① 算符的运算性质

$$e^{\lambda A} B e^{-\lambda A} = \sum_{i=0}^{+\infty} \frac{1}{i!}[A^{(i)}, B]\lambda^i = F(\lambda)$$

证明如下

$$\frac{dF(\lambda)}{d\lambda} = e^{\lambda A}(AB-BA)e^{-\lambda A} = e^{\lambda A}[A,B]e^{-\lambda A}$$

$$\frac{d^2F(\lambda)}{d\lambda} = e^{\lambda A}[A,[A,B]]e^{-\lambda A}$$

$\vdots$

对 $F(\lambda)$ 作泰勒展开 $F(\lambda) = \sum_{i=0}^{+\infty} \frac{1}{i!}\left(\frac{d^iF}{d\lambda^i}\right)_{\lambda=0}\lambda^i = \sum_{i=0}^{+\infty} \frac{1}{i!}[A^{(i)}, B]\lambda^i$

② $|x\rangle = e^{-\frac{i}{\hbar}\hat{p}x}|0_x\rangle \quad |p\rangle = e^{\frac{i}{\hbar}\hat{x}p}|0_p\rangle$

$$\langle x|p\rangle = \langle 0_x| e^{\frac{i}{\hbar}\hat{p}x} e^{\frac{i}{\hbar}\hat{x}p}|0_p\rangle = e^{\frac{i}{\hbar}px}\underline{\langle 0_x| e^{\frac{i}{\hbar}\hat{x}p}}|0_p\rangle = e^{\frac{i}{\hbar}px}\langle 0_x|0_p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$$

$$\delta(p'-p) = \langle p'|p\rangle = \int \langle p'|x\rangle\langle x|p\rangle dx = |\langle 0_x|0_p\rangle|^2 \int e^{-\frac{i}{\hbar}p'x} e^{\frac{i}{\hbar}px} dx = 2\pi\hbar\,\delta(p-p')|\langle 0_x|0_p\rangle|^2$$

证明 $\hat{p}\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi(x)$

$$\hat{p}\psi(x) = \langle x|\hat{p}|\psi\rangle = \langle 0_x| e^{\frac{i\hat{p}x}{\hbar}}\hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\langle 0_x| e^{\frac{i\hat{p}x}{\hbar}}|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x)$$

③ 角动量算符与角动量表象

$\vec{L} = \vec{R}\times\vec{p}$

$[\hat{L}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}L_k \;,\; [\hat{L}_i, \hat{L}^2] = 0$

$J^2|\lambda m\rangle = \lambda\hbar^2|\lambda m\rangle \longrightarrow J^2$ 与 J_z 共同本征态

$J_z|\lambda m\rangle = m\hbar|\lambda m\rangle$

$J_\pm = J_x \pm iJ_y \qquad [J^2, J_\pm] = 0 \qquad [J_z, J_\pm] = \pm\hbar J_\pm$

$J_z J_\pm|\lambda m\rangle = (\pm\hbar J_\pm + J_\pm m\hbar)|\lambda m\rangle = \hbar(m\pm1)J_\pm|\lambda m\rangle$

则 $J_\pm|\lambda m\rangle = C_\pm|\lambda\, m\pm1\rangle$ 　λ 写成 $\lambda = j(j+1)$

$\therefore J_\pm|jm\rangle = \sqrt{(j\mp m)(j\pm m+1)}\,|j\,(m\pm1)\rangle$

虚数单位

$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$

$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$

$\{\sigma_i, \sigma_j\} = 2i\delta_{ij}$

④ 定态薛定谔方程

变分法 猜一个解代入进去算

一维谐振子

$$\hat H = \frac{\hat p^2}{2m} + \frac{1}{2}m\omega^2\hat x^2 \qquad a^\pm = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat x \mp i\hat p)$$

$$\hat x = \sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)$$

$$\hat p = i\sqrt{\frac{m\omega\hbar}{2}}\,(a^\dagger - a)$$

$$\hat H = \hbar\omega(\underbrace{a^\dagger a}_{\text{粒子数算符 } \hat N} + \frac{1}{2})$$

$$[a, a^\dagger] = 1$$

$$[H, a] = \hbar\omega[a^\dagger a, a] = \hbar\omega[a^\dagger, a]a = -\hbar\omega a$$

$$[H, a^\dagger] = \hbar\omega a^\dagger$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad a^\dagger = \sum_{n=0}^{+\infty}\sqrt{n+1}\,|n+1\rangle\langle n|$$

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \qquad a = \sum_{n=0}^{+\infty}\sqrt{n}\,|n-1\rangle\langle n|$$

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

能量表象上看谐振子

① 将 $\hat H$ 与 $\hat x, \hat p$ 对易式求出来

$$[\hat H, \hat x] = \frac{1}{2m}[\hat p^2, \hat x] = \frac{1}{2m}(\hat p[\hat p, \hat x] + [\hat p, \hat x]\hat p) = -\frac{i\hbar}{m}\hat p$$

$$[\hat H, \hat p] = \frac{1}{2}m\omega^2[\hat x^2, \hat p] = m\omega^2 i\hbar\hat x$$

$$H_{ij} = \delta_{ij}E_i$$

$$\therefore\ H_{ij}x_{ij} - x_{ij}H_{ij} = -\frac{i\hbar}{m}p_{ij}$$

$$(E_j - E_i)\,x_{ij} = -\frac{i\hbar}{m}p_{ij}$$

$$(E_j - E_i)\,p_{ij} = m\omega^2 i\hbar\, x_{ij}$$

$$a|z\rangle = z|z\rangle$$

$$|z\rangle = \sum_{n=0}^{+\infty} C_n|n\rangle$$

$$a = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat x + i\hat p)$$

$$a|z\rangle = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat x + i\hat p)|z\rangle = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega x_0 + p_0)|z\rangle$$

$$\therefore\ \frac{1}{\sqrt{2m\omega\hbar}}(m\omega(\hat x - x_0) + i(\hat p - p_0))|z\rangle = 0$$

$$\therefore\ \langle x|z\rangle = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega(x - x_0))\langle x|z\rangle + \frac{1}{\sqrt{2m\omega\hbar}}\,i\,\langle x|\hat p - p_0|z\rangle = 0$$

