5.29.

由 e 有. $Be^{-\lambda a} = \frac{1}{2}\left(1-\frac{ik}{\lambda}\right)e^{ika}C$

$$B'e^{\lambda a} = \frac{1}{2}\left(1+\frac{ik}{\lambda}\right)e^{ika}C$$

代入 d, 有:

$$ik(A+A')+ik(A-A') = 2ikA$$

$$= ik(B+B')-\lambda(B-B') = (ik-\lambda)B+(ik+\lambda)B'$$

$$= \frac{1}{2}(ik-\lambda)\left(1-\frac{ik}{\lambda}\right)e^{\lambda a}e^{ika}C+\frac{1}{2}(ik+\lambda)\left(1+\frac{ik}{\lambda}\right)e^{-\lambda a}e^{ika}C$$

$$= \left[(\lambda+ik)^2e^{-\lambda a}-(\lambda-ik)^2e^{\lambda a}\right]\frac{e^{ika}}{2\lambda}C$$

$$\Rightarrow \quad C = \frac{4i\lambda k e^{-ika}}{(ik+\lambda)^2e^{-\lambda a}-(\lambda-ik)^2e^{\lambda a}}A$$

从而

$$B = \frac{1}{2\lambda}(\lambda-ik)e^{\lambda a}e^{ika}C = \frac{2ik(\lambda-ik)e^{\lambda a}}{(ik+\lambda)^2e^{-\lambda a}-(\lambda-ik)^2e^{\lambda a}}A$$

$$B' = \frac{1}{2\lambda}(\lambda+ik)e^{-\lambda a}e^{ika}C = \frac{2ik(\lambda+ik)e^{-\lambda a}}{(\lambda+ik)^2e^{-\lambda a}-(\lambda-ik)^2e^{\lambda a}}A$$

$$A' = \frac{1}{2ik}\left[ik(B+B')+\lambda(B-B')\right] = \frac{1}{2ik}\left[(\lambda+ik)B-(\lambda-ik)B'\right]$$

$$= \frac{(\lambda^2+k^2)(e^{\lambda a}-e^{-\lambda a})}{(\lambda+ik)^2e^{-\lambda a}-(\lambda-ik)^2e^{\lambda a}}A$$

易知

$$B = \frac{(\lambda-ik)A+(\lambda+ik)A'}{2\lambda} \qquad B' = \frac{(\lambda-ik)A'+(\lambda+ik)A}{2\lambda}$$

5.31

1. 基态波函数为

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \quad (\text{已归一化})$$

$$\Rightarrow E_0^{(1)} = \langle \psi_0 | \hat{H}^{(1)} | \psi_0 \rangle$$

$$= \int_{-\infty}^{+\infty} \psi_0^*(x) \hat{H}^{(1)} \psi_0(x)\, dx$$

$$= \int_{-\infty}^{+\infty} \psi_0^*(x)\, \lambda x^4 \psi(x)\, dx$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, \lambda \int_{-\infty}^{+\infty} x^4 e^{-\frac{m\omega}{\hbar}x^2}\, dx$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, \lambda \left.\frac{d^2}{d\alpha^2}\right|_{\alpha=\frac{m\omega}{\hbar}} \int e^{-\alpha x^2}\, dx$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, \lambda \left.\frac{d^2}{d\alpha^2}\right|_{\alpha=\frac{m\omega}{\hbar}} \left(\sqrt{\frac{\pi}{\alpha}}\right) = \frac{3\hbar^2\lambda}{4m^2\omega^2}$$

2. 基态波函数

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

$$H^{(1)} = \frac{1}{2}m\left[(\omega+\delta\omega)^2 - \omega^2\right]x^2$$

$$= \frac{1}{2}m\left(2\omega\delta\omega + \delta\omega^2\right)x^2$$

$$E_0^{(1)} = \int \psi_0^*(x) \hat{H}^{(1)} \psi_0(x)\, dx$$

$$= \frac{1}{2}m\left(2\omega\delta\omega + \delta\omega^2\right)\sqrt{\frac{m\omega}{\pi\hbar}} \int x^2 e^{-\frac{m\omega}{\hbar}x^2}\, dx$$

$$= \frac{1}{2}m\left(2\omega\delta\omega + \delta\omega^2\right)\sqrt{\frac{m\omega}{\pi\hbar}} \cdot \frac{1}{\frac{2m\omega}{\hbar}}\sqrt{\frac{\pi\hbar}{m\omega}}$$

$$= \frac{\hbar}{4\omega}\left(2\omega\delta\omega + \delta\omega^2\right) \simeq \frac{\hbar}{4\omega} 2\omega\delta\omega = \frac{1}{2}\hbar\delta\omega$$

2. $\hat{H}^{(0)}|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle$

$$(\hat{H}^{(0)}+\hat{H}^{(1)})(|\psi_n^{(0)}\rangle+|\psi_n^{(1)}\rangle+|\psi_n^{(2)}\rangle+\cdots)$$

$$=(E_n^{(0)}+E_n^{(1)}+E_n^{(2)}+\cdots)(|\psi_n^{(0)}\rangle+|\psi_n^{(1)}\rangle+|\psi_n^{(2)}\rangle+\cdots)$$

考虑二阶项:

$$\hat{H}^{(0)}|\psi_n^{(2)}\rangle+\hat{H}^{(1)}|\psi_n^{(1)}\rangle$$

$$=E_n^{(0)}|\psi_n^{(2)}\rangle+E_n^{(1)}|\psi_n^{(1)}\rangle+E_n^{(2)}|\psi_n^{(0)}\rangle$$

