

课堂练习

练习1: 证明么正算符的本征值 $|\lambda| = 1$

证明: 根据么正算符 \hat{U} 的定义, 对任意态矢 $|\lambda\rangle$, 有 $\langle\lambda|\hat{U}^\dagger\hat{U}|\lambda\rangle = \langle\lambda|\hat{I}|\lambda\rangle = \langle\lambda|\lambda\rangle$, 而算符 \hat{U} 满足 $\hat{U}|\lambda\rangle = \lambda|\lambda\rangle$, 两边取厄米共轭, 得 $\langle\lambda|\hat{U}^\dagger = \langle\lambda|\lambda^*$, 因此有 $\langle\lambda|\hat{U}^\dagger\hat{U}|\lambda\rangle = |\lambda|^2\langle\lambda|\lambda\rangle$, 从而 $|\lambda|^2 = 1$, 即 $|\lambda| = 1$ ($|\lambda|$ 作为模长, 必须满足 $|\lambda| \geq 0$)

练习2: 证明 $\psi_k(x)$ 和 $\psi_{k+K_m}(x)$, 其中 $K_m \equiv \frac{2\pi m}{a}$ (m 为任意整数), 具有相同的平移对称性, 即具有相同的平移算符本征值

证明: 因为

$$\hat{D}(na)\psi_k(x) = e^{ikna}\psi_k(x)$$

$$\hat{D}(na)\psi_{k+K_m}(x) = e^{i(k+K_m)na}\psi_{k+K_m}(x) = e^{ikna} \cdot e^{i\frac{2\pi m}{a} \cdot na}\psi_{k+K_m}(x) = e^{ikna} \cdot e^{2\pi imn}\psi_{k+K_m}(x) = e^{ikna}\psi_{k+K_m}(x)$$

所以 $\psi_k(x)$ 和 $\psi_{k+K_m}(x)$ 具有相同的平移算符本征值

第三章习题

3.1 已知 $\hat{H}(\lambda)|\psi(\lambda)\rangle = E(\lambda)|\psi(\lambda)\rangle$, λ 为一连续变化的(实)参数, 设恒有 $\langle\psi|\psi\rangle = 1$, 证明 $\frac{\partial E}{\partial \lambda} = \langle\psi|\frac{\partial \hat{H}}{\partial \lambda}|\psi\rangle$, 此结果称为费曼-海尔曼定理, 在量子化学计算中有重要应用

证明: 记态矢 $|\psi(\lambda)\rangle$ 对 λ 的导数为 $|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle$, 对原式两边求导, 得

$$\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \hat{H}(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle = \frac{\partial E(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + E(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle$$

两边左乘 $\langle\psi(\lambda)|$, 注意到哈密顿算符的厄米性, 因此 $E(\lambda)$ 为实数, 从而

$$\begin{aligned} \langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \langle\psi(\lambda)|\hat{H}(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle &= \langle\psi(\lambda)|\frac{\partial E(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \langle\psi(\lambda)|E(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle \\ \Rightarrow \langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + E(\lambda)\langle\psi(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle &= \frac{\partial E(\lambda)}{\partial \lambda}\langle\psi(\lambda)|\psi(\lambda)\rangle + E(\lambda)\langle\psi(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle \\ \Rightarrow \langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle &= \frac{\partial E(\lambda)}{\partial \lambda} \end{aligned}$$

另证: 两边先左乘 $\langle\psi(\lambda)|$, 得 $\langle\psi(\lambda)|\hat{H}(\lambda)|\psi(\lambda)\rangle = \langle\psi(\lambda)|E(\lambda)|\psi(\lambda)\rangle = E(\lambda)\langle\psi(\lambda)|\psi(\lambda)\rangle = E(\lambda)$, 接下来对两边求导, 结合哈密顿算符的厄米性, 得

$$\begin{aligned} \langle\frac{\partial \psi(\lambda)}{\partial \lambda}|\hat{H}(\lambda)|\psi(\lambda)\rangle + \langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \langle\psi(\lambda)|\hat{H}(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle &= \frac{\partial E(\lambda)}{\partial \lambda} \\ \Rightarrow \langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + E(\lambda)[\langle\frac{\partial \psi(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \langle\psi(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle] &= \frac{\partial E(\lambda)}{\partial \lambda} \end{aligned}$$

