课堂练习

练习1：为什么采用玻恩-冯·卡门边界条件后，波矢必须表示成如下形式？

$$k = l\frac{2\pi}{L} = \frac{l}{N}\frac{2\pi}{a} \quad (l = 0, \pm 1, \pm 2, \pm 3, \ldots)$$

解：玻恩-冯·卡门边界条件表明，$\phi_k(x + Na) = \phi_k(x)$，又平面波可表示为$\phi_k(x) = L^{-\frac{1}{2}}\mathrm{e}^{\mathrm{i}kx}$，其中$L = Na$，代入得

$$L^{-\frac{1}{2}}\mathrm{e}^{\mathrm{i}k(x+Na)} = L^{-\frac{1}{2}}\mathrm{e}^{\mathrm{i}kx} \Rightarrow \mathrm{e}^{\mathrm{i}kNa} = 1 \Rightarrow kNa = 2\pi l \quad (l = 0, \pm 1, \pm 2, \pm 3, \ldots)$$

由此可得$k = \frac{l}{N}\frac{2\pi}{a}(l = 0, \pm 1, \pm 2, \pm 3, \ldots)$

练习2：对于矩阵元$V_{kk'} \equiv \langle \phi_k | \hat{V} | \phi_{k'} \rangle = L^{-1}\int_0^L V(x)\mathrm{e}^{-\mathrm{i}(k-k')x}dx$，求证只有当$k - k' = \frac{2\pi}{a}l$，其中$l$为任意整数时，矩阵元才不为零，并等于周期势函数$V(x)$对应于$q = \frac{2\pi}{a}l$的傅里叶积分

证明：注意到$V(x + na) = V(x)$，其中$n \in \mathbb{Z}$，利用傅里叶级数，我们有（设$V_l \equiv a^{-1}\int_0^a V(x)\mathrm{e}^{-\mathrm{i}\frac{2\pi l}{a}x}dx$）

$$V_{kk'} = L^{-1}\int_0^L V(x)\mathrm{e}^{-\mathrm{i}(k-k')x}dx = L^{-1}\int_0^L \Big[\sum_{l=-\infty}^{+\infty} V_l\mathrm{e}^{\mathrm{i}\frac{2\pi x}{a}l}\Big]\mathrm{e}^{-\mathrm{i}(k-k')x}dx = L^{-1}\int_0^L \Big[\sum_{l=-\infty}^{+\infty} V_l\mathrm{e}^{\mathrm{i}x(\frac{2\pi}{a}l-k+k')}\Big]dx$$

这样展开似乎找不出思路，我们改用如下方法：

$$V_{kk'} = L^{-1}\int_0^L V(x)\mathrm{e}^{-\mathrm{i}(k-k')x}dx = L^{-1}\sum_{n=0}^{N-1}\int_{na}^{(n+1)a} V(x)\mathrm{e}^{-\mathrm{i}(k-k')x}dx$$

$$= L^{-1}\sum_{n=0}^{N-1}\int_0^a V(x'+na)\mathrm{e}^{-\mathrm{i}(k-k')(x'+na)}d(x'+na)$$

$$= L^{-1}\sum_{n=0}^{N-1}\int_0^a V(x')\mathrm{e}^{-\mathrm{i}(k-k')x'}\cdot\mathrm{e}^{-\mathrm{i}(k-k')na}dx'$$

$$= L^{-1}\int_0^a V(x')\mathrm{e}^{-\mathrm{i}(k-k')x'}dx'\cdot\sum_{n=0}^{N-1}\mathrm{e}^{-\mathrm{i}(k-k')na}$$

