第四章 对称性与守恒量

$$\frac{d}{dt}\langle\psi|\hat{F}|\psi\rangle = \frac{\partial}{\partial t}(\langle\psi|)\hat{F}|\psi\rangle + \langle\psi|\frac{\partial\hat{F}}{\partial t}|\psi\rangle + \langle\psi|\hat{F}\frac{\partial}{\partial t}(|\psi\rangle)$$

$\hat{H} = i\hbar\frac{\partial}{\partial t}$, $\hat{H}^{+} = \hat{H}$

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

$$= \langle\psi|\hat{F}\hat{H}-\hat{H}\hat{F} + \frac{\partial\hat{F}}{\partial t}|\psi\rangle$$

$$= \langle\psi|[\hat{F},\hat{H}] + \frac{\partial\hat{F}}{\partial t}|\psi\rangle$$

若 $[\hat{F},\hat{H}] = 0$ 且 $\hat{F}$ 不含时 ($\frac{\partial\hat{F}}{\partial t} = 0$)

则 $\frac{d}{dt}\langle\psi|\hat{F}|\psi\rangle = 0$ ， $\hat{F}$ 为守恒量（期待值不随时间变化）

2. 好量子数

守恒量对应的标记本征值的数

Ehrenfest 定理：

$$\frac{d}{dt}\langle\hat{r}\rangle = \frac{1}{i\hbar}\langle[\hat{r},\frac{\hat{p}^2}{2m}+\hat{V}(r)]\rangle = \frac{1}{2mi\hbar}\langle[\hat{r},\hat{p}^2]\rangle = \frac{\langle\hat{p}\rangle}{m}$$

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{1}{i\hbar}\langle[\hat{p},\frac{\hat{p}^2}{2m}+\hat{V}(r)]\rangle = \frac{1}{i\hbar}\langle[\hat{p},\hat{V}(r)]\rangle = -\nabla V(r)$$

$\Rightarrow$ $\frac{dr}{dt} = \frac{p}{m}$, $\frac{dp}{dt} = -\nabla V$

能量－时间不确定关系：

$$\Delta E\Delta A \geq \frac{1}{2}|[\hat{A},\hat{H}]| = \frac{\hbar}{2}|\frac{d}{dt}\langle\hat{A}\rangle|$$

定义 $\Delta t = \frac{\Delta\hat{A}}{\frac{d}{dt}|\langle\hat{A}\rangle|}$ ， $\Delta E\Delta t \geq \frac{\hbar}{2}$

$t \geq \Delta t$ 才能看出显著变化（区别于涨落）

§ 4.2 对称性与守恒量的关系

在幺正变换 $\hat{Q}$ 下

$$|\psi\rangle \to |\psi'\rangle = \hat{Q}|\psi\rangle$$

对称变换：$\langle a|b\rangle = \langle a'|b'\rangle$ $\forall |a\rangle, |b\rangle$ 成立.

Wigner定理：对称变换一定是幺正变换 / 反幺正变换

$\langle\psi|\hat{A}|\psi\rangle \to \langle\psi'|\hat{A}|\psi'\rangle = \langle\psi|\hat{Q}^\dagger\hat{A}\hat{Q}|\psi\rangle$ $|\psi'\rangle = \hat{Q}|\psi\rangle$

↳ 定义算符的变换 $\hat{A} \to \hat{A}' = \hat{Q}^\dagger\hat{A}\hat{Q}$

系统在 $\hat{Q}$ 变换下有对称性：Schrodinger方程不变.

$$\hat{Q}^\dagger\hat{H}\hat{Q} = \hat{H} \to [\hat{Q}, \hat{H}] = 0$$

连续变换 $\hat{Q}$：

幺正：$\hat{Q}^\dagger\hat{Q} = \hat{Q}\hat{Q}^\dagger = 1$

无穷小变换：$\hat{Q}(\eta) = e^{i\eta\hat{F}} = 1 + i\eta\hat{F}$

$$\hat{Q}^\dagger\hat{Q} = (1 - i\eta\hat{F}^\dagger)(1 + i\eta\hat{F}) = 1 + i\eta(\hat{F} - \hat{F}^\dagger) = 1$$

$\hat{F} = \hat{F}^\dagger$，$\hat{F}$ 是厄米算符. $\hat{F}$：变换 $\hat{Q}$ 的生成算符、

对称性：$[\hat{Q}, \hat{H}] = [e^{i\eta\hat{F}}, \hat{H}] = 0$ 诸定理.

