩阵表示 $(0, 1)^T$

$\Rightarrow (\alpha, \beta)^T = \alpha(1,0)^T + \beta(0,1)^T$

假设一个算符

$\hat{A}|1\rangle = \alpha|1\rangle + \beta|2\rangle$

$\Rightarrow \langle 1|\hat{A}|1\rangle = \alpha \quad \langle 2|\hat{A}|1\rangle = \beta.$

$\hat{A}|2\rangle = \gamma|1\rangle + \lambda|2\rangle$

$\Rightarrow \langle 1|\hat{A}|2\rangle = \gamma \quad \langle 2|\hat{A}|2\rangle = \lambda.$

$\Rightarrow$ $\hat{A}$ 在 $|1\rangle, |2\rangle$ 下表示为 $\begin{pmatrix}\alpha & \gamma \\ \beta & \lambda\end{pmatrix}$

$\Rightarrow |1\rangle\langle 1| = \begin{pmatrix}1\\0\end{pmatrix}(1, 0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$ $\quad |1\rangle\langle 2| = \begin{pmatrix}1\\0\end{pmatrix}(0 \ \ 1) = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$

$\hat{A} = \alpha|1\rangle\langle 1| + \beta|2\rangle\langle 1| + \gamma|1\rangle\langle 2| + \lambda|2\rangle\langle 2|$

例：本征问题 $\hat{A}|\psi\rangle = A|\psi\rangle$

假设某组基下 $\hat{A} \Rightarrow$ ones(2)

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix}$$

求A矩阵的本征值 $\lambda_1 = 0$ $\lambda_2 = 2$.

$\lambda = 0$ 时.

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0 \Rightarrow \begin{cases} a+b=0 \\ a^2+b^2=1 \end{cases}$$ 设该本征向量为 $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$\lambda = 2$ 时

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 2\begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{cases} a=b \\ a^2+b^2=1 \end{cases}$$ 一个本征向量为 $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

则 $|\lambda=0\rangle = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|2\rangle$

$|\lambda=2\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$

例：力学量完全集

设 $\hat{A}$ 于基 $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle\}$ 下的矩阵表示为

$$\begin{array}{cc} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} & \begin{array}{c} |\alpha\rangle \\ |\beta\rangle \\ |\gamma\rangle \end{array} \end{array}$$

$\hat{A}|\alpha\rangle = |\alpha\rangle$ $\hat{A}|\beta\rangle = -|\beta\rangle$ $\hat{A}|\gamma\rangle = -|\gamma\rangle$

引入与 $\hat{A}$ 对易的 $\hat{B}$ 算符，其矩阵表示为

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 2i \\ 0 & -2i & 0 \end{pmatrix}$$ (厄米阵，准对角阵)

$\hat{B}|\alpha\rangle = 2|\alpha\rangle$

$\left.\begin{array}{l} \hat{B}|\beta\rangle = -2i|\gamma\rangle \\ \hat{B}|\gamma\rangle = 2i|\beta\rangle \end{array}\right\}$ $\hat{B}$作用在$|\beta\rangle|\gamma\rangle$上，仍在$\{|\beta\rangle,|\gamma\rangle\}$这个简并子空间中.

对角化 $\begin{pmatrix} 0 & 2i \\ -2i & 0 \end{pmatrix}$

$$\begin{pmatrix} 0 & 2i \\ -2i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \lambda_1 = 2 \quad \lambda_2 = -2$$

$\lambda = 2$时 $\Rightarrow$ 本征矢 $\frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix} \longrightarrow |\beta'\rangle = \frac{1}{\sqrt{2}} i|\beta\rangle + \frac{1}{\sqrt{2}}|\gamma\rangle$

$\lambda = -2$时 $\Rightarrow$ 本征矢 $\frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix} \longrightarrow |\gamma'\rangle = \frac{-i}{\sqrt{2}}|\beta\rangle + \frac{1}{\sqrt{2}}|\gamma\rangle$

即 $|\beta'\rangle = (0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}})^T$ $\quad |\gamma'\rangle = (0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}})^T$

在新的基$\{|\alpha\rangle, |\beta'\rangle, |\gamma'\rangle\}$下

$\hat{A} \rightarrow \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}$ $\quad \hat{B} \rightarrow \begin{pmatrix} 2 & & 0 \\ & 2 & \\ 0 & & -2 \end{pmatrix}$

$|\alpha\rangle \rightarrow |1, 2\rangle \quad |\beta'\rangle \rightarrow |-1, 2\rangle, \quad |\gamma'\rangle \rightarrow |-1, -2\rangle$

4. 分离谱的表象变换 $\quad$ G表象 $\quad$ F表象

两个基组 $\{|\psi_n\rangle\}, \{|\alpha_n\rangle\}$ 且 $\sum|\psi_n\rangle\langle\psi_n| = \hat{I}$, $\sum|\alpha_n\rangle\langle\alpha_n| = \hat{I}$

则 $|\psi\rangle = \underbrace{\sum_n C_n|\psi_n\rangle = \sum C_m|\varphi_m\rangle}_{\text{两边同时用}\langle\varphi_k|\text{作用}}$

$$\Rightarrow C_k = \sum_n C_n \langle \varphi_k | \psi_n \rangle \hat{=} S_{kn}$$

$$(\text{新}) F \leftarrow \begin{pmatrix} \\ \\ \end{pmatrix} = \begin{pmatrix} & & \\ & S_{kn} & \\ & & \end{pmatrix} \begin{pmatrix} \\ \\ \end{pmatrix} \rightarrow G (\text{旧})$$

$$\Longrightarrow C^{(F)} = S C^{(G)}$$

下面讨论 S 矩阵.

$$\begin{aligned}(S^+ S)_{mn} &= \sum_\beta (S^+)_{m\beta} (S)_{\beta n} \\ &= \sum_\beta (S^*_{\beta m}) (S)_{\beta n} \\ &= \sum_\beta \langle \psi_m | \varphi_\beta \rangle \langle \varphi_\beta | \psi_n \rangle \\ &= \langle \psi_m | \psi_n \rangle = \delta_{mn} \end{aligned} \quad \Longrightarrow S^+ S = I = S S^+$$

我们称 S 这种变化为幺正变换

↳ 对应 Hilbert 空间的转动

对任意给定的算符 $\hat{A}$.

$$\begin{aligned} A^{(F)}_{\alpha\beta} &= \langle \varphi_\alpha | \hat{A} | \varphi_\beta \rangle \\ &= \sum_{mn} \langle \varphi_\alpha | \psi_m \rangle \langle \psi_m | \hat{A} | \psi_n \rangle \langle \psi_n | \varphi_\beta \rangle \\ &= \sum S_{\alpha m} A_{mn} S^*_{\beta n} \\ &= \sum (S)_{\alpha m} A^{(G)}_{mn} (S^+)_{n\beta} \end{aligned}$$

$$\Longrightarrow A^{(F)} = S A^{(G)} S^+ , \quad S^+ A^{(F)} S = A^{(G)}$$

性质: $\{ |\psi_n\rangle \}^G$. $\qquad \{ |\varphi_\alpha\rangle \}^F$

$\hat{A} |\psi\rangle \qquad \sum A_{mn} C_n \qquad \sum A_{\alpha\beta} C_\beta$

$\qquad A^{(G)} G \qquad A^{(F)} C^{(F)} = S A^{(G)} S^+ S C^{(G)} = S A^{(G)} C^{(G)}$

$\langle\varphi|\hat{A}|\psi\rangle = \sum_{mn} a_m^* A_{mn} C_n$ | $\sum_{\alpha\beta} a_\alpha^* A_{\alpha\beta} C_\beta$