若$\mathrm{e}^{-\mathrm{i}(k-k')a} = \mathrm{e}^{-\mathrm{i}\frac{2\pi(l-l')}{L}a} \neq 1$，则$\sum_{n=0}^{N-1}\mathrm{e}^{-\mathrm{i}(k-k')na} = \frac{1-\mathrm{e}^{-\mathrm{i}(k-k')(N-1)a}}{1-\mathrm{e}^{-\mathrm{i}(k-k')a}} = \frac{1-\mathrm{e}^{-\mathrm{i}\frac{2\pi(l-l')}{L}(N-1)a}}{1-\mathrm{e}^{-\mathrm{i}\frac{2\pi(l-l')}{L}a}} = 0$，故为使级数不为零，必须使$\mathrm{e}^{-\mathrm{i}(k-k')a} = 1$，从而有$(k-k')a = 2\pi l\ (l \in \mathbb{Z})$，即$k - k' = \frac{2\pi}{a}l$，从而

$$V_{kk'} = L^{-1}\int_0^a V(x)\mathrm{e}^{-\mathrm{i}\frac{2\pi l}{a}x}\cdot Ndx = a^{-1}\int_0^a V(x)\mathrm{e}^{-\mathrm{i}\frac{2\pi l}{a}x}dx \equiv V_l$$

练习3：写出波函数的一阶修正$\delta\psi_k^{(1)}(x)$，证明考虑了一阶修正后的波函数$\psi_k(x) = \phi_k(x) + \delta\psi_k^{(1)}(x)$满足 Bloch定理

解：对于$k \neq k'$，波函数的一阶修正$\delta\psi_k^{(1)}(x) = \sum_{k'\neq k}\frac{V_{k'k}}{\varepsilon_k-\varepsilon_{k'}}\phi_k'(x)$，由于矩阵元$V_{kk'}$只有在$k - k' = \frac{2\pi}{a}l\ (l \in \mathbb{Z})$时才不为0，因此

$$\psi_k(x) = \phi_k(x) + \delta\psi_k^{(1)}(x) = \phi_k(x) + \sum_{k' \neq k} \frac{V_{k'k}}{\varepsilon_k - \varepsilon_{k'}} \phi_k'(x)$$

$$= L^{-\frac{1}{2}} e^{ikx} + \sum_{l \neq 0} \frac{V_l^*}{\frac{\hbar^2}{2m}[k^2 - (k - \frac{2\pi}{a}l)^2]} L^{-\frac{1}{2}} e^{i(k - \frac{2\pi}{a}l)x}$$

$$= L^{-\frac{1}{2}} e^{ikx} \left\{ 1 + \frac{2m}{\hbar^2} \sum_{l \neq 0} \frac{V_l^*}{[k^2 - (k - \frac{2\pi}{a}l)^2]} e^{-i\frac{2\pi lx}{a}} \right\}$$

因此

$$\psi_k(x + na) = L^{-\frac{1}{2}} e^{ik(x+na)} \left\{ 1 + \frac{2m}{\hbar^2} \sum_{l \neq 0} \frac{V_l^*}{[k^2 - (k - \frac{2\pi}{a}l)^2]} e^{-i\frac{2\pi l(x+na)}{a}} \right\}$$

$$= e^{ikna} \cdot L^{-\frac{1}{2}} e^{ikx} \left\{ 1 + \frac{2m}{\hbar^2} \sum_{l \neq 0} \frac{V_l^*}{[k^2 - (k - \frac{2\pi}{a}l)^2]} e^{-i\frac{2\pi lx}{a}} e^{-2\pi inl} \right\}$$

$$= e^{ikna} \cdot L^{-\frac{1}{2}} e^{ikx} \left\{ 1 + \frac{2m}{\hbar^2} \sum_{l \neq 0} \frac{V_l^*}{[k^2 - (k - \frac{2\pi}{a}l)^2]} e^{-i\frac{2\pi lx}{a}} \right\} = e^{ikna} \psi_k(x)$$

从而$\psi_k(x)$满足Bloch原理，证毕

练习4：试应用简并态微扰理论，证明

$$E_\pm = \frac{\varepsilon_k + \varepsilon_{k'}}{2} + \sqrt{(\frac{\varepsilon_k - \varepsilon_{k'}}{2})^2 + |V_l|^2}$$

并推导当$\Delta \to 0$时，上式可简化为

$$E_\pm \approx \varepsilon_l(1 + \Delta^2) + \left(|V_l| + \frac{2\varepsilon_l^2 \Delta^2}{|V_l|}\right)$$