$\langle x|\hat p - p_0|z\rangle = (-i\hbar\frac{\partial}{\partial x} - p_0)\langle x|z\rangle$ 解微分方程即可

能量表象下 $|z\rangle = \sum_{n=0}^{+\infty} C_n|n\rangle$

$$a|z\rangle = \sum_{n=1}^{+\infty} C_n\sqrt{n}\,|n-1\rangle = \sum_{n=0}^{+\infty} C_{n+1}\sqrt{n+1}\,|n\rangle = z\sum_{n=0}^{+\infty} C_n|n\rangle$$

$$\therefore\ C_{n+1}\sqrt{n+1} = zC_n$$

$$\therefore\ C_{n+1} = \frac{zC_n}{\sqrt{n+1}},\quad C_n = \frac{z^n C_0}{\sqrt{n!}}$$

$\therefore\ |z\rangle = \sum_{n=0}^{+\infty}\frac{z^n C_0}{\sqrt{n!}}|n\rangle$ 而 $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$

$$\therefore\ |z\rangle = C_0\sum_{n=0}^{+\infty}\frac{(za^\dagger)^n}{n!}|0\rangle = \underbrace{C_0 e^{za^\dagger}|0\rangle}_{\text{本征态}}$$

$$a\hat Q|z\rangle = (z + \lambda)\hat Q|z\rangle$$

$$[a, \hat Q] = \lambda\hat Q$$

取 $\hat Q = e^{-\frac{i}{\hbar}\hat p\lambda}$

$$\therefore\ [a, \hat Q] = \frac{1}{\sqrt{2m\omega\hbar}}m\omega[\hat x, e^{-\frac{i}{\hbar}\hat p\lambda}] = \lambda\sqrt{\frac{m\omega}{2\hbar}}\, i\hbar \cdot -\frac{i}{\hbar}\hat Q(\lambda) = \lambda\sqrt{\frac{m\omega}{2\hbar}}\hat Q(\lambda)$$

$$\therefore\ a\hat Q|z\rangle = (\hat Q a + \lambda\sqrt{\frac{m\omega}{2\hbar}}\hat Q(\lambda))|z\rangle = (z + \lambda\sqrt{\frac{m\omega}{2\hbar}})\hat Q(\lambda)|z\rangle$$

例 $f=\hat{x}+a\hat{p}$ 本征态为 $|x_0\rangle$ 计算 $e^{-i\hat{p}\lambda/\hbar} f e^{i\hat{p}\lambda/\hbar}$

$$e^{\lambda A} B e^{-\lambda A} = \sum_{i=0}^{+\infty} \frac{1}{i!} [A^{(i)}, B] \lambda^i$$

$A=-\frac{i\hat{p}}{\hbar}$ $B=\hat{x}+a\hat{p}$

$[\hat{A},\hat{B}] = -\frac{i}{\hbar}\cdot -i\hbar = -1$

$[\hat{A},[\hat{A},\hat{B}]]=0$ $e^{-\frac{i\lambda\hat{p}}{\hbar}} f e^{\frac{i\lambda\hat{p}}{\hbar}}$

$\therefore$ 上式 $= \hat{x}+a\hat{p}-\lambda$

(2) 证明 $e^{-i\hat{p}\lambda/\hbar}|x_0\rangle$ 是 f 的本征态

$f|x_0\rangle = x_0|x_0\rangle$

$[f, e^{-i\hat{p}\lambda/\hbar}] = i\hbar\frac{\partial}{\partial p} e^{-i\hat{p}\lambda/\hbar} = \lambda e^{-i\hat{p}\lambda/\hbar}$

$\therefore$ $f e^{-i\hat{p}\lambda/\hbar}|x_0\rangle = e^{-i\hat{p}\lambda/\hbar} x_0|x_0\rangle + \lambda e^{-i\hat{p}\lambda/\hbar}|x_0\rangle = (x_0+\lambda) e^{-i\hat{p}\lambda/\hbar}|x_0\rangle$

故 $e^{-i\hat{p}\lambda/\hbar}|x_0\rangle$ 是 f 的本征态

微扰法

$H = H_0 + \lambda H_1 + \cdots \lambda^n$

$E_n^1 = \langle\psi_0|H_1|\psi_0\rangle$ 一阶

Summary

$|x\rangle = e^{-i\hat{p}x/\hbar}|0_x\rangle$ $|p\rangle = e^{i\hat{x}p/\hbar}|0_p\rangle$ 谐振子能量表象展开 $\sum_{n=0}^{+\infty}\langle n|n\rangle$

证明本征值可以取任意实数 构造 $\hat{Q}(\lambda) = e^{-i\hat{p}\lambda/\hbar}$

$$e^{\lambda A} B e^{-\lambda A} = \sum_{i=0}^{+\infty} \frac{1}{i!} [A^{(i)}, B] \lambda^i$$

$$[A^{(i)}, B] = \underbrace{[A,[A\cdots[A}_{i},B]]]$$

但当出现 $e^{-i\hat{p}\lambda/\hbar} g e^{i\hat{p}\lambda/\hbar}$ 时可以将其作用到 $|x\rangle$ 上