而对归一化条件求导得 $\langle\psi|\psi\rangle = 1 \Rightarrow \langle\frac{\partial \psi(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle + \langle\psi(\lambda)|\frac{\partial \psi(\lambda)}{\partial \lambda}\rangle = 0$, 代回上式, 即有

$$\langle\psi(\lambda)|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}|\psi(\lambda)\rangle = \frac{\partial E(\lambda)}{\partial \lambda}$$

3.2 可以用如下的势能体系作为化学键的最简单的模型

$$V(x) = \begin{cases} \infty & (x \leq a_1) \\ -V_0 & (a_1 < x < a_2) \\ 0 & (x \geq a_2) \end{cases}$$

其中 $V_0 > 0$ 。请分别在 $E > 0$ 和 $E < 0$ 的情形下求解该体系，并联系化学键的性质进行讨论。体系能够有束缚态的条件是什么？

解：

3.3 求解如下 δ 势阱的本征态，该势阱的势能函数满足 $V(x) = -\gamma\delta(x)$ ($\gamma > 0$)

解：将势能函数代入薛定谔方程得 $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \gamma\delta(x)\psi(x) = E\psi(x)$ ，即

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2} [E + \gamma\delta(x)]\psi(x)，现在分 $E > 0$ 和 $E < 0$ 的情形进行讨论。$$

若 $E > 0$ ，体系为非束缚态，由于在 $x = 0$ 处 δ 函数发散，因此此处 $\psi'(x)$ 不连续，在邻域 $U(0, \varepsilon)$ 上对薛定谔方程积分，得 $\psi'(\varepsilon) - \psi'(-\varepsilon) = -\frac{2m\gamma}{\hbar^2} \cdot 2\varepsilon - \frac{2m\gamma}{\hbar^2} \psi(0)$ ，取 $\varepsilon \rightarrow 0$ ，得

$$\psi'(0^+) - \psi'(0^-) = -\frac{2m\gamma}{\hbar^2} \psi(0)，这是 $x = 0$ 处的跃变条件。设平面波 e^{ikx} 从负无穷处入射，其中$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}，则在 $x \neq 0$ 处，波函数满足 $\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & (x < 0) \\ Se^{ikx} & (x > 0) \end{cases}$ ，其导数满足$$

$$\psi'(x) = \begin{cases} ik(e^{ikx} - Re^{-ikx}) & (x < 0) \\ ikSe^{ikx} & (x > 0) \end{cases}，根据波函数的连续性，有 $\psi(0^+) = \psi(0^-)$ ，联立这两个条件，并代入数据，得：$$

$$\begin{cases} 1 + R = S \\ ik[S - (1 - R)] = -\frac{2m\gamma}{\hbar^2} S \end{cases} \Rightarrow \begin{cases} R = -\frac{m\gamma}{ik\hbar^2 + m\gamma} \\ S = \frac{1}{1 + \frac{m\gamma}{ik\hbar^2}} = \frac{ik\hbar^2}{ik\hbar^2 + m\gamma} \end{cases}$$

$$\text{故相应的本征函数为 } \psi(x) = \begin{cases} e^{ikx} - \frac{m\gamma}{ik\hbar^2 + m\gamma} e^{-ikx} & (x < 0) \\ \frac{ik\hbar^2}{ik\hbar^2 + m\gamma} e^{ikx} & (x > 0) \end{cases}$$

若 $E < 0$ ，因 $x \neq 0$ 时， $\psi''(x) = -\frac{2mE}{\hbar^2} \psi(x)$ ，而 $-\frac{2mE}{\hbar^2} > 0$ ，因此 $\psi(x)$ 为实函数，又知

$V(-x) = V(x) = 0$ ($x \neq 0$)，故 $\psi(x)$ 必满足一定的宇称性。若 $\psi(x)$ 为奇宇称，记 $k' = \sqrt{-\frac{2mE}{\hbar^2}}$ ，则

$$\text{波函数可写为 } \psi(x) = \begin{cases} Ae^{k'x} & (x < 0) \\ -Ae^{-k'x} & (x > 0) \end{cases} \quad (\text{注意到波函数在 } x \rightarrow \infty \text{ 时必须收敛至 } 0，\text{ 否则波函数无法归一化})$$

