(2)算符的运算:

①两个算符的积通常不可交换: $\hat{A}\hat{B} \neq \hat{B}\hat{A}$ (无交换律)

② 有结合律: $\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$

$$\hat{A}^n\hat{A}^m = \hat{A}^{(n+m)}$$

③作用先后: $\hat{A}\hat{B}|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle)$

④ $\langle\phi|\hat{A}|\psi\rangle$ = 复数.

$$(\langle\phi|\hat{A})|\psi\rangle = \langle\phi|(\hat{A}|\psi\rangle)$$

(3)线性算符:

分配律: $\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1\hat{A}|\psi_1\rangle + a_2\hat{A}|\psi_2\rangle$

$$(\langle\psi_1|a_1 + \langle\psi_2|a_2)\hat{A} = a_1\langle\psi_1|\hat{A} + a_2\langle\psi_2|\hat{A}.$$

(4.) 讨论:

① 期望: $\hat{A}$ 关于一个态 $|\psi\rangle$ 的期望: $\langle\hat{A}\rangle$

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$$

② $|\phi\rangle\langle\psi|$ 是线性算符:

$$|\phi\rangle\langle\psi|\psi'\rangle = \underbrace{\langle\psi|\psi'\rangle}_{\text{复数}}|\phi\rangle.$$

不合法: $|\psi\rangle\hat{A}$. $\hat{A}\langle\psi|$.

2. 厄米特伴随(= 厄米特共轭)

对复数 α. $\alpha^+ = \alpha^*$

对 $\hat{A}$. 定义: $\langle\psi|\hat{A}^+|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$.

(1)厄米特共轭规则的性质:

为得到任何表达式的厄米伴随, 需经过以下替换:

① 复常数: $\alpha^+ = \alpha^*$

② 右矢(左矢) $(|\psi\rangle)^+ = \langle\psi|$. $(\langle\psi|)^+ = |\psi\rangle$.

③ $\hat{A} \to \hat{A}^+$

(2) 厄米运算的性质:

① $(\hat{A}^\dagger)^\dagger = \hat{A}$

② $(\alpha\hat{A})^\dagger = \alpha^*\hat{A}^\dagger$

③ $(\hat{A}^n)^\dagger = (\hat{A}^\dagger)^n$

④ $(\hat{A}+\hat{B}+\hat{C}+\hat{D})^\dagger = \hat{A}^\dagger+\hat{B}^\dagger+\hat{C}^\dagger+\hat{D}^\dagger$

⑤ $(\hat{A}\hat{B}\hat{C}\hat{D})^\dagger = \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger$

⑥ $(\hat{A}\hat{B}\hat{C}\hat{D}|\psi\rangle)^\dagger = \langle\psi|\hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger$

⑦ $(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|$.

⑧ $|a\hat{A}\psi\rangle = a\hat{A}|\psi\rangle$. $\langle a\hat{A}\psi| = a^*\langle\psi|\hat{A}^\dagger$

(同理, $\langle a\hat{A}^\dagger\psi| = a^*\langle\psi|\hat{A}\cdot$)

$$\Rightarrow \langle\psi|\hat{A}|\phi\rangle = \langle\underbrace{\hat{A}^\dagger\psi}_{=\langle\psi|\hat{A}}|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$$

(3) 厄米算符:

若 $\hat{A}=\hat{A}^\dagger$. 则 $\hat{A}$ 是厄米的.

或: $\langle\psi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$

斜厄米算符: $\hat{B}^\dagger = -\hat{B}$ = anti-..

skew-

或: $\langle\psi|\hat{B}|\phi\rangle = -\langle\phi|\hat{B}|\psi\rangle^*$

注: 对于一个算符, 通常 $\hat{A}^\dagger \neq \hat{A}^*$.