$(a^{(G)})^+ A^{(G)} (C^{(G)})$ | $(a^{F})^+ A^{(F)} C^{F}$

$= (a^{G})^+ S^+ S A^{G} S^+ S C^{(G)}$

$= (a^{G})^+ A^{(G)} C^{(G)}$

内积是一个数
与表象无关，与我们
的预期相同

例：算符$\hat{A}$在某基下的表示为$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$，求$\hat{A}$在其本征态基下的矩阵表示

解：求出$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$的本征值与本征态，如下：

$\lambda = 0 \Leftrightarrow \frac{1}{\sqrt{2}}(1,-1)^T$

$\lambda = 2 \Longleftrightarrow \frac{1}{\sqrt{2}}(1,\ 1)^T$

旧基(G)：$(1,0)^T,\ (0,1)^T$

新基(F)：$\frac{1}{\sqrt{2}}(1,-1)^T,\ \frac{1}{\sqrt{2}}(1,1)^T$

$$S_{\beta n} = \langle \underset{F}{\varphi_\beta} | \underset{G}{\psi_n} \rangle$$

$$= \frac{1}{\sqrt{2}}(1,-1)\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}}(1,-1)\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$+ \frac{1}{\sqrt{2}}(1,1)\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} + \frac{1}{\sqrt{2}}(1,1)\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \frac{\sqrt{2}}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

则 $A^{(F)} = S A^{(G)} S^+ = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$

$= \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}$ → A的本征值，预合我们的预期.

例: $f(\hat{A}) = \sum_n \frac{f^{(n)}(0)}{n!} \hat{A}^n$

$$\Rightarrow f^{(F)} = \sum_n \frac{f^{(n)}(0)}{n!} (A^F)^n$$

$$= \sum_n \frac{f^{(n)}(0)}{n!} \underbrace{SA^{(G)}S^+ SA^{(G)}S^+ \cdots SA^{(G)}S^+}_{n个}$$

$$= \sum_n \frac{f^{(n)}(0)}{n!} S (A^{(G)})^n S^+$$

$$= S\left(\sum_n \frac{f^{(n)}(0)}{n!} A^{(G)n} \right) S^+$$

$$= S f^{(G)} S^+$$

利用这种关系我们可以简化计算.

如 $\hat{A}$ 在 $F(G)$ 表象下对角, 则可简化计算.

eg $A^{(F)} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$

则 $e^{A^{(F)}} = \begin{pmatrix} e^a & 0 \\ 0 & e^b \end{pmatrix}$

若 A的特征矢 $\begin{pmatrix} \\ a_1 \\ \\ \end{pmatrix} \begin{pmatrix} \\ \lambda_2 \\ \\ \end{pmatrix} \begin{pmatrix} \\ \lambda_3 \\ \\ \end{pmatrix}$

则 $\underbrace{\begin{pmatrix} (\ \lambda_1\ ) \\ (\ \lambda_2\ ) \\ (\ \lambda_3\ ) \end{pmatrix}}_{S} A \underbrace{\left(\begin{pmatrix} \\ \lambda_1 \\ \\ \end{pmatrix} \begin{pmatrix} \\ \lambda_2 \\ \\ \end{pmatrix} \begin{pmatrix} \\ \lambda_3 \\ \\ \end{pmatrix} \right)}_{S^+} = \mathrm{diag}\{\lambda_1, \lambda_2, \lambda_3\}$

5. 连续谱表象

当表象基对应的力学量本征值连续取值时,我们称之为连续谱表象,我们大多讨论 $\{|r\rangle\}$ 与 $\{|p\rangle\}$

a. 坐标表象

$$|\psi\rangle = \int d^3r\, |r\rangle\langle r|\psi\rangle = \int d^3r\, \underbrace{\psi(r)}_{波函数.}|r\rangle$$

我们要求 $\begin{cases} \langle r|r'\rangle = \delta(r-r') \\ \int d^3r\, |r\rangle\langle r| = \hat{I} \end{cases} \xleftrightarrow{类比} \begin{cases} \langle\psi_m|\psi_n\rangle = \delta_{mn} \\ \sum |\psi_n\rangle\langle\psi_n| = \hat{I} \end{cases}$

b. 连续谱的归一化.

$$\langle\psi_n|\psi_m\rangle = \delta_{mn}$$

$$\Rightarrow \int d^3r\, d^3r' \langle\psi_n|r'\rangle\langle r'|r\rangle\langle r|r\rangle\langle r|\psi_m\rangle$$

$$= \int d^3r\, d^3r'\, \psi_n^*(r')\, \psi_m(r) \langle r'|r\rangle = \delta_{mn}$$

$$\Rightarrow \langle r|r'\rangle = \delta(r-r')$$

$$\langle \psi| = \int d^3r \langle r|\, \psi^*(r)$$

$$\langle \varphi|\psi\rangle = \int d^3r \langle \varphi|r\rangle\langle r|\psi\rangle$$

$$= \int d^3r\, \underbrace{\varphi^*(r)\, \psi(r)}$$ 交叠积分

算符的表示

$$\hat{A}|\psi\rangle = \int d^3r\, d^3r' |r\rangle\langle r|\hat{A}|r'\rangle \underbrace{\langle r'|\psi\rangle}^{\psi(r')}$$

$$= |\varphi\rangle = \int d^3r\, \underbrace{\langle r|\varphi\rangle}_{\varphi(r)} |r\rangle$$

两边用 $\langle r''|$ 作用

$$\Rightarrow \int d^3r\, d^3r' \underbrace{\langle r''|r\rangle}_{\delta(r-r'')} \langle r|\hat{A}|r'\rangle \psi(r') = \int d^3r\, \varphi(r) \underbrace{\langle r''|r\rangle}^{\delta(r''-r)}$$

$$\Rightarrow \varphi(r'') = \int d^3r' \langle r''|\hat{A}|r'\rangle \psi(r')$$

$$\Rightarrow \varphi(r) = \int d^3r' \langle r|\hat{A}|r'\rangle \psi(r')$$

$$\langle r|\hat{r}|r'\rangle = r\,\delta(r-r')$$

$$\langle r|\hat{V}(r)|r'\rangle = V(r)\,\delta(r-r')$$

下面讨论 $\langle r|\hat{p}|r'\rangle$

一维: $\langle x|[\hat{x},\hat{p}]|x'\rangle = i\hbar\,\delta(x-x')$

$$= \langle x|\hat{x}\hat{p} - \hat{p}\hat{x}|x'\rangle$$

$$= (x-x')\langle x|\hat{p}|x'\rangle$$

$$\Rightarrow (x-x')\langle x|\hat{p}|x'\rangle = i\hbar\,\delta(x-x')$$ 比较

利用 $\int f(x)\,\delta'(x)\,dx = -\int \delta(x)\, f'(x)\,dx$

令 $f(x) = x \Rightarrow x\,\delta'(x) = -\delta(x)$

$\Rightarrow \langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x')$

$\Rightarrow \langle \vec{r}|\hat{p}|\vec{r}'\rangle = -i\hbar\nabla_r\delta(\vec{r}-\vec{r}')$

那么若 $\hat{A} = A(\hat{r},\hat{p})$ ($\hat{r},\hat{p}$ 的顺序固定)

则 $\langle r|\hat{A}|r'\rangle = A(r,-i\hbar\nabla_r)\delta(r-r')$

讨论:

i) $\langle x|\hat{p}|p\rangle = p\langle x|p\rangle$

则 $\langle x|\hat{p}|p\rangle = \int dx'\langle x|\hat{p}|x'\rangle\langle x'|p\rangle$