，根据波函数的连续性，有 $\psi(0^+) = \psi(0^-)$ ，代入得 $A = -A$ ，即 $A = 0$ ，此时

$\psi(x) = 0$ ($x \neq 0$)，与束缚态相矛盾，故 $\psi(x)$ 不可能为奇宇称。

$$\text{若 } \psi(x) \text{ 为偶宇称，则波函数可写为 } \psi(x) = \begin{cases} Ae^{k'x} & (x < 0) \\ Ae^{-k'x} & (x > 0) \end{cases}，此时 \psi(0^+) = \psi(0^-) = A，满足波$$

函数连续的条件，又波函数满足归一化条件，因此有

$$\begin{aligned} \int_{-\infty}^{+\infty} |\psi(x)|^2 dx &= \int_0^{+\infty} |Ae^{-k'x}|^2 dx + \int_{-\infty}^0 |Ae^{k'x}|^2 dx = |A|^2 \left(\int_0^{+\infty} e^{-2k'x} dx + \int_{-\infty}^0 e^{2k'x} dx \right) \\ &= |A|^2 \left[\int_0^{+\infty} \frac{e^{-2k'x}}{-2k'} d(-2k'x) + \int_{-\infty}^0 \frac{e^{2k'x}}{2k'} d(2k'x) \right] \\ &= |A|^2 \left\{ \left[\frac{e^{-2k'x}}{-2k'} \right]_0^{+\infty} + \left[\frac{e^{2k'x}}{2k'} \right]_{-\infty}^0 \right\} = \frac{|A|^2}{k'} = 1 \end{aligned}$$

解得 $|A| = \sqrt{k'}$, 若 A 取正实数, 则 $A = \sqrt{k'}$, 因此 $\psi(x) = \begin{cases} \sqrt{k'} e^{k'x} & (x < 0) \\ \sqrt{k'} e^{-k'x} & (x > 0) \end{cases}$, 相应的导数为

$$\psi'(x) = \begin{cases} k'^{\frac{3}{2}} e^{k'x} & (x < 0) \\ -k'^{\frac{3}{2}} e^{-k'x} & (x > 0) \end{cases}, \text{ 结合 } x=0 \text{ 处的跃变条件, 我们有 } (-k'^{\frac{3}{2}}) - k'^{\frac{3}{2}} = -\frac{2m\gamma}{\hbar^2} k'^{\frac{1}{2}}, \text{ 解}$$

$$\text{得 } k' = \frac{m\gamma}{\hbar^2} = \sqrt{-\frac{2mE}{\hbar^2}}, \text{ 因此本征能量为 } E = -\frac{m\gamma^2}{2\hbar^2}, \text{ 本征函数为 } \psi(x) = \begin{cases} \sqrt{\frac{m\gamma}{\hbar^2}} e^{\frac{m\gamma}{\hbar^2}x} & (x < 0) \\ \sqrt{\frac{m\gamma}{\hbar^2}} e^{-\frac{m\gamma}{\hbar^2}x} & (x > 0) \end{cases}$$

3.4 推导3.5节矩形势垒体系中, $E > V_0$ 时反射和投射系数

解: 为讨论问题方便, 设 $k_1^2 = \frac{2mE}{\hbar^2}$, $k_2^2 = \frac{2m(E-V_0)}{\hbar^2}$, 并假设平面波 e^{ik_1x} 从负无穷处向正方向传播,

$$\text{则对应的解为 } \psi(x) = \begin{cases} e^{ik_1x} + Be^{-ik_1x} & (x \leq -\frac{a}{2}) \\ Ce^{ik_2x} + De^{-ik_2x} & (|x| < \frac{a}{2}) \\ Se^{ik_1x} & (x \geq \frac{a}{2}) \end{cases}, \text{ 其导函数为}$$

$$\psi'(x) = \begin{cases} ik_1(e^{ik_1x} - Be^{-ik_1x}) & (x \leq -\frac{a}{2}) \\ ik_2(Ce^{ik_2x} - De^{-ik_2x}) & (|x| < \frac{a}{2}) \\ ik_1Se^{ik_1x} & (x \geq \frac{a}{2}) \end{cases}$$

$$\text{接下来, 考虑到边界连续条件及波函数光滑条件, 体系应满足 } \begin{cases} \psi_{x \rightarrow (-\frac{a}{2})^-} = \psi_{x \rightarrow (-\frac{a}{2})^+} \\ \psi'_{x \rightarrow (-\frac{a}{2})^-} = \psi'_{x \rightarrow (-\frac{a}{2})^+} \\ \psi_{x \rightarrow (\frac{a}{2})^-} = \psi_{x \rightarrow (\frac{a}{2})^+} \\ \psi'_{x \rightarrow (\frac{a}{2})^-} = \psi'_{x \rightarrow (\frac{a}{2})^+} \end{cases}, \text{ 代入可得}$$