其中$\varepsilon_l = \frac{\hbar^2}{2m}\left(\frac{l\pi}{a}\right)^2$

证明：定义$k \equiv l\frac{\pi}{a}(1 + \Delta)$，$k' \equiv k - l\frac{2\pi}{a} = l\frac{\pi}{a}(-1 + \Delta)$，则当$\Delta \ll 1$时为近简并态，必须采用简并态微扰理论。记哈密尔顿算符为$\hat{H} = \hat{H}_0 + \hat{H}'$，其中$\hat{H}_0 = \frac{\hat{p}^2}{2m}$，$\hat{H}' = \hat{V}$，则薛定谔方程可写作$(\hat{H}_0 + \hat{H}')\psi_k = E\psi_k$，写成矩阵形式即为

$$\begin{pmatrix} \varepsilon_k & 0 \\ 0 & \varepsilon_{k'} \end{pmatrix} + \begin{pmatrix} 0 & V_{kk'} \\ V_{k'k} & 0 \end{pmatrix} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \Rightarrow \begin{pmatrix} \varepsilon_k - E & V_{kk'} \\ V_{k'k} & \varepsilon_{k'} - E \end{pmatrix} = 0$$

对应的久期方程为

$$\begin{vmatrix} \varepsilon_k - E & V_{kk'} \\ V_{k'k} & \varepsilon_{k'} - E \end{vmatrix} = 0 \Rightarrow (\varepsilon_k - E)(\varepsilon_{k'} - E) - V_{kk'}V_{k'k} = 0$$

$$\Rightarrow E^2 - (\varepsilon_k + \varepsilon_{k'})E + \varepsilon_k \varepsilon_{k'} - |V_l|^2 = 0$$

$$\Rightarrow E_\pm = \frac{(\varepsilon_k + \varepsilon_{k'}) + \sqrt{(\varepsilon_k + \varepsilon_{k'})^2 - 4(\varepsilon_k \varepsilon_{k'} - |V_l|^2)}}{2}$$

$$\Rightarrow E_\pm = \frac{\varepsilon_k + \varepsilon_{k'}}{2} + \sqrt{(\frac{\varepsilon_k - \varepsilon_{k'}}{2})^2 + |V_l|^2}$$

当$\Delta \to 0$时，由于$\varepsilon_k = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{l\pi}{a}\right)^2(1 + \Delta)^2$，$\varepsilon_{k'} = \frac{\hbar^2 k'^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{l\pi}{a}\right)^2(1 - \Delta)^2$，因此代入得

$$E_\pm = \frac{\hbar^2}{2m}(\frac{l\pi}{a})^2 \frac{(1+\Delta)^2+(1-\Delta)^2}{2} + \sqrt{[\frac{\hbar^2}{2m}(\frac{l\pi}{a})^2\frac{(1+\Delta)^2-(1-\Delta)^2}{2}]^2+|V_l|^2}$$

$$= \varepsilon_l(1+\Delta^2) + |V_l|\sqrt{(\frac{2\varepsilon_l\Delta}{|V_l|})^2+1} \approx \varepsilon_l(1+\Delta^2)+|V_l|[1+\frac{1}{2}(\frac{2\varepsilon_l\Delta}{|V_l|})^2]$$

$$= \varepsilon_l(1+\Delta^2)+(|V_l|+\frac{2\varepsilon_l^2\Delta^2}{|V_l|})$$

第六章习题

6.1 一维谐振子体系$V=\frac{1}{2}\mu\omega_0^2 x^2$受到如下微扰 (其中$\tau>0$)

$$H' = \begin{cases} 0 & (t<0) \\ a_0 x \mathrm{e}^{-\frac{t}{\tau}} & (t>0) \end{cases}$$