↳ $[\hat{F}, \hat{H}] = 0$

2. 平移算符 $\hat{T}$

$$x \to x' = x + \delta x$$

$$\hat{T}(\delta x)|x\rangle = |x + \delta x\rangle$$

$$|\psi'\rangle = \hat{T}|\psi\rangle = \int \hat{T}|x\rangle\langle x|\psi\rangle dx$$

$$= \int dx\, |x + \delta x\rangle\langle x|\psi\rangle = \int dx'\, |x'\rangle\langle x' - \delta x|\psi\rangle$$

$$= \int dx'\, |x'\rangle\, \psi(x - \delta x)$$

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

具体形式：$\langle x|\hat{T}(\delta x)|\psi\rangle$

$$= \langle x|1 + i\delta x\hat{F}|\psi\rangle = \langle x|\psi\rangle + i\delta x\langle x|\hat{F}|\psi\rangle$$

$\psi(x - \delta x)$ 展开 $= \psi(x) - \delta x\frac{\partial}{\partial x}\psi(x)$

→ $\hat{F} = -\frac{\hat{p}}{\hbar}$ 平移对称性：$[\hat{p}_x, \hat{H}] = 0$ 动量守恒.

$$\hat T(x) = \lim_{N\to\infty} \left(e^{-\frac{ix}{N}\frac{\hat p_x}{\hbar}} \right) \int e^{i\delta x \cdot \frac{\hat p_x}{\hbar}} = e^{-\frac{i\hat p_x x}{\hbar}}$$

位置算符的变换:

$$\hat x' = \hat T^{+} \hat x \hat T = e^{\frac{i\hat p_x x}{\hbar}} \hat x \, e^{-\frac{i\hat p_x x}{\hbar}} = \hat x + a$$

Baker - Hausdorff 公式:

$$f(\lambda) = e^{\lambda\hat A} \hat B e^{-\lambda \hat A}$$

$$f^{(1)}(\lambda) = e^{\lambda\hat A} \hat A \hat B e^{-\lambda \hat A} - e^{\lambda\hat A} \hat B \hat A e^{-\lambda \hat A}$$

$$= e^{\lambda\hat A} [\hat A, \hat B] e^{-\lambda \hat A}$$

$$f^{(2)}(\lambda) = e^{\lambda\hat A} (\hat A [\hat A, \hat B] - [\hat A, \hat B] \hat A) e^{-\lambda \hat A}$$

$$= e^{\lambda\hat A} [\hat A, [\hat A, \hat B]] e^{-\lambda \hat A}$$

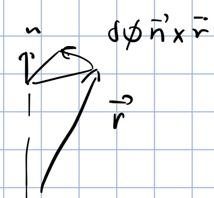
$$\vdots$$

$$f^{(n)}(\lambda) = e^{\lambda\hat A} [\hat A, \cdots \hat A, [\hat A, \hat B]] \cdots] e^{-\lambda \hat A}$$

$$\Rightarrow f(\lambda) = f(0) + \sum_n \frac{\lambda^n}{n!} f^{(n)}(\lambda)$$

$$= \sum_n \frac{\lambda^n}{n!} \hat C_n \qquad \hat C_0 = \hat B, \ \hat C_1 = [\hat A, \hat B], \ \hat C_2 = [\hat A, \hat C_1] \cdots$$

3. 旋转算符 $\hat R_n$



$$\vec r' = \vec r + \delta\phi \, \vec n \times \vec r$$

$$\hat R_n(\delta\phi), \quad \hat R_n(\delta\phi) |\vec r\rangle = |\vec r - \delta\phi \, \vec n \times \vec r\rangle$$

$$\psi'(r) = \langle \vec r | \hat R_n(\delta\phi) | \psi\rangle = \psi(\vec r - \delta\phi \, \vec n \times \vec r)$$

$$\langle \vec r | \hat R_n(\delta\phi) | \psi\rangle = \psi(r) - \delta\phi (\vec n \times \vec r) \cdot \nabla\psi(r)$$ 泰勒展开.