$$\begin{cases} e^{-\frac{ik_1a}{2}} + Be^{\frac{ik_1a}{2}} = Ce^{-\frac{ik_2a}{2}} + De^{\frac{ik_2a}{2}} \\ ik_1(e^{-\frac{ik_1a}{2}} - Be^{\frac{ik_1a}{2}}) = ik_2(Ce^{-\frac{ik_2a}{2}} - De^{\frac{ik_2a}{2}}) \\ Ce^{\frac{ik_2a}{2}} + De^{-\frac{ik_2a}{2}} = Se^{\frac{ik_1a}{2}} \\ ik_2(Ce^{\frac{ik_2a}{2}} - De^{-\frac{ik_2a}{2}}) = ik_1Se^{\frac{ik_1a}{2}} \end{cases}, \text{ 经化简为}$$

$$\begin{cases} Ce^{-\frac{ik_2a}{2}} + De^{\frac{ik_2a}{2}} = e^{-\frac{ik_1a}{2}} + Be^{\frac{ik_1a}{2}} & \text{①} \\ Ce^{-\frac{ik_2a}{2}} - De^{\frac{ik_2a}{2}} = \frac{k_1}{k_2}(e^{-\frac{ik_1a}{2}} - Be^{\frac{ik_1a}{2}}) & \text{②} \\ Ce^{\frac{ik_2a}{2}} + De^{-\frac{ik_2a}{2}} = Se^{\frac{ik_1a}{2}} & \text{③} \\ Ce^{\frac{ik_2a}{2}} - De^{-\frac{ik_2a}{2}} = \frac{k_1}{k_2}Se^{\frac{ik_1a}{2}} & \text{④} \end{cases}$$

$$\frac{\text{①}+\text{②}}{2} \cdot e^{\frac{ik_2a}{2}}, \text{ 得 } C = \frac{1}{2}e^{\frac{ik_2a}{2}} \left(\frac{k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} + \frac{-k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} \right), \frac{\text{③}+\text{④}}{2} \cdot e^{-\frac{ik_2a}{2}}, \text{ 得}$$

$$C = \frac{1}{2}e^{-\frac{ik_2a}{2}} \cdot \frac{k_1+k_2}{k_2}Se^{\frac{ik_1a}{2}} = \frac{k_1+k_2}{2k_2}Se^{\frac{i(k_1-k_2)a}{2}}, \text{ 代入可得}$$

$$\begin{aligned} \frac{1}{2}e^{\frac{ik_2a}{2}} \left(\frac{k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} + \frac{-k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} \right) &= \frac{k_1+k_2}{2k_2}Se^{\frac{i(k_1-k_2)a}{2}} \\ \Rightarrow \frac{-k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} &= \frac{k_1+k_2}{k_2}Se^{\frac{i(k_1-2k_2)a}{2}} - \frac{k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} \end{aligned} \quad \text{⑤}$$

$$\frac{\text{①}-\text{②}}{2} \cdot e^{-\frac{ik_2a}{2}}, \text{ 得 } D = \frac{1}{2}e^{-\frac{ik_2a}{2}} \left(\frac{-k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} + \frac{k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} \right); \frac{\text{③}-\text{④}}{2} \cdot e^{\frac{ik_2a}{2}}, \text{ 得}$$

$$D = \frac{1}{2}e^{\frac{ik_2a}{2}} \cdot \frac{-k_1+k_2}{k_2}Se^{\frac{ik_1a}{2}} = \frac{-k_1+k_2}{2k_2}Se^{\frac{i(k_1+k_2)a}{2}}, \text{ 代入可得}$$

$$\begin{aligned} \frac{1}{2}e^{-\frac{ik_2a}{2}} \left(\frac{-k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} + \frac{k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} \right) &= \frac{-k_1+k_2}{2k_2}Se^{\frac{i(k_1+k_2)a}{2}} \\ \Rightarrow \frac{k_1+k_2}{k_2}Be^{\frac{ik_1a}{2}} &= \frac{-k_1+k_2}{k_2}Se^{\frac{i(k_1+2k_2)a}{2}} - \frac{-k_1+k_2}{k_2}e^{-\frac{ik_1a}{2}} \end{aligned} \quad \text{⑥}$$