$(\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*)$

习题:

E26. (1) $\hat{B}_1^\dagger = (\hat{A}+\hat{A}^\dagger)^\dagger = \hat{A}^\dagger+\hat{A} = \hat{B}$. ✓

$\hat{B}_2^\dagger = (i(\hat{A}+\hat{A}^\dagger))^\dagger = -i(\hat{A}^\dagger+\hat{A}) = -\hat{B}_2$ ×

$\hat{B}_3^\dagger = (i(\hat{A}-\hat{A}^\dagger))^\dagger = -i(\hat{A}^\dagger-\hat{A}) = \hat{B}_3$. ✓

(2) $f^\dagger(\hat{A}) = f^*(\hat{A}^\dagger)$

$$(f(\hat{A}))^\dagger = \left(\frac{(1+i\hat{A}+3\hat{A}^2)(1-2i\hat{A}-9\hat{A}^2)}{5+7\hat{A}}\right)^\dagger = \frac{(1-i\hat{A}^\dagger+3\hat{A}^{\dagger 2})(1+2i\hat{A}^\dagger-9\hat{A}^{\dagger 2})}{5+7\hat{A}^\dagger}$$

(3) A 厄米算符：期望值 $\in$ 实数.

反 ………… $\in$ 虚数.

若：$\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}|\psi\rangle^*$ （$\hat{A}$ 是厄米的）

（如果 $\hat{A}=\hat{A}^\dagger$）则 $\langle\psi|\hat{A}|\psi\rangle$ = 实数.

若：$\langle\psi|\hat{B}|\psi\rangle = -\langle\psi|\hat{B}|\psi\rangle^*$ （$\hat{B}^\dagger=-\hat{B}$）.

$\therefore \langle\psi|\hat{B}|\psi\rangle$ 为虚数.

3. 投影算符

定义：$\hat{P}^\dagger=\hat{P}$. $\hat{P}^2=\hat{P}$.

示例：单位算符 $\hat{I}$.

(1) 性质

① $\hat{P}_1 \cdot \hat{P}_2$ 相乘仍是投影算符 （$\hat{P}_1 \cdot \hat{P}_2$ 为对易算符. $\hat{P}_1\hat{P}_2=\hat{P}_2\hat{P}_1$.）

$(\hat{P}_1\hat{P}_2)^\dagger=(\hat{P}_2^\dagger\hat{P}_1^\dagger)=\hat{P}_2\hat{P}_1=\hat{P}_1\hat{P}_2$ ✓.

$(\hat{P}_1\hat{P}_2)^2=\hat{P}_1^2\hat{P}_2^2=P_1P_2$. ✓

② $\hat{P}_1+\hat{P}_2$ 一般不是投影算符.

③ 若 $\hat{P}_1 \cdot \hat{P}_2$ 是投影$_{ㄅ}$. $\hat{P}_1\hat{P}_2=0$. 则正交.

④ 若 $\underset{\text{投影}_{ㄅ}}{\hat{P}_1}+\hat{P}_2+\cdots+\hat{P}_n$ 要成为投影算符 则必须两两正交.

（交叉项=0）

Example 2.7.

$|\psi\rangle\langle\psi|$. 是投影算符 $\Leftrightarrow$ $|\psi\rangle$ 是归一化的.

$(|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi|$ （厄米的） ✓.

$(|\psi\rangle\langle\psi|)^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|\psi\rangle\langle\psi|$

若 $|\psi\rangle$ 归一化. $(|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi|$.

$\Rightarrow \langle\psi|\psi\rangle=1$

4. 对易运算

定义：$[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$.

反对易：$\{\hat{A},\hat{B}\}=\hat{A}\hat{B}+\hat{B}\hat{A}$.

两个算符是对易的 $\Leftrightarrow$ $[\hat{A},\hat{B}]=0$ $\Leftrightarrow$ $\hat{A}\hat{B}=\hat{B}\hat{A}$.

恒成立：$[\hat{A},\hat{A}]=0$.