用一级微扰理论计算当t足够大后从基态向各激发态的跃迁概率

解：由于一级微扰系数为

$$c_n^{(1)}(t) = -\frac{\mathrm{i}}{\hbar}\int_0^t \langle n|\hat{H}'_I(t_1)|i\rangle dt_1 = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_n-E_i)t_1}\langle n|\hat{H}'(t_1)|i\rangle dt_1$$

$$= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{e}^{\mathrm{i}(n-i)\omega_0 t_1}\langle n|a_0\hat{x}\mathrm{e}^{-\frac{t_1}{\tau}}|i\rangle dt_1 = -\frac{\mathrm{i}a_0}{\hbar}\int_0^t \mathrm{e}^{[\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}]t_1}\langle n|\hat{x}|i\rangle dt_1$$

$$= -\frac{\mathrm{i}a_0}{\hbar}\int_0^t \mathrm{e}^{[\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}]t_1}\langle n|\sqrt{\frac{\hbar}{2\mu\omega_0}}(\sqrt{i+1}|i+1\rangle+\sqrt{i}|i-1\rangle)dt_1$$

$$= -\frac{\mathrm{i}a_0}{\hbar}\sqrt{\frac{\hbar}{2\mu\omega_0}}(\sqrt{i+1}\delta_{n,i+1}+\sqrt{i}\delta_{n,i-1})\int_0^t \mathrm{e}^{[\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}]t_1}dt_1$$

$$= -\frac{\mathrm{i}a_0}{\hbar}\sqrt{\frac{\hbar}{2\mu\omega_0}}(\sqrt{i+1}\delta_{n,i+1}+\sqrt{i}\delta_{n,i-1})\frac{\mathrm{e}^{[\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}]t}-1}{\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}}$$

$$= -\frac{\mathrm{i}a_0}{\hbar}\sqrt{\frac{\hbar}{2\mu\omega_0}}(\sqrt{i+1}\delta_{n,i+1}+\sqrt{i}\delta_{n,i-1})\frac{\mathrm{e}^{\mathrm{i}(n-i)\omega_0 t}-\mathrm{e}^{\frac{1}{\tau}t}}{\mathrm{e}^{\frac{1}{\tau}t}[\mathrm{i}(n-i)\omega_0-\frac{1}{\tau}]}$$

因此一级微扰下，从第i能级跃迁至第n能级的概率为

$$P_{n\leftarrow i}^{(1)}(t) = |c_n^{(1)}(t)|^2 = ?$$

由题意，$i=0$，结合上式可知，当$n=1$时，有$P_{1\leftarrow 0}^{(1)}(t)=?$，从而$t$足够大时，可得

$$\lim_{t\to\infty} P_{1\leftarrow 0}^{(1)}(t) = ?$$

6.2 精确求解一个带电为q的离子在谐振子势能面上同时受到均匀外电场ε的作用的问题，与§6.3节的结果比较。将极化率α定义为诱导偶极矩μ与外场强度ε之比，证明能量改变为$-\frac{\alpha\varepsilon^2}{2}$

解：

6.3 势能函数为如下形式的体系

$$V(x) = \begin{cases} \infty & (x\le 0, x\ge a) \\ 0 & (0<x<\frac{a}{3}, \frac{2a}{3}<x<a) \\ \frac{\hbar^2\pi^2}{20ma^2} & (\frac{a}{3}\le x\le\frac{2a}{3}) \end{cases}$$

(1)取 $\hat{H}_0$ 的势能函数为 $V_0(x) = \begin{cases} \infty & (x \le 0, x \ge a) \\ 0 & (0 < x < a) \end{cases}$，求 $\hat{H}$ 体系基态的一级微扰能量和展开到第5个能级的一级微扰波函数

(2)以 $\psi(x) = \sin(\frac{\pi}{a}x) + \lambda \sin(\frac{3\pi}{a}x)$ 作为试探波函数，λ 作为变分参数，求体系基态的能量

(3)以 $\psi(x) = \sin(\frac{\pi}{a}x) + \lambda_1 \sin(\frac{3\pi}{a}x) + \lambda_2 \sin(\frac{5\pi}{a}x)$ 作为试探波函数，λ_1, λ_2 作为变分参数，求体系基态的能量。对以上过程和结果进行讨论