$$= \langle r | \psi\rangle - \frac{i}{\hbar} \delta\phi \langle r | (\vec n \times \vec r) \cdot \hat p | \psi\rangle \qquad \hat p = -i\hbar\nabla$$

$$= \langle r | \psi\rangle - \frac{i}{\hbar} \delta\phi \langle r | (\vec r \times \hat p) \cdot \vec n | \psi\rangle$$

$$= \langle r | 1 - \frac{i}{\hbar} (\hat L \cdot \vec n) \delta\phi | \psi\rangle$$

$$\rightarrow \hat R_n(\delta\phi) = 1 - \frac{i}{\hbar} (\hat L \cdot \vec n) \delta\phi = e^{-\frac{i(\hat L \cdot \vec n)\delta\phi}{\hbar}}$$

$$\hat R_n(\phi) = \int \hat R_n(\delta\phi) = e^{-i\frac{\hat L \cdot \vec n}{\hbar}\phi}$$

旋转对称: $[\hat L \cdot \vec n, \hat H] = 0$ 角动量守恒.

离散对称性.

空间反演：$\hat{\pi}$：$\vec{r} \to -\vec{r}$

$\hat{\pi}|r\rangle = |-r\rangle$ ，$\hat{\pi}|p\rangle = |-p\rangle$

坐标、动量算符的变换：

$$\hat{\pi}\hat{\vec{r}}\hat{\pi}^{-1}\hat{\pi}|\vec{r}\rangle = \hat{\pi}\hat{\vec{r}}|\vec{r}\rangle = \hat{\pi}\vec{r}|r\rangle$$

$$= \vec{r}\hat{\pi}|r\rangle = \vec{r}|-r\rangle$$

$$= -\hat{\vec{r}}|-r\rangle = -\hat{\vec{r}}\hat{\pi}|\vec{r}\rangle$$

$\Rightarrow \hat{\pi}^{+}\hat{\vec{r}}\hat{\pi} = -\hat{\vec{r}}$ 同理：$\hat{\pi}^{+}\hat{\vec{p}}\hat{\pi} = -\hat{\vec{p}}$

$\hat{\pi}^{+}[\hat{\vec{x}},\hat{\vec{p}}]\hat{\pi} = \hat{\pi}^{+}(\hat{\vec{x}}\hat{\vec{p}} - \hat{\vec{p}}\hat{\vec{x}})\hat{\pi}$ * $\hat{\pi}^{+}i\hbar\hat{\pi} = i\hbar$

$= \hat{\pi}^{+}\hat{\vec{x}}\hat{\pi}\hat{\pi}^{+}\hat{\vec{p}}\hat{\pi} - \hat{\pi}^{+}\hat{\vec{p}}\hat{\pi}\hat{\pi}^{+}\hat{\vec{x}}\hat{\pi}$ ↳ $\hat{\pi}$是幺正算符.

$= \hat{\vec{x}}\hat{\vec{p}} - \hat{\vec{p}}\hat{\vec{x}} = [\hat{\vec{x}},\hat{\vec{p}}]$

$$\hat{\pi}|\psi\rangle = \hat{\pi}\int dr^3 |r\rangle\langle r|\psi\rangle = \int dr^3 |-r\rangle\langle r|\psi\rangle$$

$r \to -r$ $$= -\int_{+\infty}^{-\infty} dr^3 |r\rangle\langle -r|\psi\rangle = -\int_{+\infty}^{-\infty} dr^3 |r\rangle \psi(-r)$$

$$= \int_{-\infty}^{+\infty} dr^3 |r\rangle \psi(-r) = |\psi(-r)\rangle$$

$\psi'(r) = \langle r|\hat{\pi}|\psi\rangle = \psi(r)$

$\hat{\pi}^2|r\rangle = |r\rangle$ $\hat{\pi}^2 = 1$ → $\hat{\pi}$是厄米算符

本征方程：$\hat{\pi}|\psi\rangle = \lambda|\psi\rangle$

$\hat{\pi}^2|\psi\rangle = \lambda^2|\psi\rangle = |\psi\rangle$ → $\lambda = \pm 1$ $\lambda = 1$，偶宇称.