若两算符厄米且乘积厄米 $\Rightarrow$ $(\hat{A}\hat{B})^{+}=\hat{A}\hat{B}$

$(\hat{A}\hat{B})^{+}=\hat{B}^{+}\hat{A}^{+}=\hat{B}\hat{A}$ 相等.

① 举例：动量算符 $\hat{p}$

坐标算符 $\hat{x}$. $\hat{p}=-i\hbar\frac{\partial}{\partial x}$.

$[\hat{x},\hat{p}_x]=i\hbar\hat{I}$

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

$\hat{p}_x\hat{x}|\psi\rangle=-i\hbar\frac{\partial}{\partial x}(\hat{x}|\psi\rangle)=\hat{x}\cdot(-i\hbar\frac{\partial}{\partial x})|\psi\rangle-i\hbar|\psi\rangle$

$\therefore [\hat{x},\hat{p}_x]=\hat{x}\hat{p}_x-\hat{p}_x\hat{x}=i\hbar\hat{I}$.

同理：$[\hat{y},\hat{p}_y]=i\hbar\hat{I}$. $[\hat{z},\hat{p}_z]=i\hbar\hat{I}$

② 性质：

1) 反对称性：$[\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$

2) 线性性：$[\hat{A},\hat{B}+\hat{C}+\cdots]=[\hat{A},\hat{B}]+[\hat{A},\hat{C}]+\cdots$

3) 对易运算的厄米共轭：

$[\hat{A},\hat{B}]^{+}=[\hat{B}^{+},\hat{A}^{+}]$

4) 分配律：$[\hat{A},\hat{B}\hat{C}]=[\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}]$ (*)

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

5) 雅各比恒等式：$[\hat{A},[\hat{B},\hat{C}]]+[\hat{B},[\hat{C},\hat{A}]]+[\hat{C},[\hat{A},\hat{B}]]=0$.

注：李代数 2). $[X,[Y,Z]]+[Y,[Z,X]]+[Z,[X,Y]]=0$.

注：满足 2) 的代数不一定具有反对称性.

6). 从 (*) 式：$[\hat{A},\hat{B}^{n}]=\sum_{j=0}^{n-1}\hat{B}^{j}[\hat{A},\hat{B}]\hat{B}^{n-j-1}$.

$[\hat{A}^{n},\hat{B}]=\sum_{j=0}^{n-1}\hat{A}^{n-j-1}[\hat{A},\hat{B}]\hat{A}^{j}$

7). $\hat{A}$ 和常数 b 一定是对易的：$[\hat{A},b]=0$

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Example 2.8.

(1) 两个厄米算符的对易是反厄米算符.

$$[\hat{A},\hat{B}]^+ = (\hat{A}\hat{B}-\hat{B}\hat{A})^+ = \hat{B}^+\hat{A}^+ - \hat{A}^+\hat{B}^+ = \hat{B}\hat{A}-\hat{A}\hat{B} = -[\hat{A},\hat{B}]$$

$$\Rightarrow [\hat{A},\hat{B}]^+ = -[\hat{A},\hat{B}] \qquad (\{\hat{A},\hat{B}\}^+ = \{\hat{A},\hat{B}\})$$

厄米的.

(2) 计算: $[\hat{A},[\hat{B},\hat{C}]\hat{D}]$

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

$$= [\hat{A},\hat{B}\hat{C}-\hat{C}\hat{B}]\hat{D} + (\hat{A}\hat{D}-\hat{D}\hat{A})(\hat{B}\hat{C}-\hat{C}\hat{B})$$

$$= \hat{C}\hat{B}\hat{D}\hat{A} - \hat{B}\hat{C}\hat{D}\hat{A} + \hat{A}\hat{B}\hat{C}\hat{D} - \hat{A}\hat{C}\hat{B}\hat{D}.$$

5. 两算符之间的不确定关系:

定义: $\langle\hat{A}\rangle$ $\langle\hat{B}\rangle$ 是两厄米算符 $\hat{A}$. $\hat{B}$ 关于已归一化的态 $|\psi\rangle$ 的期望:

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

$$\langle\hat{B}\rangle = \langle\psi|\hat{B}|\psi\rangle.$$

$$\Delta\hat{A} = \hat{A}-\langle\hat{A}\rangle. \qquad \Delta\hat{B} = \hat{B}-\langle\hat{B}\rangle.$$

$$(\Delta\hat{A})^2 = \hat{A}^2+\langle\hat{A}\rangle^2-2\hat{A}\langle\hat{A}\rangle. \qquad (\Delta\hat{B})^2 = \hat{B}^2+\langle\hat{B}\rangle^2-2\hat{B}\langle\hat{B}\rangle$$

$$\langle\psi|(\Delta\hat{A})^2|\psi\rangle = \langle\Delta\hat{A}\rangle^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 \qquad (\langle\hat{A}^2\rangle = \langle\psi|\hat{A}^2|\psi\rangle)$$

$$(\Delta\hat{B})^2 = \langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2.$$

不确定度 ΔA. ΔB.

(是数)

$$\Delta A = \sqrt{\langle(\Delta\hat{A})^2\rangle} = \sqrt{\langle\hat{A}^2\rangle-\langle\hat{A}\rangle^2}$$

$$\Delta B = \sqrt{\langle\hat{B}^2\rangle-\langle\hat{B}\rangle^2}$$

$$|\chi\rangle = \Delta\hat{A}|\psi\rangle = (\hat{A}-\langle\hat{A}\rangle)|\psi\rangle.$$

$$|\phi\rangle = \Delta\hat{B}|\psi\rangle = (\hat{B}-\langle\hat{B}\rangle)|\psi\rangle.$$

$\cancel{Su}$ Schwartz 不等式:

$$\langle\chi|\chi\rangle\langle\phi|\phi\rangle \geq |\langle\chi|\phi\rangle|^2. \quad (*)$$

由于 $\hat{A}$. $\hat{B}$ 是厄米的. $\Delta\hat{A}^+ = \hat{A}^+ - \langle\hat{A}\rangle = \hat{A}-\langle\hat{A}\rangle = \Delta\hat{A}$ (厄米).

$\Delta\hat{B}$ 同理.

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$\langle \chi|\chi\rangle = (\Delta\hat{A}|\psi\rangle)^+|\chi\rangle$

$= \langle\psi|\Delta\hat{A}^+|\chi\rangle = \langle\psi|\Delta\hat{A}\cdot\Delta\hat{A}|\psi\rangle = \langle\psi|(\Delta\hat{A})^2|\psi\rangle$

$= \langle(\Delta\hat{A})^2\rangle$

同理，$\langle\phi|\phi\rangle = \langle\phi|(\Delta\hat{B})^2|\phi\rangle$.

$\langle\chi|\phi\rangle = \langle\psi|\Delta\hat{A}\Delta\hat{B}|\psi\rangle$

(*)：$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq |\langle\Delta\hat{A}\Delta\hat{B}\rangle|^2$ ①

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

由于 $[\hat{A},\hat{B}] = [\Delta\hat{A},\Delta\hat{B}]$

(证明：左 $= \hat{A}\hat{B}-\hat{B}\hat{A}$.

右 $= [\hat{A}-\langle\hat{A}\rangle, \hat{B}-\langle\hat{B}\rangle]$

都是数

$= \hat{A}\hat{B} - \hat{A}\langle\hat{B}\rangle - \hat{B}\langle\hat{A}\rangle\hat{B} - \langle\hat{A}\rangle\langle\hat{B}\rangle$

$-(\hat{B}\hat{A} - \langle\hat{B}\rangle\hat{A} - \hat{B}\langle\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle)$

$= \hat{A}\hat{B} - \hat{B}\hat{A}$

$= [\hat{A},\hat{B}]$.)

由于 $[\hat{A},\hat{B}]$ 是反厄米的.