运动方程 $i\hbar\frac{\partial}{\partial t}\psi(t) = \hat{H}\psi(t)$

时间演化算符

$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$

$U(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t)dt}$

绘景变换 (Picture)

态矢的演化 —— 薛定谔绘景 $i\hbar\frac{\partial}{\partial t}|\psi\rangle_s = \hat{H}_s|\psi\rangle_s$

算符的演化 —— 海森堡绘景 $|\psi\rangle_H = U^{-1}(t,0)|\psi\rangle_s = |\psi(0)\rangle_s$

$\hat{H}_H = U^{-1}(t,0)\hat{H}_s U(t,0)$ (H不含时)

$$i\hbar\frac{\partial}{\partial t}A^H(t) = i\hbar\frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}Ht}A^s e^{-\frac{i}{\hbar}Ht}\right) = -e^{\frac{i}{\hbar}Ht}HAe^{-\frac{i}{\hbar}Ht} + e^{\frac{i}{\hbar}Ht}AHe^{-\frac{i}{\hbar}Ht} = H_H - A_H + A_H H_H = -[H_H, A_H]$$

得到海森伯方程 $i\hbar\frac{\partial}{\partial t}A^H(t) = -[H^H, A^H(t)]$

如何写出海森伯绘景下的算符表达

① 写出时间演化算符 $\hat{F}^H = U^{-1}(t)\hat{F}^S U(t)$

or 通过海森堡方程直接得出

例: $\hat{H} = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2 + mgx$ 求 $x^H(t)$, $p^H(t)$

$i\hbar\dot{x}^H(t) = [x^H(t), \hat{H}^H] = \frac{1}{2m}[x^H(t), p^{H2}(t)] = \frac{1}{m}i\hbar p^H(t)$

$\therefore \dot{x}^H(t) = \frac{1}{m}p^H(t)$

$i\hbar\dot{p}^H(t) = [p^H(t), H^H] = [p^H(t), \frac{1}{2}mw^2x_H^2 + mgx_H] = mw^2 - i\hbar x_H(t) - i\hbar mg$

$\dot{p}^H(t) = -mw^2 x_H(t) - mg$

$\ddot{p}^H(t) = -\cancel{m}w^2 p^H(t)$

谐振子 $a^H(t)$ 咋算

↓

套 Heisenberg方程

谐振子相干态

$|z\rangle = D(z)|0\rangle$

↓

$D(z) = e^{zA^\dagger - z^*A}$ $e^Ae^Be^{-\frac{1}{2}[A,B]} = e^{A+B}$

$\therefore D(z) = e^{zA^\dagger}e^{-z^*A}e^{-\frac{1}{2}|z|^2 \cdot 1 \cdot -1}$

$\therefore |z\rangle = e^{-\frac{1}{2}|z|^2}e^{zA^\dagger}|0\rangle = e^{-\frac{1}{2}|z|^2}\frac{1}{C_0}|z\rangle$, $C_0 = e^{-\frac{1}{2}|z|^2}$

而 $|z\rangle=\sum_{n=0}^{+\infty}C_n|n\rangle \qquad C_n=\frac{z^n C_0}{\sqrt{n!}}$

$$=e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}|n\rangle$$

$$|z(t)\rangle=e^{-i\omega t a^\dagger a}|z\rangle$$

$$|z(t)\rangle=e^{-i\omega t\hat{n}}e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}|n\rangle=e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}(e^{-i\omega t})^n|n\rangle=e^{-\frac{1}{2}|ze^{-i\omega t}|^2}\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}(e^{-i\omega t})^n|n\rangle=|ze^{-i\omega t}\rangle$$

关心其位置 $\langle x|z(t)\rangle$

$$x'=\sqrt{\frac{m\omega}{\hbar}}x$$

$$a^\dagger+a=\sqrt{2}X',\ X'|x'\rangle=x'|x'\rangle$$

$$e^{za^\dagger}=e^{(\sqrt{2}X'-a)z}=e^{\sqrt{2}zX'}e^{-az}e^{-\frac{1}{2}z^2}$$

$$\langle x'|z\rangle=\langle x'|e^{-\frac{1}{2}|z|^2}e^{\sqrt{2}zX}e^{-az}e^{-\frac{1}{2}z^2}|0\rangle=e^{-\frac{1}{2}(|z|^2+z^2)}\langle x'|e^{\sqrt{2}zX'}e^{-az}|0\rangle=e^{-\frac{1}{2}(|z|^2+z^2)}e^{\sqrt{2}zX'}\langle x|0\rangle\rightarrow\psi_0(x')$$

$$\psi_0(x')=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{1}{2}x'^2}$$

$$\therefore\langle x'|z\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{1}{2}(|z|^2+z^2)}e^{\sqrt{2}zx'}e^{-\frac{1}{2}x'^2}$$

例：证明 $\langle z(t)|X|z(t)\rangle=\sqrt{\frac{2\hbar}{m\omega}}|z|\cos(\omega t+\varphi)$?