$\lambda = 1$，奇宇称.

系统有空间反演对称性：

$[\hat{\pi}, \hat{H}] = 0$ 宇称守恒.

例：一维谐振子.

$\hat{\pi}|n\rangle = \alpha_n|n\rangle$，$\alpha_n = \pm 1$ $\hat{\pi}\hat{a}^{+}\hat{\pi} = -\hat{a}$

$$\hat{\pi}|n\rangle = \hat{\pi}\frac{1}{\sqrt{n}}\hat{a}^{+}|n-1\rangle = -\frac{1}{\sqrt{n}}\hat{a}^{+}\hat{\pi}|n-1\rangle$$

$$= -\frac{1}{\sqrt{n}}\hat{a}^{+}\alpha_{n-1}|n-1\rangle = -\alpha_{n-1}|n\rangle$$

↳ $\alpha_n = -\alpha_{n-1}$，$\alpha_n = (-1)^n\alpha_0$

基态：偶宇称 $\alpha_n = (-1)^n$，$\hat{\pi}|n\rangle = (-1)^n|n\rangle$

§ 4.3 时间反演对称性

$t \to -t$

$\Theta|\vec r\rangle = |\vec r\rangle$, $\Theta|\vec p\rangle = |-\vec p\rangle$

反幺正算符 : $\Theta^\dagger\Theta = 1$

$|\alpha'\rangle = \Theta|\alpha\rangle$, $|\beta'\rangle = \Theta|\beta\rangle$ $\quad \langle\alpha'|\beta'\rangle = \langle\alpha|\beta\rangle^*$

反线性 $\Theta(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha^*\Theta|\alpha\rangle + c_\beta^*\Theta|\beta\rangle$

$\hat\Theta\hat r\hat\Theta = \hat r$, $\hat\Theta\hat p\hat\Theta = -\hat p$

表示：

$$|\psi'\rangle = \hat\Theta|\psi\rangle = \sum_n \hat\Theta|n\rangle\langle n|\psi\rangle^*$$

$$= \sum_n |n'\rangle\langle\psi|n\rangle$$

$\hat\Theta = \hat U\hat K$ $\quad$ $\hat U$为幺正算符，负责对基矢变换。

Wigner定理 $\quad$ $\hat K$负责对展开系数取复共轭。(反线性)

$$\hat\Theta^{-1} = \hat K^{-1}\hat U^{-1} = \hat K\hat U^\dagger$$

对态矢量的变换 :

$$\hat\Theta|\psi\rangle = \hat\Theta\int d^3r\,|r\rangle\langle r|\psi\rangle = \int d^3r\,|r\rangle\langle r|\psi\rangle^*$$

$\hookrightarrow \quad \psi'(r) = \langle r|\hat\Theta|\psi\rangle = \psi^*(r)$

$\hat K$对算符的变换: $\quad \hat K^2 = 1$, $\hat K = \hat K^{-1}$

$$\hat K\hat A\hat K^{-1}|\psi\rangle = \hat K\hat A\hat K|\psi\rangle = \hat K\hat A|\psi^*\rangle \quad (\hat K|\psi\rangle = |\psi^*\rangle)$$

$$= (\hat A|\psi^*\rangle)^* = \hat A^*|\psi\rangle$$

$\to \quad \hat K\hat A\hat K^{-1} = \hat A^*$

Schur引理：若一个有限维不可约表示空间$\mathcal{H}$上有线性算符A满足A和所有表示中的变换D(g)对易，则$A \propto I$

$$\hat\Theta^2 = \hat U\hat K\hat U\hat K$$

$= \hat U\hat K\hat U\hat K^{-1} = \hat U\hat U^* = \alpha$ $\quad$ α为相位因子，为实数.