$\{\Delta\hat{A},\Delta\hat{B}\}$ 是厄米的 $\cdot$($\{\Delta\hat{A},\Delta\hat{B}\}^+ = [(\Delta\hat{A}\Delta\hat{B}+\Delta\hat{B}\Delta\hat{A})]^+$

$= \{\Delta\hat{A},\Delta\hat{B}\}$)

$\Rightarrow \langle\Delta\hat{A}\Delta\hat{B}\rangle$ 由 $\langle\frac{1}{2}\{\Delta\hat{A},\Delta\hat{B}\}\rangle$ 作为实部.

$\langle\frac{1}{2}[\hat{A},\hat{B}]\rangle$ 作为虚部.

$\Rightarrow \langle\Delta\hat{A}\Delta\hat{B}\rangle^2 = \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2 + \underbrace{\frac{1}{4}|\langle\{\Delta\hat{A},\Delta\hat{B}\}\rangle|^2}_{\geq 0.}$

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

①② 对比：

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

开根号：$\Delta A\,\Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$ (☆)

(见上页)

应用在 $\hat{p}$. $\hat{x}$ 上：Heisenberg 测不准原理.

Example 2.9. Heisenberg 测不准关系.

利用(的)式: ~~ΔA~~ $\hat{A}=\hat{x}$, $\hat{B}=\hat{p_x}$

数字. $\Delta x \Delta p_x \geq \frac{1}{2}\mathbb{E}|\langle[\hat{x},\hat{p_x}]\rangle|$.

$\because [\hat{x},\hat{p_x}] = i\hbar\hat{I}$

$\Rightarrow \Delta x \Delta p_x \geq \frac{1}{2}\hbar$

同理: $\Delta y \Delta p_y \geq \frac{1}{2}\hbar$

$\Delta z \Delta p_z \geq \frac{1}{2}\hbar$

6. 算符的函数:

$F(\hat{A})$. 若 $\hat{A}$ 是线性算符. 则 Taylor 展开:

$$F(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n$$

$e^{a\hat{A}}$. (a: 标量)

$$\Rightarrow e^{a\hat{A}} = \sum_{n=0}^{\infty}\frac{a^n}{n!}A^n = \hat{I} + a\hat{A} + \frac{\hat{a}^2}{2!}\hat{A}^2 + \frac{\hat{a}^3}{3!}\hat{A}^3 + \cdots \quad (*)$$

(1) 涉及函数算符的对易:

若 $[\hat{A},\hat{B}]=0$. $\Rightarrow [\hat{B}, F(\hat{A})]=0$.

特别地. $[\hat{A}, F(\hat{A})]=0$.

$[\hat{A}^n, F(\hat{A})]=0$.

$[F(\hat{A}), G(\hat{A})]=0$.

(2) 厄米共轭:

$$[F(\hat{A})]^{\dagger} = F^*(\hat{A}^{\dagger})$$

① 若 $\hat{A}$ 是厄米的. $F(\hat{A})$ 不一定厄米.

② $F(\hat{A})$ 厄米 $\Leftrightarrow$ F是一个实函数, 且 $\hat{A}$ 厄米.

例: $(e^{\hat{A}})^{\dagger} = e^{\hat{A}^{\dagger}}$ $\quad (e^{i\hat{A}})^{\dagger} = e^{-i\hat{A}^{\dagger}}$

$(e^{ia\hat{A}})^{\dagger} = e^{-ia^*\hat{A}^{\dagger}}$.

若 $\hat{A}$ 是厄米的. $F(\hat{A}) = \sum_{n=0}^{\infty} a_n\hat{A}^n$ 厄米 $\Leftrightarrow$ a_n 是实数.

但一般来说不满足. $\Rightarrow$ $\underline{[F(\hat{A})]^{\dagger} = F^*(\hat{A}^{\dagger}) = \sum_{n=0}^{\infty} a_n^*(\hat{A}^{\dagger})^n}$