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

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

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

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

$\int dx'\left[\frac{\partial}{\partial x}\delta(x-x')\right]\langle x'|p\rangle = \frac{\partial}{\partial x}\langle x|p\rangle.$

我们得到 $-i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$

$\Rightarrow \langle x|p\rangle \propto e^{ipx/\hbar}$

$\Rightarrow \langle \vec{r}|\vec{p}\rangle \propto e^{i\vec{p}\cdot\vec{r}/\hbar}$

ii) $\psi(r) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int\varphi(p)\, e^{i\vec{p}\cdot\vec{r}/\hbar}d^3p.$

$\Updownarrow$

$\langle r|\psi\rangle = \int d^3p\,\langle p|\psi\rangle\langle r|p\rangle$

☆ 坐标变约矩阵元

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

• 系数的由来:

$\int\langle r|p\rangle\langle p|r'\rangle d^3p = \delta(r-r') = \frac{1}{(2\pi\hbar)^3}\int e^{i\vec{p}(\vec{r}-\vec{r}')/\hbar}d^3p.$

$$\langle r|\hat{p}|r'\rangle = \int d^3p \langle r|\hat{p}|p\rangle\langle p|r'\rangle$$
$$= \int d^3p\ \vec{p}\ \frac{1}{(2\pi\hbar)^3} e^{i\vec{p}(\vec{r}-\vec{r}')/\hbar}$$
$$= -\frac{i\hbar}{(2\pi\hbar)^3}\nabla_r \int d^3p\, e^{i\vec{p}\cdot(\vec{r}-\vec{r}')/\hbar}$$
$$= -i\hbar\nabla_r\delta(r-r')$$ 自洽.

iii) $\langle r|\hat{l}|r'\rangle = -i\hbar\,\vec{r}\times\nabla_r\delta(r-r')$

$$\langle r|\hat{H}|r'\rangle = \langle r|[\frac{\hat{p}^2}{2m}+V(\hat{r})]|r'\rangle$$
$$= [-\frac{\hbar^2\nabla^2}{2m}+V(r)]\delta(r-r')$$

Schrödiger's equation:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$
$$\Rightarrow i\hbar\frac{\partial}{\partial t}\langle r|\psi\rangle = \int\langle r|\hat{H}|r'\rangle\langle r'|\psi\rangle d^3r'$$
$$\Rightarrow i\hbar\frac{\partial}{\partial t}(\psi(r)) = \int[-\frac{\hbar^2}{2m}\nabla^2+V(r)]\delta(r-r')\psi(r')d^3r'$$
$$\Rightarrow i\hbar\frac{\partial}{\partial t}\psi(r) = [-\frac{\hbar^2}{2m}\nabla^2+V(r)]\psi(r)$$

iv) 期望值.

$$\langle\psi|\hat{A}|\psi\rangle = \int dr^3dr'^3\,\psi^*(r)\langle r|\hat{A}|r'\rangle\psi(r')$$
$$= \int dr^3dr'^3\,\psi^*(r)A(r,-i\hbar\nabla)\delta(r-r')\psi(r')$$

v) $\hat{p}$ 的厄米性.

需证明: $\langle\varphi|\hat{p}|\psi\rangle = \langle\varphi|\hat{p}^\dagger|\psi\rangle = (\hat{p}|\varphi\rangle)^\dagger|\psi\rangle$

证明: $\langle\varphi|\hat{p}|r\rangle = \int dr'^3\langle\varphi|r'\rangle\langle r'|\hat{p}|r\rangle$
$$= \int dr'^3\,\varphi^*(r')[-i\hbar\nabla_{r'}\delta(r'-r)]$$

$$= i\hbar \nabla_r \varphi^*(r)$$
$$= [-i\hbar\nabla_r \varphi(r)]^*$$
$$= \langle r|\hat{p}|\varphi\rangle^*$$
$$= (\hat{p}|\varphi\rangle)^\dagger |r\rangle$$

即 $\langle\varphi|\hat{p}|r\rangle = (\hat{p}|\varphi\rangle)^\dagger |r\rangle$

或 $\langle\varphi|\hat{p}|\psi\rangle = \int dr^3\ \varphi^*(r)(-i\hbar\nabla_r)\psi(r)$

$$= i\hbar\int dr^3\, \psi(r)\,(\nabla_r)\,\varphi^*(r)$$
$$= \int \langle r|\psi\rangle\ (\hat{p}|\varphi\rangle)^\dagger |r\rangle\, d^3r$$
$$= \langle\varphi|\hat{p}^\dagger|\psi\rangle \Rightarrow \hat{p} = \hat{p}^\dagger$$

b. 动量表象

$|\psi\rangle = \int d^3p\ \ \varphi(p)|p\rangle$ $\quad \begin{cases} \langle p|p'\rangle = \delta(p-p') \\ \int d^3p\, |p\rangle\langle p| = \hat{I} \end{cases}$

$\langle p|\hat{p}|p'\rangle = p\,\delta(p-p')$

$\langle p|A(\hat{p})|p'\rangle = A(p)\delta(p-p')$

$\langle p|\hat{r}|p'\rangle = \int d^3r d^3r'\ \langle p|r\rangle\langle r|\hat{r}|r'\rangle\langle r'|p'\rangle$

$$= \int d^3r\ \vec{r}\,\langle p|r\rangle\langle r|p'\rangle$$
$$= i\hbar\nabla_p\delta(p-p')$$ 无负号!!

$\langle p|A(\hat{r})|p'\rangle = A(i\hbar\nabla_p)\,\delta(p-p')$

6. 连续谱的表象变换

$\{|r\rangle\} \Longleftrightarrow \{|p\rangle\}$ Fourier transform. 矩阵元: $\langle r|p\rangle$.

$$\begin{cases} \psi(r) = \int d^3p\ \ \varphi(p)\langle r|p\rangle \\ \varphi(p) = \int d^3r\ \psi(r)\langle p|r\rangle \end{cases}$$

$$\langle r|\hat{A}|r'\rangle = \int \langle r|p\rangle\langle p|\hat{A}|p'\rangle\langle p'|r'\rangle d^3p\, d^3p'$$

连续谱 $\Longleftrightarrow$ 分离谱

- $|\psi\rangle = \sum_n C_n|\psi_n\rangle \qquad C_n = \langle\psi_n|\psi\rangle = \int d^3r\langle\psi_n|r\rangle\langle r|\psi\rangle$

$$= \int d^3r\, \psi_n^*(r)\,\psi(r)$$

$$A_{mn} = \langle\psi_m|\hat{A}|\psi_n\rangle = \int d^3r\, d^3r'\langle\psi_m|r\rangle\langle r|\hat{A}|r'\rangle\langle r'|\psi_n\rangle$$

- $|\psi\rangle = \int d^3r\, \psi(r)|r\rangle$

$$\psi(r) = \langle r|\psi\rangle = \sum_n \langle r|\psi_n\rangle\langle\psi_n|\psi\rangle$$

$$= \sum_n C_n\psi_n(r).$$

$\Rightarrow \psi(r) = \sum_n C_n\psi_n(r).$

总结: $\begin{cases} \langle\psi_m|\psi_n\rangle = \delta_{mn} \\ \sum|\psi_n\rangle\langle\psi_n| = \hat{I} \end{cases} \Longleftrightarrow \begin{cases} \int \psi_m^*(r)\,\psi_m(r)\,d^3r = \delta_{mn} \\ \sum_n \psi_n^*(r)\,\psi_n(r') = \delta(r-r') \end{cases}$

例: $e^{i\hat{p}a/\hbar}|\psi\rangle$

$$\Rightarrow \int\langle x|e^{i\hat{p}a/\hbar}|x'\rangle\langle x'|\psi\rangle dx'$$

$$= \int e^{i(-i\frac{\partial}{\partial x}a)}\delta(x-x')\,\psi(x')\,dx'$$

$$= e^{a\frac{\partial}{\partial x}}\psi(x)$$

$$= \sum_n \frac{1}{n!}a^n\frac{\partial^n}{\partial x^n}\psi(x) = \psi(x+a)$$

$e^{i\hat{p}a/\hbar} \longrightarrow$ 平移算符 ☆

类比 $e^{\alpha\hat{a}^+}|0\rangle = |\alpha\rangle$

第五章 时间演化与三种绘景

背景与问题

a. 时间与空间不同，$t \to$ 参数，$\hat{r} \to$ 算符.

b. $|\psi(t)\rangle \longrightarrow |\psi(t')\rangle$ 如何演化.

c. 存在多种描述时间演化的方式，但在可观测的意义下应给出相同的结果.