先求 $\langle z|X|z\rangle \qquad |z\rangle=e^{-\frac{1}{2}|z|^2}e^{za^\dagger}|0\rangle$

$$\langle z'|z\rangle=e^{-\frac{1}{2}(|z|^2+|z'|^2)}\langle 0|e^{z'^*a}e^{za^\dagger}|0\rangle=e^{-\frac{1}{2}(|z|^2+|z'|^2)}\langle 0|e^{za^\dagger+z'^*a}e^{+\frac{1}{2}zz'^*}|0\rangle=e^{-\frac{1}{2}(|z|^2+|z'|^2)}\langle 0|e^{za^\dagger}e^{z'^*a}e^{zz'^*}|0\rangle$$

$$=e^{-\frac{1}{2}(|z|^2+|z'|^2+2zz'^*)}$$

---

§ 密度矩阵

纯态 $\rho=|\psi\rangle\langle\psi|$

混态 $\rho=\sum_i p_i|\psi\rangle\langle\psi|=\sum_i|\psi_i\rangle p_i\langle\psi_i|$

$$\langle A\rangle=\sum_n\sum_i p_i\langle\psi_i|n\rangle\langle n|A|\psi_i\rangle=\sum_n\langle n|A[\sum_i|\psi_i\rangle p_i\langle\psi_i|]|n\rangle=tr(A\rho)$$

$$\langle A\rangle=\sum_i p_i\langle\psi_i|A|\psi_i\rangle$$

刘维尔方程

$$i\hbar\frac{\partial}{\partial t}\rho=\sum_i p_i i\hbar\frac{\partial}{\partial t}|\psi\rangle\langle\psi|=\sum_i p_i\left[\left(i\hbar\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi|+\left(i\hbar|\psi\rangle\frac{\partial}{\partial t}\langle\psi|\right)\right]=\sum_i p_i\left(\hat{H}|\psi\rangle\langle\psi|-|\psi\rangle\langle\psi|\hat{H}\right)=[\hat{H},\rho]$$

(薛定谔绘景)

$$tr(\rho)=\sum_n\sum_i\langle n|\psi_i\rangle p_i\langle\psi_i|n\rangle=\sum_i\langle\psi_i|\psi_i\rangle p_i=1$$

§ 约化密度矩阵

粒子1，2各有一组基矢 $\{|\varphi_i^1\rangle\}$，$\{|\varphi_i^2\rangle\}$

则 $|\psi\rangle=\sum_i\sum_j|\varphi_i^1\rangle|\varphi_j^2\rangle C_{ij}$

系数应满足 $\sum_i\sum_j|C_{ij}|^2=1$

$$\rho=\sum_{ii'}\sum_{jj'}|\varphi_i^1\rangle|\varphi_j^2\rangle C_{ij}C_{i'j'}^*\langle\varphi_{i'}^1|\langle\varphi_{j'}^2|$$

只关心粒子1的某物理量均值

$$\langle F(1)\rangle=\underline{tr}(F(1)\rho)$$

$$=\sum_{ii'}\sum_{jj'}\langle\varphi_i^1|\langle\varphi_j^2|F(1)\rho|\varphi_j^2\rangle|\varphi_i^1\rangle=\sum_{ii'}\langle\varphi_i^1|F(1)|\varphi_{i'}^1\rangle\underbrace{\sum_j\langle\varphi_{i'}^1|\langle\varphi_j^2|\rho|\varphi_j^2\rangle|\varphi_i^1\rangle}_{tr_2(\rho)=\rho(1)}=tr_1(F(1)\rho(1))$$

例 $\rho_{AB}=|01\rangle\langle 01|$

求 ρ_A

$\rho_A=tr_B(\rho_{AB})=(I\otimes\langle 0|)\rho_{AB}(I\otimes|0\rangle)+(I\otimes\langle 1|)\rho_{AB}(I\otimes|1\rangle)$

$=|0\rangle\langle 0|$

已知混态 $|\psi\rangle=\frac{\sqrt{3}}{3}(|001\rangle+|011\rangle+|111\rangle)$ $\rho_{123}=\frac{1}{3}(|001\rangle+|011\rangle+|111\rangle)(\langle 001|+\langle 011|+\langle 111|)=\frac{1}{3}(|001\rangle\langle 001|+|001\rangle\langle 011|+|001\rangle\langle 111|+|011\rangle\langle 011|+|111\rangle\langle 111|+|011\rangle\langle 001|+|011\rangle\langle 111|$

$+|111\rangle\langle 001|+|111\rangle\langle 011|)$

求 ρ_1，$\rho_1=tr_{23}(\rho_{123})=(I\otimes\langle 0|\otimes\langle 0|\rho_{123}I\otimes|0\rangle\otimes|0\rangle)+(I\otimes\langle 0|\otimes\langle 1|\rho_{123}I\otimes|0\rangle\otimes|1\rangle)$

$+(I\otimes\langle 1|\otimes\langle 0|\rho_{123}|I\otimes|1\rangle\otimes|0\rangle)+(I\otimes\langle 1|\otimes\langle 1|\rho_{123}I\otimes|1\rangle\otimes|1\rangle)$

$=\frac{1}{3}(|0\rangle\langle 0|)+\frac{1}{3}(|0\rangle\langle 0|+|1\rangle\langle 1|)=\frac{2}{3}|0\rangle\langle 0|+\frac{1}{3}|1\rangle\langle 1|+\frac{1}{3}|0\rangle\langle 1|+\frac{1}{3}|1\rangle\langle 0|$

$+\frac{1}{3}|0\rangle\langle 1|+\frac{1}{3}|1\rangle\langle 0|$

对称性理论

§空间对称变换

平移变换 ——→ 动量守恒

$\hat{D}|x\rangle=|x+\lambda\rangle$

$\hat{D}\psi(x)=\langle x|\hat{D}|\psi\rangle=\int dx'\langle x|\hat{D}|x'\rangle\langle x'|\psi\rangle=\int dx'\langle x|x'+\lambda\rangle\langle x'|\psi\rangle=\psi(x-\lambda)$

$$\hat{D}_\lambda=e^{-i\hat{p}\lambda/\hbar}$$

$\hat{x}\longrightarrow$ 平移变换之后 $\hat{D}_\lambda\hat{x}\hat{D}_\lambda^{-1}|x\rangle=\hat{D}_\lambda\hat{x}|x-\lambda\rangle=(x-\lambda)|x\rangle=(\hat{x}-\lambda\hat{I})|x\rangle$