解：(1)由题目可知，哈密尔顿算符的微扰项为 $\hat{H}' = \begin{cases} 0 & (x < \frac{a}{3}, x > \frac{2a}{3}) \\ \frac{\hbar^2\pi^2}{20ma^2} & (\frac{a}{3} \le x \le \frac{2a}{3}) \end{cases}$，因此基态能量的一级微扰为

$$\delta E_0^{(1)} = \langle\psi_0^{(0)}|\hat{H}'|\psi_0^{(0)}\rangle = \int_{\frac{a}{3}}^{\frac{2a}{3}} \frac{\hbar^2\pi^2}{20ma^2}[\sqrt{\frac{2}{a}}\sin(\frac{\pi}{a}x)]^2 dx = \frac{\hbar^2\pi^2}{20ma^2} \cdot \frac{2}{a}\int_{\frac{a}{3}}^{\frac{2a}{3}} \frac{1-\cos(\frac{2\pi}{a}x)}{2}dx = \frac{\hbar^2\pi^2}{10ma^2}(\frac{1}{6} - \frac{\sqrt{3}}{4\pi})$$

从而考虑一级微扰后的修正基态能量为

$$E_0^{(1)} = E_0^{(0)} + \delta E_0^{(1)} = \frac{\hbar^2\pi^2}{2ma^2} + \frac{\hbar^2\pi^2}{10ma^2}(\frac{1}{6} - \frac{\sqrt{3}}{4\pi}) = \frac{\hbar^2\pi^2}{10ma^2}(\frac{31}{6} - \frac{\sqrt{3}}{4\pi})$$

若展开到第5个能级，则基态波函数的一级微扰为

$$|\delta\psi_0^{(1)}\rangle = \sum_{i=1}^{4} \frac{H'_{i0}}{E_0^{(0)} - E_i^{(0)}}|\psi_i^{(0)}\rangle = \sum_{i=1}^{4} \frac{\int_{\frac{a}{3}}^{\frac{2a}{3}} \frac{\hbar^2\pi^2}{20ma^2}(\sqrt{\frac{2}{a}})^2 \sin[\frac{(i+1)\pi}{a}x]\sin(\frac{\pi}{a}x)dx}{\frac{\hbar^2\pi^2}{2ma^2} - \frac{(i+1)^2\hbar^2\pi^2}{2ma^2}}|\psi_i^{(0)}\rangle$$

$$= \sum_{i=1}^{4} \frac{\frac{\hbar^2\pi^2}{10ma^3}\int_{\frac{a}{3}}^{\frac{2a}{3}} \frac{1}{2}\{\cos(\frac{i\pi}{a}x) - \cos[\frac{(i+2)\pi}{a}x]\}dx}{-\frac{i(i+2)\hbar^2\pi^2}{2ma^2}}|\psi_i^{(0)}\rangle$$

$$= -\sum_{i=1}^{4} \frac{1}{10i(i+2)a} \cdot [\frac{\sin(\frac{i\pi}{a}x)}{\frac{i\pi}{a}} - \frac{\sin[\frac{(i+2)\pi}{a}x]}{\frac{(i+2)\pi}{a}}]_{\frac{a}{3}}^{\frac{2a}{3}}|\psi_i^{(0)}\rangle$$

$$= \frac{3\sqrt{3}}{320\pi}|\psi_2^{(0)}\rangle - \frac{\sqrt{3}}{960\pi}|\psi_4^{(0)}\rangle$$

故考虑一级微扰后的基态波函数为

$$|\psi_0^{(1)}\rangle = |\psi_0^{(0)}\rangle + |\delta\psi_0^{(1)}\rangle = |\psi_0^{(0)}\rangle + \frac{3\sqrt{3}}{320\pi}|\psi_2^{(0)}\rangle - \frac{\sqrt{3}}{960\pi}|\psi_4^{(0)}\rangle$$

写成坐标形式即为

$$\psi_0^{(1)}(x) = \psi_0^{(0)}(x) + \frac{3\sqrt{3}}{320\pi}\psi_2^{(0)}(x) - \frac{\sqrt{3}}{960\pi}\psi_4^{(0)}(x) = \sin(\frac{\pi}{a}x) + \frac{3\sqrt{3}}{320\pi}\sin(\frac{3\pi}{a}x) - \frac{\sqrt{3}}{960\pi}\sin(\frac{5\pi}{a}x)$$