1. Schrödiger's picture. 与定态

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \quad (\text{基本假设})$$

若 $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$

$$\Rightarrow |\psi_E(t)\rangle = e^{-iEt/\hbar}|\psi_E(0)\rangle$$ 只是相位上的改变.

若 $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r})$

则 $\langle r|\frac{\hat{p}^2}{2m} + V(\hat{r})|\psi\rangle = E\langle r|\psi\rangle$

$$\int d^3r' \langle r|\frac{\hat{p}^2}{2m} + V(\hat{r})|r'\rangle\langle r'|\psi\rangle = E\psi(r)$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m} + V(r)\right]\psi(r) = E\psi(r)$$

在一组完备的函数基下展开：$\psi(r) = \sum_n C_n \psi_n(r)$

$$\Rightarrow \sum_n \int \psi_m^* \left[-\frac{\hbar^2\nabla^2}{2m} + V(r)\right]\psi_n d^3r\, C_n = E\, C_m$$

形式上为

$$\begin{pmatrix} H_{mn} \end{pmatrix}\begin{pmatrix} C_n \end{pmatrix} = E\begin{pmatrix} C_m \end{pmatrix}$$

坐标表象下（数理方程练习）

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

令 $\psi(r,t) = \psi(r)T(t)$，代入方程并分离变量得到

$$\frac{i\hbar}{T(t)}\frac{dT(t)}{dt} = \underbrace{\frac{1}{\psi(r)}\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r)}_{\text{定态薛定谔方程.}} = E \to \text{const}$$

$$\Rightarrow T(t) = e^{-iEt/\hbar}$$

$$\Rightarrow \psi(r,t) = e^{-iEt/\hbar}\psi_E(t)$$

其中 $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi_E(r) = E\psi_E(r)$

定态：任意不含时的力学量在定态下的期望值与测量值的几率分布不随时间变化.

Prof: $\langle\psi_E(t)| = \langle\psi_E(0)|\, e^{iEt/\hbar}$

$|\psi_E(t)\rangle = |\psi_E(0)\rangle\, e^{-iEt/\hbar}$

$$\langle A\rangle = \langle\psi_E(t)|\hat{A}|\psi_E(t)\rangle$$
$$= \langle\psi_E(0)|\, e^{iEt/\hbar}\hat{A}\, e^{-iEt/\hbar}|\psi_E(0)\rangle$$
$$= \langle\psi_E(0)|\hat{A}|\psi_E(0)\rangle$$

$$|C_n|^2 = |\langle\psi_n|\, e^{-iEt/\hbar}|\psi_E(0)\rangle|^2 = |\langle\psi_n|\psi_E(0)\rangle|^2$$

2、任意态的时间演化.

$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ 则 $|\psi(t)\rangle = \sum_n C_n(t)|\psi_n\rangle$

$$i\hbar\sum_n \frac{\partial}{\partial t}C_n(t)|\psi_n\rangle = \sum_n C_n(t)E_n|\psi_n\rangle$$

用 $\langle\psi_m|$ 作用后为

$$i\hbar\frac{\partial}{\partial t}C_m = E_m C_m \Rightarrow C_m(t) = e^{-iE_mt/\hbar}\underbrace{C_m(0)}_{\langle\psi_m|\psi(0)\rangle}$$

$$\Rightarrow |\psi(t)\rangle = \sum_n C_n(0)\, e^{-iE_nt/\hbar}|\psi_n\rangle$$

标准流程:

① 求解 $\hat{H}$ 的本征问题 $\{E_n, |\psi_n\rangle\}$

② 用 $|\psi_n\rangle$ 为基，展开 $|\psi(0)\rangle$

③ 演化系数 $C_n(t) = e^{-iE_n t/\hbar} C_n(0)$ 必考

3. 时间演化算符

$\hat{U}$ → 时间演化算符

令 $|\psi(t)\rangle = \hat{U}|\psi(0)\rangle$

则 $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \Rightarrow i\hbar\frac{\partial}{\partial t}\hat{U}|\psi(0)\rangle = \hat{H}\hat{U}|\psi(0)\rangle$

$\Rightarrow i\hbar\frac{\partial}{\partial t}\hat{U} = \hat{H}\hat{U}$

如果 $\hat{H}$ 不显含时 $\hat{U} = e^{-i\hat{H}t/\hbar}$

(证明时将 $\hat{U}$ 展开, 即 $\hat{U} = \sum_n \left(\frac{-it}{\hbar}\right)^n \frac{\hat{H}^n}{n!}$)

$$\hat{U}|\psi(0)\rangle = \hat{U}\sum_n C_n(0)|\psi_n\rangle = \sum_n C_n(0)e^{-i\hat{H}t/\hbar}|\psi_n\rangle$$
$$= \sum_n C_n(0)e^{-iE_n t/\hbar}|\psi_n\rangle$$

归一化要求

任意时刻 t. $\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\hat{U}^+\hat{U}|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle$

$\Rightarrow \hat{U}^+\hat{U} = \hat{I}$

同理: $\langle\psi(0)|\psi(0)\rangle = \langle\psi(t)|\hat{U}\hat{U}^+|\psi(t)\rangle = \langle\psi(t)|\psi(t)\rangle$

$\Rightarrow \hat{U}\hat{U}^+ = \hat{I}$ (此性质不依赖于 $\hat{H}$ 是否含时)

当 $\hat{H}$ 不含时时, $\hat{U} = e^{-i\hat{H}t/\hbar}$ $\hat{U}^+ = e^{i\hat{H}t/\hbar}$

$\hat{U}^+|\psi(t)\rangle = |\psi(0)\rangle$ (即 $\hat{U}^+$ 为"逆时"算符)

$\hat{H}$ 含时时, 形式解.

$$\hat{U} = \int_0^t \left(-\frac{i}{\hbar}\right)\hat{H}(t')\hat{U}(t')dt' + \hat{I} \quad (\hat{U}(0))$$

通过迭代

$$\Rightarrow \hat{U} = \hat{I} + \int_0^t \left(-\frac{i}{\hbar}\right)\hat{H}(t')dt' + \int_0^t dt'\int_0^{t'} dt''\hat{H}(t')\hat{H}(t'') + \cdots$$
$$= \mathcal{T} e^{-\frac{i}{\hbar}\int_0^{t'}\hat{H}(t')dt'}$$

→ 排序用.