$\hookrightarrow \quad \hat U = \alpha\hat U^T$, $\hat U^T = \alpha\hat U$ $\quad \to \quad \hat U = \alpha^2\hat U$, $\alpha = \pm 1$

例：一个具有时间反演对称性的系统，如果能级E_n不简并，则相应本征函数可以表示为实函数.

$$\hat{\Theta}\hat{H}|n\rangle = \hat{H}\hat{\Theta}|n\rangle = E_n\hat{\Theta}|n\rangle , \quad \hat{H}|n\rangle = E_n|n\rangle$$

$$\Rightarrow \hat{\Theta}|n\rangle = k_n|n\rangle$$

$$\langle r|\hat{\Theta}|n\rangle = \langle r|n\rangle^* \rightarrow \langle r|n\rangle = e^{i\delta}\langle r|n\rangle^*$$

所以 $\langle r|n\rangle$ 为实数

§ 4.4. 轨道角动量本征态的性质

本征态: $|l,m\rangle$

旋转: $\hat{R}_z(2\pi)|l,m\rangle = e^{-i2m\pi}|l,m\rangle$

宇称: 在空间反演下 $\hat{\pi}^+\hat{L}\hat{\pi} = \hat{\pi}^+\hat{r}\hat{\pi} \times \hat{\pi}^+\hat{p}\hat{\pi} = (-\hat{r})\times(-\hat{p}) = \hat{L}$

↳ $[\hat{\pi},\hat{L}] = 0$, $[\hat{\pi},\hat{L}^2] = 0$

共同本征态 $|l,m\rangle$ 有确定的宇称.

$[\hat{\pi},\hat{L}_\pm] = 0$ → $\hat{L}_\pm$ 不改变 $|l,m\rangle$ 的宇称.

↳ $|l,m\rangle$ 的宇称与 m 无关, 只与 l 有关

具体关系:

$$[\hat{r},\hat{L}^2] = -2i\hbar\,\hat{r}\times\hat{L} - 2\hbar^2\hat{r}$$

证: $[\hat{r}_i,\hat{L}_j] = \varepsilon_{jkm}[\hat{r}_i,\hat{r}_k\hat{p}_m] = \varepsilon_{jkm}\hat{r}_k[\hat{r}_i,\hat{p}_m] = i\hbar\,\varepsilon_{ijk}\hat{r}_k$

$[\hat{r}_i,\hat{L}_j\hat{L}_j] = [\hat{r}_i,\hat{L}_j]\hat{L}_j + \hat{L}_j[\hat{r}_i,\hat{L}_j]$

或: $[\hat{r},\hat{L}^2] = [\hat{r},\hat{L}]\hat{L} + \hat{L}[\hat{r},\hat{L}]$

$= i\hbar\,\varepsilon_{ijk}(\hat{r}_k\hat{L}_j + \hat{L}_j\hat{r}_k)$

$[\hat{r},\hat{L}] = i\hbar(\hat{r}\times\hat{I})$

$= -i\hbar\,\varepsilon_{ikj}\,2r_kL_j + i\hbar\,\varepsilon_{ijk}(-\hat{r}_k\hat{L}_j + \hat{L}_j\hat{r}_k)$

↳ $[\hat{r},\hat{L}^2] = i\hbar[(\hat{r}\times\hat{I})\cdot\hat{L} + \hat{L}\cdot(\hat{r}\times\hat{I})]$

$= -2i\hbar(\hat{r}\times\hat{L})_i - i\hbar\,\varepsilon_{ijk}[\hat{r}_k,\hat{L}_j]$

$= i\hbar(\hat{L}\times\hat{r} - \hat{r}\times\hat{L})$

$= -2i\hbar(\hat{r}\times\hat{L})_i - (i\hbar)^2\varepsilon_{ijk}\varepsilon_{kji}r_i$

$= i\hbar\ -2(\hat{r}\times\hat{L}$

$= -2i\hbar(\hat{r}\times\hat{L})_i - \hbar^2 r_i$ □.