(2)由于总哈密尔顿算符为

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(\hat{x}) = \begin{cases} \infty & (x \le 0, x \ge a) \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} & (0 < x < \frac{a}{3}, \frac{2a}{3} < x < a) \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar^2\pi^2}{20ma^2} & (\frac{a}{3} \le x \le \frac{2a}{3}) \end{cases}$$

因此变分法得到的基态能量为

$$\langle \widetilde{E}_0 \rangle = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_0^a \psi(x) \cdot (-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2})dx + \frac{\hbar^2\pi^2}{20ma^2}\int_{\frac{a}{3}}^{\frac{2a}{3}} |\psi(x)|^2 dx}{\int_0^a |\psi(x)|^2 dx}$$

$$= \frac{-\frac{\hbar^2}{2m}\int_0^a [\sin(\frac{\pi}{a}x) + \lambda\sin(\frac{3\pi}{a}x)] \cdot (-\frac{\pi^2}{a^2})[\sin(\frac{\pi}{a}x) + 9\lambda\sin(\frac{3\pi}{a}x)]dx}{\int_0^a [\sin(\frac{\pi}{a}x) + \lambda\sin(\frac{3\pi}{a}x)]^2 dx}$$

$$+ \frac{\frac{\hbar^2\pi^2}{20ma^2}\int_{\frac{a}{3}}^{\frac{2a}{3}} [\sin(\frac{\pi}{a}x) + \lambda\sin(\frac{3\pi}{a}x)]^2 dx}{\int_0^a [\sin(\frac{\pi}{a}x) + \lambda\sin(\frac{3\pi}{a}x)]^2 dx}$$

$$= \frac{\frac{\hbar^2\pi^2}{2ma^2}\int_0^a [\sin(\frac{\pi}{a}x)^2 + 10\lambda\sin(\frac{\pi}{a}x)\sin(\frac{3\pi}{a}x) + 9\lambda^2\sin^2(\frac{3\pi}{a}x)]dx}{\int_0^a [\sin^2(\frac{\pi}{a}x) + 2\lambda\sin(\frac{\pi}{a}x)\sin(\frac{3\pi}{a}x) + \lambda^2\sin^2(\frac{3\pi}{a}x)]dx}$$

$$+ \frac{\frac{\hbar^2\pi^2}{20ma^2}\int_{\frac{a}{3}}^{\frac{2a}{3}} [\sin^2(\frac{\pi}{a}x) + 2\lambda\sin(\frac{\pi}{a}x)\sin(\frac{3\pi}{a}x) + \lambda^2\sin^2(\frac{3\pi}{a}x)]dx}{\int_0^a [\sin^2(\frac{\pi}{a}x) + 2\lambda\sin(\frac{\pi}{a}x)\sin(\frac{3\pi}{a}x) + \lambda^2\sin^2(\frac{3\pi}{a}x)]dx}$$

$$= \frac{\frac{\hbar^2\pi^2}{2ma^2}\int_0^a \{\frac{1-\cos(\frac{2\pi}{a}x)}{2} + 5\lambda[\cos(\frac{2\pi}{a}x) - \cos(\frac{4\pi}{a}x)] + 9\lambda^2\frac{1-\cos(\frac{6\pi}{a}x)}{2}\}dx}{\int_0^a \{\frac{1-\cos(\frac{2\pi}{a}x)}{2} + \lambda[\cos(\frac{2\pi}{a}x) - \cos(\frac{4\pi}{a}x)] + \lambda^2\frac{1-\cos(\frac{6\pi}{a}x)}{2}\}dx}$$