如不同时刻 $\hat{H}$ 对易 $\hat{U} = e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'}$

例 期望值的时间演化

$$\frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle$$

$$= \left(\frac{\partial}{\partial t}\langle\psi(t)|\right)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial}{\partial t}\hat{A}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left(\frac{\partial}{\partial t}|\psi(t)\rangle\right)$$

而 $\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{1}{i\hbar}\hat{H}|\psi(t)\rangle$, $\frac{\partial}{\partial t}\langle\psi(t)| = -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}$

代入后得到:

$$= \frac{1}{i\hbar}\langle\psi(t)|\hat{A}\hat{H}-\hat{H}\hat{A}|\psi(t)\rangle + \langle\frac{\partial}{\partial t}\hat{A}\rangle_{\psi(t)}$$

$$= \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle_{\psi(t)} + \langle\frac{\partial}{\partial t}\hat{A}\rangle_{\psi(t)}$$

Ehrenfest 关系

$$\Longrightarrow i\hbar\frac{\partial}{\partial t}\langle\hat{A}\rangle_{\psi(t)} = \langle[\hat{A},\hat{H}]\rangle_{\psi(t)} + i\hbar\langle\frac{\partial}{\partial t}\hat{A}\rangle_{\psi(t)}$$

例: 在某组基下, $H = \begin{pmatrix} 0 & \frac{A}{2} \\ \frac{A}{2} & 0 \end{pmatrix}$, 初态为 $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, 求任意时刻的态

a. 求 H 的本征问题:

$$E_1 = \frac{A}{2} \quad |\alpha\rangle = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} ; \quad E_2 = -\frac{A}{2} \quad |\beta\rangle = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

则 $\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\sqrt{2}}{2}\left[\frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\right]$

则 t 时刻态为

$$\frac{1}{2}e^{-i\frac{At}{2\hbar}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2}e^{\frac{iAt}{2\hbar}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} \cos\frac{At}{2\hbar} \\ -i\sin\frac{At}{2\hbar} \end{pmatrix}$$

(在 $\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ 基下旋转)

b. 由于 $\hat{H}$ 不含时

$$e^{-i\hat{H}t/\hbar}|\psi(0)\rangle \Rightarrow e^{-i\begin{pmatrix}0 & \frac{A}{2}\\ \frac{A}{2} & 0\end{pmatrix}t/\hbar}\begin{pmatrix}1\\0\end{pmatrix}$$

H 的本征向量为 $\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix}$ $\frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}$

$$S^+ = \frac{\sqrt{2}}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \Rightarrow S = \frac{\sqrt{2}}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

则 $e^{-i\begin{pmatrix}\frac{A}{2} & 0\\ 0 & -\frac{A}{2}\end{pmatrix}t/\hbar} = S^+ e^{i\begin{pmatrix}0 & \frac{A}{2}\\ \frac{A}{2} & 0\end{pmatrix}t/\hbar} S$

守恒量 $i\hbar\frac{\partial\langle\hat{A}\rangle_\psi}{\partial t} = \langle[\hat{A},\hat{H}]\rangle_\psi + \frac{\partial}{\partial t}\langle\hat{A}\rangle_\psi$

若 $\hat{A}$ 不显含时且与 $\hat{H}$ 对易，则 $\hat{A}$ 对应守恒量.

守恒量在体系的任意态上的期望值与几率分布不变.

$[\hat{A},\hat{H}]=0 \Rightarrow$ 共同本征值.

(Ps：假设 $\hat{A}$ 的本征态有 $|\psi_n\rangle$，$|\psi_{m_1}\rangle$ $|\psi_{m_2}\rangle$，则若 $|\psi\rangle = C_1|\psi_n\rangle + C_2|\psi_{m_1}\rangle + C_3|\psi_{m_2}\rangle$

则测到 $\hat{A}$ 为 ψ_m 的概率为 $|C_2|^2 + |C_3|^2$)

4. 三种绘景

a. Schrödiger 绘景

$|\psi(t)\rangle$ 满足 $i\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$

算符 $\hat{A}$ 不随时间演化.

可观测量

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \sum|C_n(t)|^2 A_n$$

b. Heisenberg 绘景

仿照经典力学，令态不演化，力学量随时间演化.

由 $|\psi(0)\rangle_S = |\psi(0)\rangle_H \qquad |\psi(t)\rangle_S = \hat{U}|\psi(0)\rangle_S$

$\Rightarrow |\psi\rangle_H = \hat{U}^+|\psi(t)\rangle_S$

即 $|\psi\rangle_H = |\psi(0)\rangle_S$

为保证 $\langle\psi|\hat{A}|\psi\rangle$ 不变

$${}_H\langle\psi|\hat{A}_H|\psi\rangle_H = {}_S\langle\psi(t)|\hat{U}\hat{A}_H\hat{U}^+|\psi(t)\rangle_S = {}_S\langle\psi(t)|\hat{A}_S|\psi(t)\rangle_S$$

$\Rightarrow \hat{U}\hat{A}_H\hat{U}^+ = \hat{A}_S \Rightarrow \hat{A}_H = \hat{U}^+\hat{A}_S\hat{U}$ （若 $\hat{A}_S$ 不显含时，$\hat{A}_H$ 会含时）

$$\frac{d\hat{A}_H}{dt} = \left(\frac{d}{dt}\hat{U}^+\right)\hat{A}_S\hat{U} + \hat{U}^+\hat{A}_S\left(\frac{d}{dt}\hat{U}\right) + \hat{U}^+\left(\frac{\partial}{\partial t}\hat{A}_S\right)\hat{U}$$

$\hat{U}$ 的演化方程：$i\hbar\frac{d\hat{U}}{dt} = \hat{H}\hat{U}$

则 $\begin{cases} \frac{d}{dt}\hat{U} = \left(-\frac{i}{\hbar}\right)\hat{H}\hat{U} \\ \frac{d}{dt}\hat{U}^+ = \left(\frac{i}{\hbar}\right)\hat{U}^+\hat{H} \end{cases}$

$$\Rightarrow \frac{d\hat{A}_H}{dt} = \frac{i}{\hbar}\hat{U}^+\hat{H}\hat{A}_S\hat{U} - \frac{i}{\hbar}\hat{U}^+\hat{A}_S\hat{H}\hat{U} + \hat{U}^+\left(\frac{\partial}{\partial t}\hat{A}_S\right)\hat{U}$$

$$= \frac{i}{\hbar}\hat{U}^+\hat{H}\hat{U}\hat{U}^+\hat{A}_S\hat{U} - \frac{i}{\hbar}\hat{U}^+\hat{A}_S\hat{U}\hat{U}^+\hat{H}\hat{U} + \hat{U}^+\left(\frac{\partial}{\partial t}\hat{A}_S\right)\hat{U}$$

假设 $\hat{H}$ 不显含时，$\hat{U} = e^{-i\hat{H}t/\hbar} \qquad \hat{U}^+\hat{H}_S\hat{U} = \hat{H}_H = \hat{H}_S$

$$= \frac{i}{\hbar}[\hat{H}, \hat{A}_H] + \left(\frac{\partial}{\partial t}\hat{A}\right)_H$$

$$\Rightarrow i\hbar\frac{d}{dt}\hat{A}_H = [\hat{A}_H, \hat{H}] + i\hbar\left(\frac{\partial}{\partial t}\hat{A}\right)_H$$

Schrödiger 绘景下：

$$i\hbar\frac{d}{dt}\langle\hat{A}\rangle_\psi = \langle[\hat{A}, \hat{H}]\rangle_\psi$$

例：$\hat{H} = \hat{p}^2/2m$. 求 $i\hbar\frac{d}{dt}\hat{x}$ (in Heisenberg's picture).