故联立⑤与⑥得

$$(-k_1+k_2)[(-k_1+k_2)Se^{\frac{i(k_1+2k_2)a}{2}} - (-k_1+k_2)e^{-\frac{ik_1a}{2}}] = (k_1+k_2)[(k_1+k_2)Se^{\frac{i(k_1-2k_2)a}{2}} - (k_1+k_2)e^{-\frac{ik_1a}{2}}]$$

解得,

3.5 计算谐振子势场中算符 $\hat{x}, \hat{p}, \hat{x}^2, \hat{p}^2$ 在基态的期望值, 并验证坐标和动量之间的测不准关系

解: 由于湮灭和产生算符的定义为 $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i\hat{p}}{m\omega})$, $\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i\hat{p}}{m\omega})$, 因此有

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a}), \quad \text{从而有}$$

$$\begin{aligned}\hat{x}^2 &= \frac{\hbar}{2m\omega}[\hat{a}^2 + (\hat{a}^\dagger)^2 + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger] = \frac{\hbar}{2m\omega}[\hat{a}^2 + (\hat{a}^\dagger)^2 + (\hat{N} + \hat{N} + 1)] = \frac{\hbar}{2m\omega}[\hat{a}^2 + (\hat{a}^\dagger)^2 + 2\hat{N} + 1] \\ \hat{p}^2 &= -\frac{m\hbar\omega}{2}[\hat{a}^2 + (\hat{a}^\dagger)^2 - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger] = -\frac{m\hbar\omega}{2}[\hat{a}^2 + (\hat{a}^\dagger)^2 - \hat{N} - (\hat{N} + 1)] = -\frac{m\hbar\omega}{2}[\hat{a}^2 + (\hat{a}^\dagger)^2 - 2\hat{N} - 1]\end{aligned}$$

因此

$$\begin{aligned}\langle 0|\hat{x}|0\rangle &= \langle 0|\sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle 0|\hat{a}|0\rangle + \langle 0|\hat{a}^\dagger|0\rangle) = \sqrt{\frac{\hbar}{2m\omega}}(\langle 0|\cdot\mathbf{0} + \langle 0|\cdot\mathbf{1}\rangle) = 0 \\ \langle 0|\hat{p}|0\rangle &= \langle 0|i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})|0\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(\langle 0|\hat{a}^\dagger|0\rangle - \langle 0|\hat{a}|0\rangle) = \sqrt{\frac{\hbar}{2m\omega}}(\langle 0|\cdot\mathbf{1}\rangle - \langle 0|\cdot\mathbf{0}\rangle) = 0 \\ \langle 0|\hat{x}^2|0\rangle &= \langle 0|\hat{x}|0\rangle = \langle 0|\frac{\hbar}{2m\omega}[\hat{a}^2 + (\hat{a}^\dagger)^2 + 2\hat{N} + 1]|0\rangle = \frac{\hbar}{2m\omega}[\langle 0|\hat{a}^2|0\rangle + \langle 0|(\hat{a}^\dagger)^2|0\rangle + 2\langle 0|\hat{N}|0\rangle + \langle 0|0\rangle] \\ &= \frac{\hbar}{2m\omega}[(\langle 0|\hat{a}\rangle \cdot \langle \hat{a}|0\rangle) + (\langle 0|\hat{a}^\dagger\rangle \cdot \langle \hat{a}^\dagger|0\rangle) + 2\langle 0|\cdot\mathbf{0}|0\rangle + 1] = \frac{\hbar}{2m\omega}[\langle \mathbf{1}|\cdot\mathbf{0} + \mathbf{0}\cdot\mathbf{1}\rangle + 1] = \frac{\hbar}{2m\omega} \\ \langle 0|\hat{p}^2|0\rangle &= \langle 0|-\frac{m\hbar\omega}{2}[\hat{a}^2 + (\hat{a}^\dagger)^2 - 2\hat{N} - 1]|0\rangle = -\frac{m\hbar\omega}{2}[\langle 0|\hat{a}^2|0\rangle + \langle 0|(\hat{a}^\dagger)^2|0\rangle - 2\langle 0|\hat{N}|0\rangle - \langle 0|0\rangle] \\ &= -\frac{m\hbar\omega}{2}[(\langle 0|\hat{a}\rangle \cdot \langle \hat{a}|0\rangle) + (\langle 0|\hat{a}^\dagger\rangle \cdot \langle \hat{a}^\dagger|0\rangle) - 2\langle 0|\cdot\mathbf{0}|0\rangle - 1] = -\frac{m\hbar\omega}{2}[\langle \mathbf{1}|\cdot\mathbf{0} + \mathbf{0}\cdot\mathbf{1}\rangle - 1] = \frac{m\hbar\omega}{2}\end{aligned}$$