$$+ \frac{\frac{\hbar^2\pi^2}{20ma^2}\int_{\frac{a}{3}}^{\frac{2a}{3}} \{\frac{1-\cos(\frac{2\pi}{a}x)}{2} + \lambda[\cos(\frac{2\pi}{a}x) - \cos(\frac{4\pi}{a}x)] + \lambda^2\frac{1-\cos(\frac{6\pi}{a}x)}{2}\}dx}{\int_0^a \{\frac{1-\cos(\frac{2\pi}{a}x)}{2} + \lambda[\cos(\frac{2\pi}{a}x) - \cos(\frac{4\pi}{a}x)] + \lambda^2\frac{1-\cos(\frac{6\pi}{a}x)}{2}\}dx}$$

$$= \frac{\frac{\hbar^2\pi^2}{2ma^2} \cdot \frac{a}{2}(1+9\lambda^2)}{\frac{a}{2}(1+\lambda^2)} + \frac{\frac{\hbar^2\pi^2}{20ma^2} \cdot [(\frac{a}{6} + \frac{\sqrt{3}a}{4\pi}) + \lambda \cdot (-\frac{3\sqrt{3}a}{4\pi}) + \lambda^2 \cdot \frac{a}{6}]}{\frac{a}{2}(1+\lambda^2)}$$

$$= \frac{\hbar^2\pi^2}{2ma^2}[\frac{1+9\lambda^2}{1+\lambda^2} + \frac{1}{10}\frac{(\frac{1}{3} + \frac{\sqrt{3}}{2\pi}) - \frac{3\sqrt{3}}{2\pi}\lambda + \frac{1}{3}\lambda^2}{1+\lambda^2}]$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\frac{(\frac{31}{30} + \frac{\sqrt{3}}{20\pi}) - \frac{3\sqrt{3}}{20\pi}\lambda + \frac{271}{30}\lambda^2}{1+\lambda^2}$$

将 $\langle \widetilde{E}_0 \rangle$ 对 λ 求导，得

$$\frac{d\langle \widetilde{E}_0 \rangle}{d\lambda} = \frac{\hbar^2\pi^2}{2ma^2}\frac{(-\frac{3\sqrt{3}}{20\pi} + \frac{271}{15}\lambda)(1+\lambda^2) - [(\frac{31}{30} + \frac{\sqrt{3}}{20\pi}) - \frac{3\sqrt{3}}{20\pi}\lambda + \frac{271}{30}\lambda^2] \cdot 2\lambda}{(1+\lambda^2)^2}$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\frac{[-\frac{3\sqrt{3}}{20\pi} + \frac{271}{15}\lambda - \frac{3\sqrt{3}}{20\pi}\lambda^2 + \frac{271}{15}\lambda^3] - [(\frac{31}{15} + \frac{\sqrt{3}}{10\pi})\lambda - \frac{3\sqrt{3}}{10\pi}\lambda^2 + \frac{271}{15}\lambda^3]}{(1+\lambda^2)^2}$$

$$= \frac{\hbar^2\pi^2}{2ma^2}\frac{-\frac{3\sqrt{3}}{20\pi} + (16 - \frac{\sqrt{3}}{10\pi})\lambda + \frac{3\sqrt{3}}{20\pi}\lambda^2}{(1+\lambda^2)^2}$$

解得

$$\lambda = \frac{-(16 - \frac{\sqrt{3}}{10\pi}) \pm \sqrt{(16 - \frac{\sqrt{3}}{10\pi})^2 + 4(\frac{3\sqrt{3}}{20\pi})^2}}{2 \cdot \frac{3\sqrt{3}}{20\pi}} = \frac{\sqrt{3} - 160\pi}{3\sqrt{3}} \pm \frac{10\pi}{3\sqrt{3}}\sqrt{256 - \frac{16\sqrt{3}}{5\pi} + \frac{3}{10\pi^2}}$$

根据一阶导数的性质，我们取 $\lambda = \frac{\sqrt{3} - 160\pi}{3\sqrt{3}} + \frac{10\pi}{3\sqrt{3}}\sqrt{256 - \frac{16\sqrt{3}}{5\pi} + \frac{3}{10\pi^2}} \approx 5.19 \times 10^{-3}$，代回能量的表达式，得 $\langle \widetilde{E}_0 \rangle \approx 0.530\frac{\hbar^2\pi^2}{ma^2}$