解: $i\hbar\frac{d}{dt}\hat{x}=[\hat{x},\frac{\hat{p}^2}{2m}]$

$=\frac{i\hbar}{m}\hat{p} \Rightarrow \frac{d\hat{x}}{dt}=\frac{\hat{p}}{m}$

而 $i\hbar\frac{d}{dt}\hat{p}=[\hat{p},\hat{p}^2/2m]=0$ 即 $\hat{p}$ 不演化.

则 $\hat{x}(t)=\hat{x}(0)+\frac{\hat{p}}{m}t$

若考察 $[\hat{x}(t),\hat{x}(0)]\neq 0$. 但 $[\hat{x}(t),\hat{p}(t)]=i\hbar$.

回想经典力学: 时间的演化是正则变换! 保泊松括号

例: $\hat{H}=\hat{p}^2/2m+V(\hat{x})$

$i\hbar\frac{d}{dt}\hat{x}=[\hat{x},\hat{p}^2/2m+V(\hat{x})]=\frac{i\hbar}{m}\hat{p}$

$\Rightarrow \frac{d}{dt}\hat{x}=\hat{p}/m$.

而 $i\hbar\frac{d}{dt}\hat{p}=[\hat{p},\hat{p}^2/2m+V(\hat{x})]$

$=[\hat{p},\sum_n\frac{V^{n}(0)}{n!}\hat{x}^n]$

$=(-i\hbar)\sum\frac{V^{(n)}(0)}{n!}n\hat{x}^{n-1}=-i\hbar[\frac{d}{dt}V(\hat{x})]$

$$\begin{cases}\frac{d}{dt}\hat{p}=-\frac{d}{dx}\hat{V}(x)\\ \frac{d}{dt}\hat{x}=\hat{p}/m\end{cases}\Rightarrow m\frac{d^2\hat{x}}{dt^2}=-\frac{d}{dx}V(\hat{x})$$

(以上为期中考试内容)

C. 相互作用绘景

我们将 $\hat{H}$ 分为两部分: $\hat{H}=\hat{H}_0+\hat{V}$, 其中 $\hat{H}_0$ 为已知部分, $\hat{V}$ 为未知/微扰部分, $\hat{H}_0$ 与 $\hat{V}$ 不对易 这样相当于"先前进 $\hat{H}$, 再后退 $\hat{H}_0$"

定义 $|\psi(t)\rangle_I=e^{i\hat{H}_0t/\hbar}|\psi(t)\rangle_S=e^{i\hat{H}_0t/\hbar}e^{-i\hat{H}t/\hbar}|\psi(0)\rangle_S$

相应的 $\hat{A}_I=e^{i\hat{H}_0t/\hbar}\hat{A}_S e^{-i\hat{H}_0t/\hbar} \Leftarrow$ 保证 ${}_I\langle\psi(t)|\hat{A}_I|\psi(t)\rangle_I$

$={}_S\langle\psi(t)|\hat{A}_S|\psi(t)\rangle_S$

动力学方程

$$\begin{cases} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle_I = \hat{V}_I|\psi(t)\rangle_I \\ i\hbar\frac{d}{dt}\hat{A}_I = [\hat{A}_I, \hat{H}_0] + \left(\frac{\partial \hat{A}}{\partial t}\right)_I \end{cases} \qquad \hat{V}_I = e^{i\hat{H}_0 t/\hbar}\hat{V}_s e^{-i\hat{H}_0 t/\hbar}$$

态的演化由 $\hat{V}$ 驱动，算符的演化由 $\hat{H}_0$ 驱动.

我们仍有: $|\psi(t)\rangle_I = \hat{U}_I|\psi(0)\rangle_I$.

$$i\hbar\frac{d}{dt}\hat{U}_I = \hat{V}_I\hat{U}_I \Rightarrow \hat{U}_I = \hat{I} + \frac{1}{i\hbar}\int_0^t \hat{V}_I(t')\hat{U}_I(t')dt'$$

第六章 坐标表象下的定态问题.

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$$

$$\Rightarrow \sum_n H_{mn}C_n = EC_m$$

$$H_{mn} = \int \psi_m^*(r)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi_n(r)d^3r$$

1. 一维常数势.(分段常数)

$$\psi''(x) + \frac{2m}{\hbar^2}(E-V)\psi(x) = 0$$

① $E>V$, 振荡解.

$$\psi(x) = A\sin kx + B\cos kx, \text{ 或 } Ae^{ikx} + Be^{-ikx}.$$

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$$

② $E<V$, 指数解.

$$\psi(x) = Ae^{kx} + Be^{-kx} \qquad k = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

③ 边界条件:

$|x|\to\infty$ $\psi(x)\to 0$ (束缚态)

$\psi(x)$ 与 $\psi'(x)$ 在边界上连续（如 V 有限）

$$\psi''(x) = -\frac{2m}{\hbar^2}(E-V)\psi(x).$$

在边界 R 处积分.

$$\int_{R^-}^{R^+} \psi''(x)\,dx = \int_{R^-}^{R^+} -\frac{2m}{\hbar^2}(E-V)\psi(x)\,dx$$

$$\Rightarrow \psi''(R^+) - \psi''(R^-) = \lim_{R^+\to R^-} -\frac{2m}{\hbar^2}(E-V)\psi(R)(R^+-R^-)$$

当 V 有限时右边为 0，此时 $\psi'(x)$ 连续

但若 $V \sim \delta(x)$，则 $\psi'(x)$ 不连续

处理问题的一般性流程.

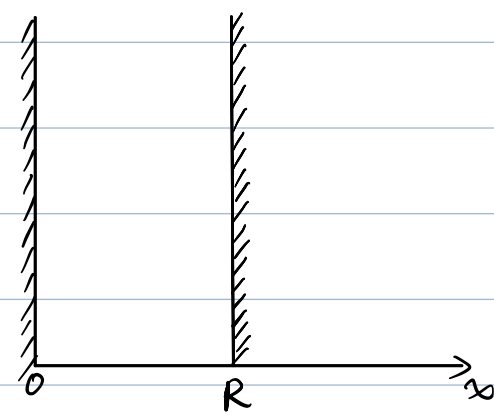
① 分区域写出通解.

② 区配边界条件.

③ 归一化条件.

a. 一维无限深势井.

$$V(x) = \begin{cases} 0, & 0<x<R \\ \infty, & x\le 0,\text{ 或 } x\ge R \end{cases}$$



则 $\psi(x) = A\sin kx + B\cos kx \quad (0<x<R) \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$

由边界条件: $\psi(0) = \psi(R) = 0$

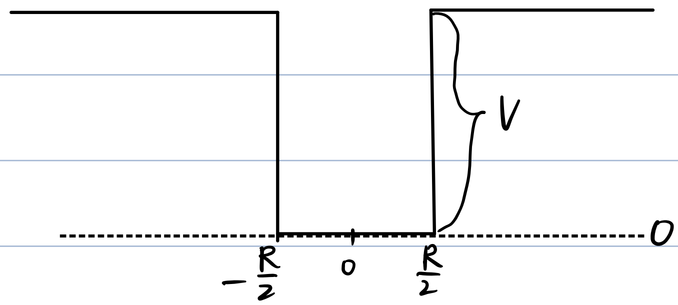
$$\Rightarrow B=0. \quad \sin kR = 0$$

$$\Rightarrow k_n = \frac{n\pi}{R}. \Rightarrow E_n = \frac{n^2\hbar^2\pi^2}{2mR^2}, \quad n=1,2\ldots$$

利用归一化条件 $A = \sqrt{\frac{2}{R}} \qquad \psi_n(x) = \sqrt{\frac{2}{R}}\sin\frac{n\pi}{R}x.$

b. 有限深势阱

$$V(x)=\begin{cases}0, & |x|<\frac{R}{2}\\ V, & |x|>\frac{R}{2}\end{cases}$$



① $E<V$

$|x|>\frac{R}{2}$： $\psi(x)=\begin{cases}Ae^{-Kx}, & x>\frac{R}{2}\\ Ce^{Kx}, & x<-\frac{R}{2}\end{cases}$ $K=\sqrt{\frac{2m(V-E)}{\hbar^2}}$

$|x|<\frac{R}{2}$： $\psi(x)=B\sin(kx+\varphi)$ $k=\sqrt{\frac{2mE}{\hbar}}$

注意到 $V(x)=V(-x)$

且 $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V\psi(x)=E\psi(x)$

$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(-x)+V(-x)\psi(x)=E\psi(-x)$

即 $\psi(-x)$ 也为 Schrödiger 方程的解.