另一方面, 设 $\Delta\hat{x} = \hat{x} - \langle\hat{x}\rangle$, $\Delta\hat{p} = \hat{p} - \langle\hat{p}\rangle$, 其中 $\langle\hat{x}\rangle, \langle\hat{p}\rangle$ 为相应算符在态矢上的期望值, 满足 $\langle x\rangle = \langle n|\hat{x}|n\rangle$, $\langle p\rangle = \langle n|\hat{p}|n\rangle$, 则对任意本征态矢, 有

$$\begin{aligned}\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle &= \langle n|(\hat{x} - \langle\hat{x}\rangle)^2|n\rangle\langle n|(\hat{p} - \langle\hat{p}\rangle)^2|n\rangle = \langle n|\hat{x}^2 - 2\langle\hat{x}\rangle\hat{x} + \langle\hat{x}\rangle^2|n\rangle\langle n|\hat{p}^2 - 2\langle\hat{p}\rangle\hat{p} + \langle\hat{p}\rangle^2|n\rangle \quad (\text{此处用到期望值为实数的性质}) \\ &= (\langle\hat{x}^2\rangle - 2\langle\hat{x}\rangle^2 + \langle\hat{x}\rangle^2)(\langle\hat{p}^2\rangle - 2\langle\hat{p}\rangle^2 + \langle\hat{p}\rangle^2) = (\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2)(\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2) \\ &= (\frac{(2n+1)\hbar}{2m\omega} - 0)(\frac{(2n+1)m\hbar\omega}{2} - 0) = \frac{(2n+1)^2\hbar^2}{4}\end{aligned}$$

$$\frac{1}{4}|\langle[\hat{x}, \hat{p}]\rangle|^2 = \frac{1}{4}|\langle n|[\hat{x}, \hat{p}]|n\rangle|^2 = \frac{1}{4}|\mathbf{i}\hbar\langle n|n\rangle|^2 = \frac{\hbar^2}{4}$$

从而 $\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle = \frac{(2n+1)^2\hbar^2}{4} \geq \frac{(2\times 0+1)^2\hbar^2}{4} = \frac{\hbar^2}{4} = \frac{1}{4}|\langle[\hat{x}, \hat{p}]\rangle|^2$, 即谐振子体系满足不确定性原理

注: 对任意状态 (无论是基态还是激发态) 验证 \hat{x} 和 \hat{p} 的对易关系, 得

$$\begin{aligned}[\hat{x}, \hat{p}]|n\rangle &= [\sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})]|n\rangle = \frac{i\hbar}{2}[\hat{a} + \hat{a}^\dagger, \hat{a}^\dagger - \hat{a}]|n\rangle = \frac{i\hbar}{2}([\hat{a} + \hat{a}^\dagger, \hat{a}^\dagger] - [\hat{a} + \hat{a}^\dagger, \hat{a}])|n\rangle \\ &= \frac{i\hbar}{2}([\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}^\dagger] - [\hat{a}, \hat{a}] - [\hat{a}^\dagger, \hat{a}])|n\rangle = \frac{i\hbar}{2}[1 + 0 - 0 - (-1)]|n\rangle = i\hbar|n\rangle\end{aligned}$$

因此 $[\hat{x}, \hat{p}] = i\hbar$, 满足对易关系

课堂练习 (续)

练习3: 升降算符满足如下的对易关系: (1) $[\hat{J}^2, \hat{J}_\pm] = 0$; (2)

$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z; \quad (3) \quad [\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$$