(3)

6.4 一维谐振子体系，势能为 $V(x) = \frac{1}{2}m\omega^2 x^2$，请用 $\psi(x) = Ae^{-\frac{\lambda^2}{2}x^2}$ 作为试探波函数，用变分法获得最低能级的能量，其中λ为调节参数，并与精确解比较

解：一维谐振子体系的总哈密尔顿算符为 $\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\hat{x}^2$，因此变分法得到最低能级的能量为

$$\langle \widetilde{E}_0 \rangle = \frac{\langle \psi | \hat{H}_0 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{-\infty}^{+\infty} A^* e^{-\frac{\lambda^2}{2}x^2} \cdot (-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 \hat{x}^2)(A e^{-\frac{\lambda^2}{2}x^2}) dx}{\int_{-\infty}^{+\infty} |A|^2 e^{-\lambda^2 x^2} dx}$$

$$= \frac{\int_{-\infty}^{+\infty} |A|^2 \cdot [-\frac{\hbar^2}{2m} e^{-\frac{\lambda^2}{2}x^2} \frac{d^2(e^{-\frac{\lambda^2}{2}x^2})}{dx^2} + \frac{1}{2}m\omega^2 x^2 e^{-\lambda^2 x^2}] dx}{\int_{-\infty}^{+\infty} |A|^2 e^{-\lambda^2 x^2} dx}$$

$$= \frac{\int_{-\infty}^{+\infty} [-\frac{\hbar^2}{2m} e^{-\frac{\lambda^2}{2}x^2} \frac{d(-\lambda^2 x e^{-\frac{\lambda^2}{2}x^2})}{dx} + \frac{1}{2}m\omega^2 x^2 e^{-\lambda^2 x^2}] dx}{\int_{-\infty}^{+\infty} e^{-\lambda^2 x^2} dx}$$

$$= \frac{\int_{-\infty}^{+\infty} [-\frac{\hbar^2}{2m} e^{-\frac{\lambda^2}{2}x^2}(-\lambda^2 e^{-\frac{\lambda^2}{2}x^2} + \lambda^4 x^2 e^{-\frac{\lambda^2}{2}x^2}) + \frac{1}{2}m\omega^2 x^2 e^{-\lambda^2 x^2}] dx}{\int_{-\infty}^{+\infty} e^{-\lambda^2 x^2} dx}$$

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

$$= \frac{\frac{\hbar^2 \lambda^2}{2m} \frac{\sqrt{\pi}}{\lambda} + (-\frac{\hbar^2 \lambda^4}{2m} + \frac{m\omega^2}{2}) \frac{\sqrt{\pi}}{2\lambda^3}}{\frac{\sqrt{\pi}}{\lambda}} = \frac{\hbar^2 \lambda^2}{2m} + (-\frac{\hbar^2 \lambda^4}{2m} + \frac{m\omega^2}{2}) \frac{1}{2\lambda^2}$$

$$= \frac{\hbar^2 \lambda^2}{4m} + \frac{m\omega^2}{4\lambda^2} \geq 2\sqrt{\frac{\hbar^2 \lambda^2}{4m} \cdot \frac{m\omega^2}{4\lambda^2}} = \frac{\hbar\omega}{2}$$

等号在 $\frac{\hbar^2 \lambda^2}{4m} = \frac{m\omega^2}{4\lambda^2}$，即 $\lambda = \pm\sqrt{\frac{m\omega}{\hbar}}$ 成立，取 $\lambda = \sqrt{\frac{m\omega}{\hbar}}$，则 $\psi(x) = A e^{-\frac{m\omega x^2}{2\hbar}}$，根据归一化条件，有

$$\langle \psi | \psi \rangle = \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-\infty}^{+\infty} |A|^2 e^{-\lambda^2 x^2} dx = |A|^2 \cdot \frac{\sqrt{\pi}}{\lambda} = |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

解得 $|A| = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}$，若 A 取正实数，则 $\psi(x) = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}$，与精确解完全一致