$$[[\hat{r},\hat{L}^2],\hat{L}^2] = [-2i\hbar\,\hat{r}\times\hat{L},\hat{L}^2] - 2\hbar^2[\hat{r},\hat{L}^2]$$

$$= -2i\hbar[\hat{r},\hat{L}]\times\hat{L} - 2\hbar^2\hat{r}(i\hbar) = 4\hbar^2\hat{r}\times\hat{L} - 2i\hbar^4$$

$$[\hat{A},(\hat{B}\times\hat{C})_i] = [\hat{A},\sum_{j,k}\varepsilon_{ijk}B_jC_k]$$

$$= \sum_{j,k}\varepsilon_{ijk}\{[\hat{A},B_j]\hat{C}_k + B_j[\hat{A},\hat{C}_k]\}$$

$$= \{[\hat{A},\hat{B}]\times\hat{C} + \hat{B}\times[\hat{A},\hat{C}]\}_i$$

$$\langle l',m'|\,[[\hat{\vec r},\hat{L}^2],\hat{L}^2]\,|l,m\rangle$$

① $= 2\hbar^2\langle l',m'|(\hat{\vec r}\hat{L}^2+\hat{L}^2\hat{\vec r})|l,m\rangle$

$= 2\hbar^2\left[\langle l',m'|\hat{L}^2\hat{r}|l,m\rangle+\langle l',m'|\hat{r}\hat{L}^2|l,m\rangle\right]$

$= 2\hbar^4\left[l'(l'+1)+l(l+1)\right]\langle l',m'|\hat{r}|l,m\rangle$

② $= \langle l',m'|\,[\hat{\vec r},\hat{L}^2]\hat{L}^2-\hat{L}^2[\hat{\vec r},\hat{L}^2]\,|l,m\rangle$

$= \hbar^2\left[l(l+1)-l'(l'+1)\right]\langle l',m'|[\hat{\vec r},\hat{L}^2]|l,m\rangle$

$= \hbar^2\left[l(l+1)-l'(l'+1)\right]\langle l',m'|\hat{r}\hat{L}^2-\hat{L}^2\hat{r}|l,m\rangle$

$= \hbar^4\left[l(l+1)-l'(l'+1)\right]^2\langle l',m'|\hat{r}|l,m\rangle$

$\langle l',m'|\hat{r}|l,m\rangle\neq 0$

$\rightarrow \left[l(l+1)-l'(l'+1)\right]^2 = 2\left[l'(l'+1)+l(l+1)\right]$

$l^2(l+1)^2+l'^2(l'+1)^2-2l(l+1)l'(l'+1)-2l'(l'+1)-2l(l+1)=0$

$\left[(l'+l+1)^2-1\right]\left[(l'-l)^2-1\right]=0$

解得 $l'=-l-1\pm1$ (舍), $l\pm1$

作业：

$\hat{H}^+ = \hat{H}$

$\Rightarrow \hat{H}^+ = (\alpha(\hat{L}_x\hat{p}_y - \hat{L}_y\hat{p}_x) + \beta\hat{p}_z)^*$

$= \alpha^*(\hat{p}_y\hat{L}_x - \hat{p}_x\hat{L}_y) + \beta^*\hat{p}_z$ $\quad [\hat{L}_x, \hat{p}_y] = \quad [\hat{L}_y, \hat{p}_x] =$

$= \alpha^*(\hat{L}_x\hat{p}_y - \hat{L}_y\hat{p}_x) + (\beta^* - 2i\hbar\alpha)\hat{p}_z$

α 为实数，$\mathrm{Im}\beta = \hbar\alpha$

$[\hat{H}, \hat{p}] = \alpha[(\hat{L}_x\hat{p}_y - \hat{L}_y\hat{p}_x), \hat{p}] \neq 0$

$\rightarrow$ $\alpha = 0$ 时才有平移对称性.

$[H, \hat{L}_z] = 0$ $\rightarrow$ 系统具有绕z轴的旋转对称性.

$\hat{\pi}^+\hat{H}\hat{\pi} = -\hat{H} \neq \hat{H}$ $\quad (\vec{p} \to -\vec{p})$

$\hat{\Theta}^+\hat{H}\hat{\Theta} = \alpha^*(L_xp_y - L_yp_x) - \beta^*p_z$ $\quad \vec{p} \to -\vec{p}$, $\vec{L} \to -\vec{L}$ $\quad i \to -i$

$\Rightarrow$ $\beta = -i\hbar\alpha$.

β 为纯虚数，$\beta^* = -\beta$

$= \alpha^*(L_xp_y - L_yp_x) + \beta p_z$