$\langle x|\hat{D}_\lambda|p\rangle=\langle x-\lambda|p\rangle=\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}p(x-\lambda)}=e^{-\frac{i}{\hbar}p\lambda}\langle x|p\rangle$

$\therefore\hat{D}_\lambda|p\rangle=e^{-ip\lambda/\hbar}|p\rangle$

注意插入 $\hat{D}_\lambda^{-1}\hat{D}_\lambda$

$\hat{D}_\lambda\hat{p}\hat{D}_\lambda^{-1}|p\rangle=\hat{D}_\lambda\hat{p}e^{ip\lambda/\hbar}|p\rangle=\hat{p}|p\rangle$

$\hat{D}_\lambda\hat{L}\hat{D}_\lambda^{-1}=\hat{D}_\lambda\varepsilon_{ijk}\hat{x}_i\hat{p}_j\hat{D}_\lambda^{-1}=\varepsilon_{ijk}\hat{D}_\lambda\hat{x}_i\hat{D}_\lambda^{-1}\hat{D}_\lambda\hat{p}_j\hat{D}_\lambda^{-1}=\varepsilon_{ijk}(\hat{x}_i-\lambda)\hat{p}_j=\hat{L}-\vec{\lambda}\times\hat{\vec{p}}$

$\hat{D}_{d\lambda}=1-\frac{i}{\hbar}\hat{p}\,d\lambda$（无限小平移变换）

$\hat{D}_\lambda=\lim_{N\to+\infty}(1-\frac{i}{\hbar}\hat{p}\,d\lambda)^N=e^{-\frac{i}{\hbar}\hat{p}\lambda}$

空间反演

$\hat{P}|x\rangle=|-x\rangle$

$\langle x|\hat{P}|p\rangle=\langle -x|p\rangle=\frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}=\langle x|-p\rangle$

$\langle x|\hat{P}|\psi\rangle=\int dx'\langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle=\psi(-x)$

$\hat{P}|p\rangle=|-p\rangle$

则空间反演变换下

$\hat{P}\hat{x}\hat{P}^{-1}|x\rangle = \hat{P}\hat{x}|-x\rangle = -x|x\rangle = -\hat{x}|x\rangle$

$\hat{P}p\hat{P}^{-1}|p\rangle = -\hat{p}|p\rangle$

$\hat{P}\hat{L}\hat{P}^{-1} = \varepsilon_{ijk}\hat{P}\hat{x}_i\hat{p}_j\hat{P}^{-1} = \varepsilon_{ijk}\hat{P}\hat{x}_i\hat{P}^{-1}\hat{P}\hat{p}_j\hat{P}^{-1} = \varepsilon_{ijk}\hat{x}_i\hat{p}_j = \hat{L}$

若 $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

$\hat{P}\hat{H}\hat{P}^{-1} = \frac{1}{2m}\hat{P}\hat{p}^2\hat{P}^{-1} + \frac{1}{2}m\omega^2\hat{P}\hat{x}^2\hat{P}^{-1} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

$|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|0\rangle$

$\hat{P}\hat{a}^+\hat{P}^{-1} = -\hat{a}^+$

$\therefore \hat{P}|n\rangle = \frac{1}{\sqrt{n!}}\hat{P}(a^+)^n\hat{P}^{-1}\hat{P}|0\rangle = \frac{1}{\sqrt{n!}}(-1)^n(a^+)^n|0\rangle = (-1)^n|n\rangle$

空间转动

Rodrigues' rotation formula

$\vec{V}_{rot} = \vec{V}\cos\theta + (\vec{K}\times\vec{V})\sin\theta + \vec{K}(\vec{K}\cdot\vec{V})(1-\cos\theta)$ （$\vec{K}$为转轴方向单位向量）

无限小转动 $\underset{\text{绕}\hat{n}\text{转}d\varphi}{\hat{D}(\hat{n}d\varphi)} = 1 - \frac{i}{\hbar}d\varphi\,\hat{n}\cdot\underset{\text{角动量}}{\hat{L}}$, $\hat{D}(\hat{n}\varphi) = e^{-\frac{i}{\hbar}\varphi\hat{n}\cdot\hat{L}}$

$\hat{Q}(\hat{n}d\varphi)\vec{r} = \vec{r} + (\vec{n}\times\vec{r})d\varphi$

$\vec{R}' = \hat{D}(\hat{n}d\varphi)\vec{R}\hat{D}^{-1}(\hat{n}d\varphi) = (1-\frac{i}{\hbar}d\varphi\,\hat{n}\cdot\hat{L})\vec{R}(1+\frac{i}{\hbar}d\varphi\,\hat{n}\cdot\hat{L}) = \vec{R} - \frac{i}{\hbar}d\varphi[\hat{n}\cdot\hat{L},\vec{R}] = \vec{R} - d\varphi\,\vec{n}\times\vec{R} = Q^{-1}(\hat{n}d\varphi)\vec{R}$

$[\vec{n}\cdot\vec{L},\vec{R}] = [n_iL_i, R_j] = n_iL_iR_j - n_iR_jL_i = n_k\varepsilon_{ijk}R_iP_jR_j - n_kR_j\varepsilon_{ijk}R_iP_j = \varepsilon_{ijk}n_kR_i[P_j,R_j] = \varepsilon_{ijk}n_kR_i\cdot(-i\hbar) = -i\hbar\,\vec{n}\times\vec{R}$

$\hat{D}(\hat{n}\varphi)\hat{\vec{x}}\hat{D}^{-1}(\hat{n}\varphi)|x\rangle = \hat{Q}^{-1}(\hat{n}\varphi)\hat{\vec{x}}|x\rangle$