左右两边同时用 $\langle\psi_n^{(0)}|$ 作用:

$$左边=\langle\psi_n^{(0)}|\hat{H}^{(0)}|\psi_n^{(2)}\rangle+\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_n^{(1)}\rangle$$

$$=E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle+\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_n^{(1)}\rangle$$

$$=右边=\langle\psi_n^{(0)}|E_n^{(0)}|\psi_n^{(2)}\rangle+\langle\psi_n^{(0)}|E_n^{(1)}|\psi_n^{(1)}\rangle$$

$$+\langle\psi_n^{(0)}|E_n^{(2)}|\psi_n^{(0)}\rangle$$

$$=E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle+E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle+E_n^{(2)}$$

$$\Rightarrow E_n^{(2)}=\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_n^{(1)}\rangle-E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle$$

因 $|\psi_n^{(1)}\rangle = \sum_{m\neq n} \frac{H_{mn}^{(1)}}{E_n^{(0)}-E_m^{(0)}}|\psi_m^{(0)}\rangle$

$\Rightarrow \langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = 0$

$\Rightarrow E_n^{(2)} = \langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_n^{(1)}\rangle$

$$= \sum_{m\neq n} \frac{H_{mn}^{(1)}}{E_n^{(0)}-E_m^{(0)}}\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle$$

$$= \sum_{m\neq n} \frac{H_{mn}^{(1)}H_{nm}^{(1)}}{E_n^{(0)}-E_m^{(0)}}$$

$$= \sum_{m\neq n} \frac{|H_{mn}^{(1)}|^2}{E_n^{(0)}-E_m^{(0)}}$$

3. 取 $\hat{H}^{(0)} = \hat{T} + \hat{V}^{(0)}$

其中 $V^{(0)}(x) = 0 \quad (0<x<L)$

$\hat{H} = \hat{T} + \hat{V}$

其中 $V(x) = V_0\cos(\frac{4\pi}{L}x) \quad (0<x<L)$

则 $\hat{H}^{(1)} = \hat{H} - \hat{H}^{(0)} = \hat{V} = V_0 \cos(\frac{4\pi}{L} x)$

简并态 ψ_1、ψ_{-1} 的零级修正需要对角化矩阵

$$\begin{bmatrix} H_{11}^{(1)} & H_{12}^{(1)} \\ H_{21}^{(1)} & H_{22}^{(1)} \end{bmatrix}$$

其中：$H_{11}^{(1)} = \langle \psi_1 | \hat{H}^{(1)} | \psi_1 \rangle = \frac{1}{L} \int_0^L V_0 \cos(\frac{4\pi}{L} x) dx = 0$

$$H_{22}^{(1)} = \langle \psi_{-1} | \hat{H}^{(1)} | \psi_{-1} \rangle = \frac{1}{L} \int_0^L V_0 \cos(\frac{4\pi}{L} x) dx = 0$$

$$H_{12}^{(1)} = \langle \psi_1 | \hat{H}^{(1)} | \psi_{-1} \rangle = \frac{1}{L} \int_0^L V_0 \cos(\frac{4\pi}{L} x) e^{-i\frac{4\pi}{L} x} dx$$

$$= \frac{V_0}{2L} \int_0^L (1 + e^{-i\frac{8\pi}{L} x}) dx = \frac{1}{2} V_0$$

$$H_{21}^{(1)} = \langle \psi_{-1} | H^{(1)} | \psi_1 \rangle = \langle \psi_1 | \hat{H}^{(1)} | \psi_{-1} \rangle^* = \frac{1}{2} V_0$$

$\Rightarrow$ $\hat{H}^{(1)}$ 的与 ψ_1、ψ_{-1} 对应的子矩阵为：

$$\tilde{H}^{(1)} = \frac{V_0}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{V_0}{2} \sigma_x$$

对角化 $\tilde{H}^{(1)}$，即求其本征值和本征矢量：

利用σ_x的结论，有$\tilde{H}^{(1)}$有两个本征值：

$\lambda_1 = +\frac{V_0}{2}$

对应的本征态为：$|\tilde{\psi}_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

把基矢$|\psi_1\rangle$、$|\psi_{-1}\rangle$代入，有：

$|\tilde{\psi}_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_{-1}\rangle\right)$

或$\tilde{\psi}_1(x) = \frac{1}{\sqrt{2}}\left[\psi_1(x) + \psi_{-1}(x)\right] = \sqrt{\frac{2}{L}}\cos\frac{2\pi x}{L}$

$\lambda_2 = -\frac{V_0}{2}$

对应的本征态为 $|\tilde{\psi}_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$

把基矢$|\psi_1\rangle$、$|\psi_{-1}\rangle$代入，有：

$|\tilde{\psi}_2\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle - |\psi_{-1}\rangle\right)$

或 $\tilde{\psi}_2(x) = \frac{1}{\sqrt{2}}\left[\psi_1(x) - \psi_{-1}(x)\right] = i\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}$

⇒ 修正后的零级波函数为：

$\phi_1^{(0)}(x) = \tilde{\psi}_1(x) = \sqrt{\frac{2}{L}}\cos\frac{2\pi x}{L}$

$\phi_{-1}^{(0)}(x) = \tilde{\psi}_2(x) = i\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}$

一级修正后的能量为：

$$E_1 = \frac{2\hbar^2\pi^2}{mL^2} + \frac{1}{2}V_0$$

$$E_{-1} = \frac{2\hbar^2\pi^2}{mL} - \frac{1}{2}V_0$$