即 $\psi(x)$ 有奇与偶的对称性.

i) 偶宇称 (偶函数)

$\psi(x)=B\cos kx,\ |x|<\frac{R}{2}$.

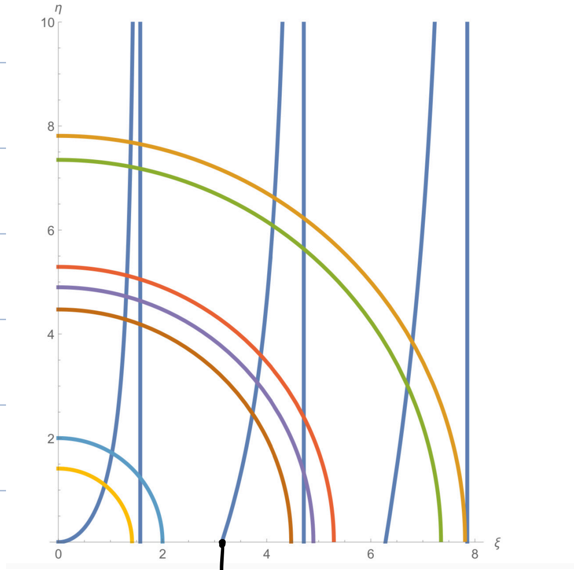
讨论能量 (k, K 量子态 常用方法)：要求 $[\ln\psi(x)]'$ 在边界连续

利用对数导数在 $x=\frac{R}{2}$, $x=-\frac{R}{2}$ 处连续得到：

$k\tan\frac{kR}{2}=K$ 令 $\xi=\frac{kR}{2}$ $\eta=\frac{KR}{2}$

$$\Rightarrow\begin{cases}\xi\tan\xi=\eta\\ \xi^2+\eta^2=\frac{mVR^2}{2\hbar^2}\end{cases}$$

作图如下：



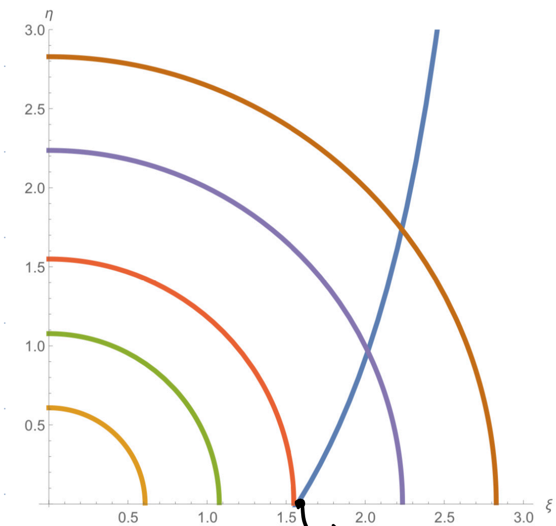
$\xi = \pi$

我们可以看到，不论势井多浅，总有至少一个偶宇称的解，而当V大一个使两曲线在 $(\pi, 0)$ 以右有交点，才有第二个解

ii) 奇宇称（奇函数）

$\psi(x) = B\sin kx, \quad |x| < \frac{R}{2}$

$\Rightarrow \quad -k\cot\frac{kR}{2} = K \quad \Rightarrow \quad \begin{cases} -\xi\cot\xi = \eta \\ \xi^2 + \eta^2 = \frac{mVR^2}{2\hbar^2} \end{cases}$



$\frac{\pi}{2}$

我们注意到 $V \geq \frac{\pi^2\hbar^2}{2mR^2}$ 时，才有第一个奇宇称的束缚态的解

宇称的讨论（对称性）

$\hat{P}\psi(x) = \psi(-x) \qquad \hat{P}$：宇称算符

$\hat{P}^2 = \hat{I}, \quad \hat{P}^+ = \hat{P}$

利用 $\hat{P}|\psi\rangle = \lambda|\psi\rangle \Rightarrow \hat{P}^2|\psi\rangle = \lambda^2|\psi\rangle = |\psi\rangle$

$\lambda^2 = \pm 1 \Rightarrow \hat{P}$ 的本征态为奇/偶函数.

若$\hat{H}$有宇称对称性，我们有 $\hat{P}\hat{H}\hat{P}^{-1}=\hat{H}$

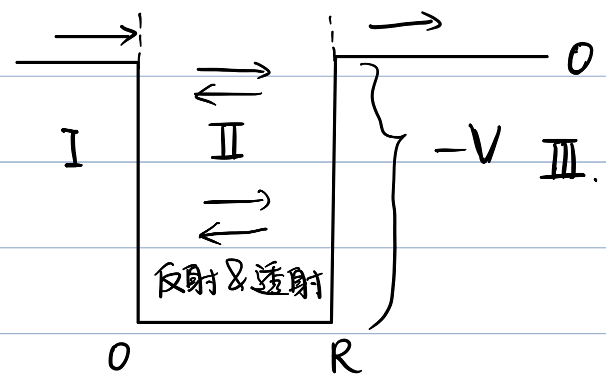
即 $[\hat{H},\hat{P}]=0 \Rightarrow \hat{H},\hat{P}$有共同本征态

而$\hat{P}$的本征态为奇、偶函数 $\Rightarrow$ $\hat{H}$的本征态也为奇/偶函数.

(若有简并，则利用线性组合)

可以查阅"对称性自发破缺"

② $E>V$，散射态，为方便讨论，我们挪动坐标系

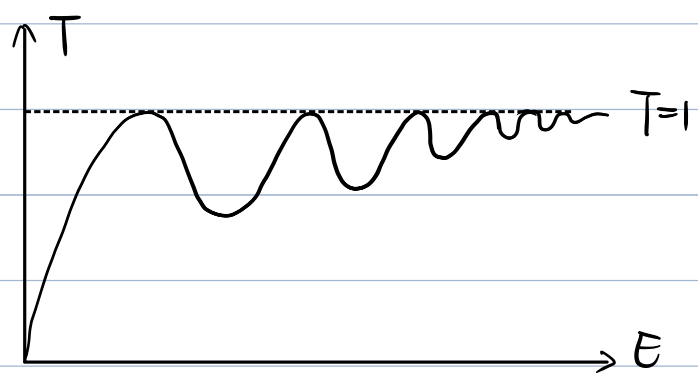


$$\psi(x)=\begin{cases} e^{ikx}+Re^{-ikx}, & \text{I.} \\ Ae^{ik'x}+Be^{-ik'x}, & \text{II.} \\ Se^{ikx}, & \text{III.} \end{cases}$$

$$k=\sqrt{\frac{2mE}{\hbar^2}} \qquad k'=\sqrt{\frac{2m(E+V)}{\hbar^2}}$$

由 $x=0, R$处 $\frac{\psi'}{\psi}$ 连续，求解得

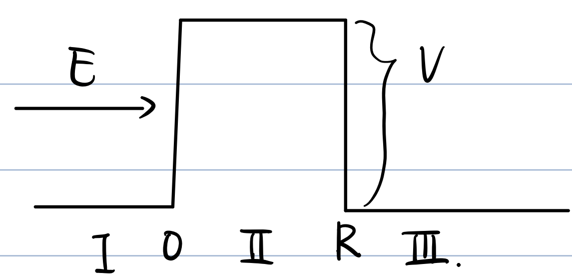
$$T=|S|^2=\left[1+\frac{\sin^2 k'R}{4\frac{E}{V}(1+\frac{E}{V})}\right]^{-1}$$



$$E=-V+\frac{n^2\pi^2\hbar^2}{2mR^2}$$

即当有驻波条件时，发生相干相消，透射率为1.