矢量算符 $\hat{\vec{V}}$ 满足

$\hat{D}(\hat{n}\varphi)\hat{\vec{V}}\hat{D}^{-1}(\hat{n}\varphi) = \hat{Q}^{-1}(\hat{n}\varphi)\hat{\vec{V}}$

$\hat{D}(\hat{n}\varphi)\hat{\vec{V}}\cdot\hat{\vec{m}}\hat{D}^{-1}(\hat{n}\varphi) = \hat{\vec{V}}\cdot(Q(\hat{n}\varphi)\vec{m})$ （求证）已知 $[\vec{n}\cdot\vec{L},\vec{m}\cdot\vec{V}] = i\hbar\,\vec{n}\times\vec{m}\cdot\vec{V}$

$e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot\vec{L}}\,\hat{\vec{V}}\cdot\hat{\vec{m}}\,e^{\frac{i}{\hbar}\varphi\vec{n}\cdot\vec{L}}$

空间变换对称性

必须满足 $D(Q)HD^{-1}(Q)=H$

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§ 时间平移

$\hat{U}(\tau)\psi(x,t)=\psi(x,t-\tau)$

$\hat{U}(\tau)\vec{x}\hat{U}^{-1}(\tau)=\vec{x}$

§ 时间反演

$i\hbar\frac{\partial}{\partial t}\psi(x,t)=\hat{H}\psi(x,t)$

$-i\hbar\frac{\partial}{\partial t}\psi^*(x,t)=\hat{H}\psi^*(x,t)$

故 $i\hbar\frac{\partial}{\partial(-t)}\psi^*(x,-t)=\hat{H}\psi^*(x,-t)$

时间反演算符 $\hat{T}_0\psi(\vec{r},t)=\psi^*(\vec{r},-t)$

$\hat{T}_0\hat{x}\hat{T}_0^{-1}=\hat{x}$

$\hat{T}_0\hat{x}\hat{T}_0^{-1}\psi(x,t)=\hat{T}_0\hat{x}\psi^*(x,-t)=x\psi(x,t)=\hat{x}\psi(x,t)$

$\hat{T}_0\hat{p}\hat{T}_0^{-1}\psi(x,t)=\hat{T}_0\,(-i\hbar\frac{\partial}{\partial x})\psi^*(x,-t)=i\hbar\frac{\partial}{\partial x}\psi(x,t)=-\hat{p}\psi(x,t)$

$\hat{T}_0\varepsilon_{ijk}x_ip_j\hat{T}_0^{-1}=\varepsilon_{ijk}\hat{T}_0\hat{x}_i\hat{T}_0^{-1}\hat{T}_0p_j\hat{T}_0^{-1}=\varepsilon_{ijk}\hat{x}_i(-\hat{p}_j)=-\hat{L}$

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§ 二次量子化

第i个粒子的希尔伯特空间 $R^{(i)}$

则总希尔伯特空间 $R_{tot}=R^{(1)}\otimes R^{(2)}\otimes\cdots R^{(n)}$

设第i个粒子的本征矢为 $|b^{\alpha}\rangle_i\cdots|b^{\nu}\rangle_i$

n个粒子,设每一个粒子有k的本征矢,则巨希尔伯特空间的本征矢个数为 k^n

记为 $|b_1^{\alpha}\rangle\otimes|b_2^{\beta}\rangle\cdots|b_n^{\nu}\rangle$

此矢量必须对称/反对称.

由于全同粒子条件的限制

构成两个子空间 R_{nb} R_{nf}

则对称化的基矢 $|n;b^{\alpha}b^{\beta}\cdots b^{\nu}\rangle=\frac{1}{n!}\sum_p P|b_1^{\alpha}\rangle|b_2^{\beta}\rangle\cdots|b_n^{\nu}\rangle$ 举例子

反对称化 $|n;b^{\alpha}b^{\beta}\cdots b^{\nu}\rangle=\frac{1}{n!}\sum_p(-1)^p|b_1^{\alpha}\rangle\cdots|b_n^{\nu}\rangle$

由于 $R=R_c\otimes R_s \longrightarrow$ 自旋空间

位形空间

内积定理

$\langle\alpha_1',\alpha_2'\cdots\alpha_n'|\alpha_1\cdots\alpha_n\rangle=\frac{1}{n}\big(\delta(\alpha_1'-\alpha_1)\langle\alpha_2'\cdots\alpha_n'|\alpha_2\cdots\alpha_n\rangle$
$+\cdots\varepsilon^{n-1}(\alpha_1'-\alpha_n)\langle\alpha_2'\cdots\alpha_n'|\alpha_1\cdots\alpha_{n-1}\rangle\big)$

$=\frac{1}{n!}\sum_p\varepsilon^P P\,\delta(\alpha_1'-\alpha_1)\cdots\delta(\alpha_n'-\alpha_n)$

产生 湮灭算符

$a^+(a_1)|0\rangle = |1,a_1\rangle$, $a^+(a_2)|1,a_1\rangle = \sqrt{2}|2,a_1a_2\rangle$

真空态

玻色子 $a^+(a_2)\sqrt{2}|2,a_1a_2\rangle = \sqrt{3}|3,a_1a_2a_2\rangle$

费米子 $a^+(a_2)\sqrt{2}|2,a_1a_2\rangle = \sqrt{2}|2,a_1a_2\rangle$

对于任意一个态 $|n;b^\alpha b^\beta\cdots b^\gamma\rangle = \frac{1}{\sqrt{n!}}a^+(b^\alpha)\cdots a^+(b^\gamma)|0\rangle$