证明: 首先证明引理 $[\hat{J}^2, \hat{J}_x] = [\hat{J}^2, \hat{J}_y] = [\hat{J}^2, \hat{J}_z] = 0$, 显然

$$[\hat{J}^2, \hat{J}_x] = [\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \hat{J}_x] = [\hat{J}_x^2, \hat{J}_x] + [\hat{J}_y^2, \hat{J}_x] + [\hat{J}_z^2, \hat{J}_x] = 0 + \hat{J}_y[\hat{J}_y, \hat{J}_x] + [\hat{J}_y, \hat{J}_x]\hat{J}_y + \hat{J}_z[\hat{J}_z, \hat{J}_x] + [\hat{J}_z, \hat{J}_x]\hat{J}_z \\ = \hat{J}_y \cdot (-\hat{J}_z) + (-\hat{J}_z) \cdot \hat{J}_y + \hat{J}_z\hat{J}_y + \hat{J}_y\hat{J}_z = 0$$

$$[\hat{J}^2, \hat{J}_y] = [\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \hat{J}_y] = [\hat{J}_x^2, \hat{J}_y] + [\hat{J}_y^2, \hat{J}_y] + [\hat{J}_z^2, \hat{J}_y] = \hat{J}_x[\hat{J}_x, \hat{J}_y] + [\hat{J}_x, \hat{J}_y]\hat{J}_x + 0 + \hat{J}_z[\hat{J}_z, \hat{J}_y] + [\hat{J}_z, \hat{J}_y]\hat{J}_z \\ = \hat{J}_x\hat{J}_z + \hat{J}_z\hat{J}_x + \hat{J}_z \cdot (-\hat{J}_x) + (-\hat{J}_x) \cdot \hat{J}_z = 0$$

$$[\hat{J}^2, \hat{J}_z] = [\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \hat{J}_z] = [\hat{J}_x^2, \hat{J}_z] + [\hat{J}_y^2, \hat{J}_z] + [\hat{J}_z^2, \hat{J}_z] = 0 + \hat{J}_y[\hat{J}_y, \hat{J}_z] + [\hat{J}_y, \hat{J}_z]\hat{J}_y + \hat{J}_x[\hat{J}_x, \hat{J}_z] + [\hat{J}_x, \hat{J}_z]\hat{J}_x \\ = \hat{J}_y \cdot (-\hat{J}_x) + (-\hat{J}_x) \cdot \hat{J}_y + \hat{J}_x\hat{J}_y + \hat{J}_y\hat{J}_x = 0$$

(1) 由于 $\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$, 因此 $[\hat{J}^2, \hat{J}_{\pm}] = [\hat{J}^2, \hat{J}_x] \pm i[\hat{J}^2, \hat{J}_y] = 0$

(2) 易知

$$[\hat{J}_+, \hat{J}_-] = \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+ = (\hat{J}_x + i\hat{J}_y)(\hat{J}_x - i\hat{J}_y) - (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y) \\ = (\hat{J}_x^2 - \hat{J}_y^2 - i[\hat{J}_x, \hat{J}_y]) - (\hat{J}_x^2 - \hat{J}_y^2 + i[\hat{J}_x, \hat{J}_y]) = -2i[\hat{J}_x, \hat{J}_y] \\ = -2i \cdot i\hbar\hat{J}_z = 2\hbar\hat{J}_z$$

(3) 易知

$$[\hat{J}_z, \hat{J}_{\pm}] = [\hat{J}_z, \hat{J}_x \pm i\hat{J}_y] = [\hat{J}_z, \hat{J}_x] \pm i[\hat{J}_z, \hat{J}_y] = i\hbar\hat{J}_y \pm i(-i\hbar\hat{J}_x) = \hbar(i\hat{J}_y \pm \hat{J}_x) = \pm\hbar\hat{J}_{\pm}$$

练习4: 推导 $\langle jm' | \hat{J}_x | jm \rangle$ 的表达式

解: 由于 $\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$, 即 $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$, 因此

$$\langle jm' | \hat{J}_x | jm \rangle = \langle jm' | \frac{1}{2}(\hat{J}_+ + \hat{J}_-) | jm \rangle = \frac{1}{2}(\langle jm' | \hat{J}_+ | jm \rangle + \langle jm' | \hat{J}_- | jm \rangle) \\ = \frac{1}{2}(\sqrt{j(j+1) - m(m+1)}\hbar\langle jm' | j(m+1) \rangle + \sqrt{j(j+1) - m(m-1)}\hbar\langle jm' | j(m-1) \rangle) \\ = \frac{\hbar}{2}(\sqrt{(j+m+1)(j-m)}\delta_{m',m+1} + \sqrt{(j-m+1)(j+m)}\delta_{m',m-1})$$