C. 方势垒



$$V(x)=\begin{cases} V, & 0<x<R \\ 0, & \text{else.} \end{cases}$$

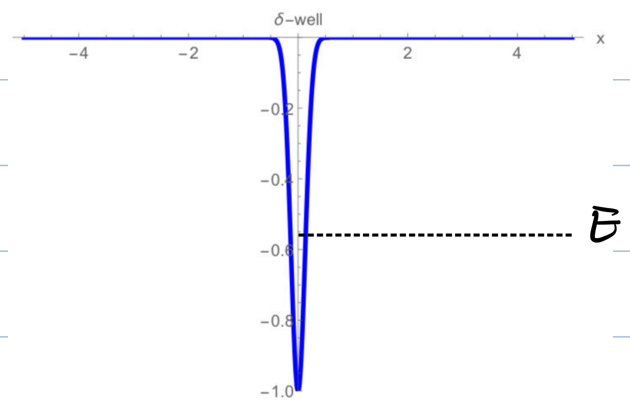
$$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx}, & \mathrm{I} \\ Ae^{Kx} + Be^{-Kx}, & \mathrm{II}. \\ Se^{ikx}, & \mathrm{III}. \end{cases}$$

$k = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad K = \sqrt{\frac{2m(V-E)}{\hbar^2}}$

由 $x=0, R$ 处 $\frac{\psi'}{\psi}$ 连续

$$T = |S|^2 = \left[1 + \frac{1}{\frac{E}{V}(1-\frac{E}{V})} \sinh^2 KR\right]^{-1}$$

2. 一维 δ 势阱



$V(x) = -\gamma\delta(x)$ $\quad (\gamma > 0)$

$\psi'(0^+) - \psi'(0^-) = -\frac{2m}{\hbar^2}\gamma\psi(0)$

对 $x \neq 0$, $\psi'' = -\frac{2mE}{\hbar^2}\psi$

设 $k = \sqrt{\frac{-2mE}{\hbar^2}}$ $\quad (E<0)$

则 $\psi(x) \propto e^{-k|x|}$

① 偶宇称: $\psi(x) = \begin{cases} Ae^{-kx}, & x>0 \\ Ae^{kx}, & x<0 \end{cases}$

加上边界条件: $k = \frac{m\gamma}{\hbar^2} \Rightarrow E = -\frac{m\gamma^2}{2\hbar^2}$

只有一个解.

由归一化条件: $\int_{-\infty}^{+\infty} |\psi(x)|^2 = 1 \Rightarrow A = \sqrt{k}$

$\psi(x) = \sqrt{k}\, e^{-k|x|}$

② 奇宇称: $\psi(x) = \begin{cases} Be^{-kx}, & x>0 \\ -Be^{kx}, & x<0 \end{cases}$

在 $x=0$ 处连续 $\Rightarrow$ $B=0$，因此不存在奇宇称解.

注：δ 势可以用来近似只有很小距离才会有很大势能的情况.

3. 一维谐振子问题.

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi(x)=E\psi(x)$$ 无量纲化

定义 $\alpha=\sqrt{\frac{m\omega}{\hbar}}$ 则 $\xi=\alpha x$ 为无量纲的长度.

定义 $\lambda=E/\frac{1}{2}\hbar\omega$ 为无量纲的能量.

则 $H\psi(x)=E\psi(x)$

$$\Rightarrow \frac{2}{\hbar\omega}\left(-\frac{\hbar^2}{2m}\right)\alpha^2\frac{d^2}{d(\alpha x)^2}\psi=\frac{E}{\frac{1}{2}\hbar\omega}-\frac{1}{2}m\omega^2\frac{1}{\alpha^2}(\alpha x)^2\frac{2}{\hbar\omega}$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2}+(\lambda-\xi^2)\psi=0$$

渐近行为

$\xi\to\pm\infty$ $\Rightarrow$ $\frac{d^2\psi}{d\xi^2}=\xi^2\psi$ $\quad\psi\sim Ae^{-\frac{1}{2}\xi^2}+Be^{\frac{1}{2}\xi^2}$

令 $\psi=e^{-\frac{1}{2}\xi^2}\mu(\xi)$

代入 $\psi(x)$ 的方程，得到关于 $\mu(\xi)$ 的方程.

$$\frac{d^2\mu}{d\xi^2}-2\xi\frac{d\mu}{d\xi}+(\lambda-1)\mu=0$$ $\longrightarrow$ 厄米方程.

解得 $H_n(\xi)=(-1)^n e^{\xi^2}\frac{d^n}{dx^n}(e^{-\xi^2})$ $\longrightarrow$ 厄米多项式

级数解法：

令 $\mu(\xi)=\sum_{k=0}^{\infty} C_k \xi^k$，$|\xi|<\infty$

代入方程可以得到系数的递推关系为

$$C_{k+2}=\frac{2k-\lambda+1}{(k+1)(k+2)}C_k$$

$k\to\infty$ 时，$C_{k+2}\sim\frac{2}{k}C_k \Rightarrow C_k\sim\frac{1}{(\frac{k}{2})!}$

$$\Rightarrow \mu(\xi)\sim\sum_{k=0}^{\infty}\frac{1}{(\frac{k}{2})!}\xi^{2(\frac{k}{2})}=e^{\xi^2}$$

但这样的话 $\psi\sim e^{-\frac{1}{2}\xi^2}e^{\xi^2}=e^{\frac{1}{2}\xi^2}$ 发散.

因此级数必须被截断，否则会发散.

考察 $C_{k+2}=\frac{2k-\lambda+1}{(k+1)(k+2)}C_k$，可以让 $(2k-\lambda+1)=0$ 或 $C_0=0$

截断方式：

$\underbrace{\lambda=2k+1}$ 若 k 在取奇数满足时，令 $C_0=0$

只能满足奇或偶 若 k 在取偶数满足时，令 $C_1=0$.

截断，另一个数列靠首项 $=0$

则 $E/\frac{1}{2}\hbar\omega=\lambda=2k+1 \Rightarrow E_k=(k+\frac{1}{2})\hbar\omega$；$k=0,1,2\ldots$

$\psi_k(x)=\underbrace{N_k}_{\text{归一化系数}}e^{-\frac{1}{2}\xi^2}H_k(\xi)$

三维情况则为 x,y,z 方向的厄米多项式 $|n_x,n_y,n_z\rangle$

球坐标下我们用球谐函数 + 广义 Laguerre 多项式求解

$Y_l^m(\theta,\varphi)$ L_n^l

$$E_{nl}=(\underbrace{2n+l}_{N=n_x+n_y+n_z}+\frac{3}{2})\hbar\omega$$