左矢为湮灭算符 $\langle n;b^\alpha b^\beta\cdots b^\gamma| = \frac{1}{\sqrt{n!}}\langle 0|a(b^\gamma)\cdots a(b^\alpha)$

湮灭算符作用到右矢上 $\langle n;b^{\alpha'}\cdots b^{\gamma'}|n;b^\alpha\cdots b^\gamma\rangle = \langle n-1;b^{\beta'}\cdots b^{\gamma'}|\frac{1}{\sqrt{n}}a(b^{\alpha'})|n;b^\alpha\cdots b^\gamma\rangle$ 内积定理 $\frac{1}{n}(\delta(b^{\alpha'}-b^\alpha)\langle b^{\beta'}\cdots b^{\gamma'}|b^\beta\cdots b^\gamma\rangle$
$+\cdots\varepsilon^{n-1}\delta(b^{\alpha'}-b^\gamma)\langle b^{\beta'}\cdots b^{\gamma'}|b^\alpha\cdots b^\gamma\rangle)$

$\therefore a(b^{\alpha'})|n;b^\alpha\cdots b^\gamma\rangle = \frac{1}{\sqrt{n}}(\delta(b^{\alpha'}-b^\alpha)|b^\beta\cdots b^\gamma\rangle + \cdots \varepsilon^{n-1}\delta(b^{\alpha'}-b^\gamma)|b^\alpha\cdots b^\gamma\rangle)$

关注 $[a(b),a^+(b')]_\mp = \delta(b-b')$, $[a(b),a(b)]_\mp = 0$

$a(b)a^+(b')|n;b_1\cdots b_n\rangle = a(b)\sqrt{n+1}|n+1;b'b_1\cdots b_n\rangle = \delta(b-b')|b_1\cdots b_n\rangle + \varepsilon\delta(b-b_1)|b'b_2\cdots b_n\rangle\cdots\varepsilon^n\delta(b-b_n)|b'b_1\cdots b_{n-1}\rangle$

$a^+(b')a(b)|n,b_1\cdots b_n\rangle = a^+(b')\frac{1}{\sqrt{n}}(\delta(b-b_1)|b_2\cdots b_n\rangle + \delta(b-b_2)|b_1b_3\cdots b_n\rangle\cdots) = \delta(b-b_1)|b'b_2\cdots b_n\rangle+\cdots+\varepsilon^{n-1}\delta(b-b_n)|b'b_1\cdots b_{n-1}\rangle$

$\therefore (a(b)a^+(b')-\varepsilon a^+(b')a(b))|b_1\cdots b_n\rangle = \delta(b-b')|b_1\cdots b_n\rangle$

$\therefore a(b)a^+(b')-\varepsilon a^+(b')a(b) = \delta(b-b')$

总粒子数算符 $N(b) = a^+(b)a(b)$ [占有数密度算符]

$N(b)|n;b_1\cdots b_n\rangle = a^+(b)a(b)|n;b_1\cdots b_n\rangle = a^+(b)\frac{1}{\sqrt{n}}(\delta(b-b_1)|b_2\cdots b_n\rangle + \varepsilon\delta(b-b_2)|b_1b_3\cdots b_n\rangle+\cdots\varepsilon^{n-1}\delta(b-b_n)|b_1\cdots b_{n-1}\rangle)$

$= \delta(b-b_1)|bb_2\cdots b_n\rangle + \varepsilon\delta(b-b_2)|bb_1b_3\cdots b_n\rangle\cdots\varepsilon^{n-1}\delta(b-b_n)|bb_1\cdots b_{n-1}\rangle$

$= \delta(b-b_1)|bb_2\cdots b_n\rangle + \delta(b-b_2)|b_1bb_3\cdots b_n\rangle + \cdots\delta(b-b_n)|b_1\cdots b_{n-1}b\rangle$

$= \sum_{i=1}^{n}\delta(b-b_i)|b_1b_2\cdots b_n\rangle$

$[N(b),a^+(b')] = [a^+(b)a(b),a^+(b')] = a^+(b)[a(b),a^+(b')]$

Boson $[N(b),a^+(b')] = a^+(b)\delta(b-b')$, $[N(b),a(b')] = -a(b)\delta(b-b')$

Fermi $[a^+(b)a(b),a^+(b')] = a^+(b)[a(b),a^+(b')]+[a^+(b),a^+(b')]a(b) = a^+(b)(\delta(b-b')-2a^+(b')a(b)) = a^+(b)\delta(b-b')-2\{a^+(b),a^+(b')\}a(b)$
$+ \ -2a^+(b')a^+(b)a(b)$ $= a^+(b)\delta(b-b')$

积分之后对总粒子数算符 $[N,a^+(b)] = a^+(b)$, $[N,a(b)] = -a(b)$

$\psi^+(x)|n;x_1\cdots x_n\rangle = \sqrt{n+1}\,|n+1;xx_1\cdots x_n\rangle$

产生一个位置在x的粒子

$\psi(x)|n;x_1\cdots x_n\rangle = \frac{1}{\sqrt{n!}}\{\delta(x-x_1)|n-1;x_2\cdots x_n\rangle + \varepsilon\delta(x-x_2)|n-1;x_1x_3\cdots x_n\rangle+\cdots\varepsilon^{n-1}\delta(x-x_n)|n-1;x_1\cdots x_{n-1}\rangle\}$

对称化基矢

$$|n; x_1 \cdots x_n\rangle = \frac{1}{\sqrt{n!}}\psi^+(x_1)\cdots\psi^+(x_n)|0\rangle$$

对易关系与上述相同

$$[\psi(x), \psi^+(x')]_\mp = \delta(x-x')$$

$$[\psi(x), \psi(x')]_\mp = [\psi^+(x), \psi^+(x')]_\mp = 0$$

对密度算符 $N(x) = \psi^+(x)\psi(x)$

$$[N(x), \psi^+(x')] = \psi^+(x)\delta(x-x')$$

$$[N(x), \psi(x')] = -\psi(x)\delta(x-x')$$

x表象与之前谈到的a表象如何转换呢

$$a^+(b) = \int dx \langle x|b\rangle \psi^+(x)$$

$$a(b) = \int dx \langle b|x\rangle \psi(x)$$

$$\psi^+(x) = \int db \langle b|x\rangle a^+(b)$$

$$\psi(x) = \int db \langle x|b\rangle a(b)$$

例如 $b=p$

$$\left.\begin{aligned}\psi^+(x) &= \int dp\, e^{-\frac{i}{\hbar}px} a^+(p)\cdot\left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \\ \psi(x) &= \int dp\, e^{\frac{i}{\hbar}px} a(p)\left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3\end{aligned}\right\}\text{归一化系数}$$

对于一个态 $|\phi\rangle$ 求 $\langle\phi|\psi^+(x)\psi(x)|\phi\rangle$

将 $|\phi\rangle$ 放到 $|x\rangle$ 表象下

$$|\phi\rangle = \int dx' |x'\rangle \phi(x')$$

$$\therefore \psi(x)|\phi\rangle = \int dx' \underbrace{\psi(x)|x'\rangle}_{\delta(x-x')|0\rangle} \phi(x') = \phi(x)|0\rangle$$

$$\therefore \langle\phi|\psi^+(x)\psi(x)|\phi\rangle = |\phi(x)|^2$$

$$\psi(x_1, x_2 \cdots x_n) = \frac{1}{\sqrt{n!}}\begin{vmatrix}\phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_n(x_2) \\ \vdots & & \ddots & \vdots \\ \phi_1(x_n) & \cdots & & \phi_n(x_n)\end{vmatrix}$$

费米子
对称化基矢

$$\equiv |x_1 \cdots x_n\rangle$$

ϕ^+ —— 单粒子产生算符

$$\phi^+|0\rangle = |\phi\rangle,\quad \langle 0|\phi = \langle\phi|$$

$$|\phi\rangle = \int dx |x\rangle\phi(x) = \underline{\int dx\, \psi^+(x)\phi(x)}|0\rangle$$

$$[\psi^+(x'), \phi^+]_\mp = \int dx [\psi^+(x'), \psi^+(x)]_\mp \phi(x) = 0$$

$$[\psi^+(x), \phi]_\mp = \int dx\, \phi^*(x)[\psi^+(x), \psi(x)]_\mp = -\phi^*(x)$$

$$[\psi(x), \phi^+]_\mp = \phi(x)$$

$$\langle x_1 x_2| = \langle 0|\psi(x_2)\psi(x_1)\frac{1}{\sqrt{2}}$$

$$\psi^+(x_1)\psi^+(x_2)|0\rangle = |x_1 x_2\rangle\frac{1}{\sqrt{2}}$$

$$\langle 0|\psi(x_2)\psi(x_1)\phi_1^+\phi_2^+|0\rangle = \langle 0|\psi(x_2)(\phi_1(x_1) - \phi_1^+\psi(x_1))\phi_2^+|0\rangle = \phi_1(x_1)\langle 0|\psi(x_2)\phi_2^+|0\rangle - \langle 0|\psi(x_2)\phi_1^+\psi(x_1)\phi_2^+|0\rangle$$

$$= \phi_1(x_1)\phi_2(x_2) - \langle 0|\psi(x_2)\phi_1^+(\phi_2(x_1) - \phi_2^+\psi(x_1))|0\rangle$$

$$= \phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)$$

算符的二次量子化形式

单体 $F=\sum_{i=1}^{n} F_i$

两体 $F=\frac{1}{2!}\sum_{i=1}^{n}\sum_{j=1(j\neq i)}^{n} F_{ij}$

① 写出矩阵元（x表象下），② 两边夹得到结果

$\langle x|F|x'\rangle$

例如对动量算符 $\vec{P}=\sum_i \vec{P}_i$

① $\langle x|\vec{P}_i|x'\rangle=\langle x|\frac{\hbar}{i}\nabla|x'\rangle=\frac{\hbar}{i}\nabla\delta(x-x')$

② $\vec{P}=\int dx\int dx'\ |x\rangle\langle x|\vec{P}|x'\rangle\langle x'|=\int dx\int dx'\ |0\rangle\ \psi^{+}(x)\frac{\hbar}{i}\nabla\delta(x-x')\ \psi(x')\langle 0|=\int dx\,\psi^{+}(x)\frac{\hbar}{i}\nabla\psi(x)dx$

对两体算符同样有

① 矩阵元 $\langle x_i x_j|F_{ij}|x_i' x_j'\rangle$

② $F=\int dx_i dx_j dx_i' x_j'\ |x_i x_j\rangle\langle x_i x_j|F_{ij}|x_i' x_j'\rangle\langle x_i' x_j'|$

例如 $F=\delta(x_i-x_j)$

$F=\frac{1}{2}\int dx_i dx_j dx_i' dx_j'\ \psi^{+}(x_i)\psi^{+}(x_j)\ \langle x_i x_j|x_i' x_j'\rangle\ \psi(x_i')\psi(x_j')=\frac{1}{2}\int dx_i\ dx_i' dx_j'\ \psi^{+}(x_i)\psi^{+}(x_i)\ \delta(x_i-x_i')\ \delta(x_i-x_j')\psi(x_i')\ \psi(x_j')$

$$=\frac{1}{2}\int dx_i[\psi^{+}(x_i)]^2[\psi(x_i)]^2$$