2022秋易为老师量子力学B
习题十二参考解答

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1　第一题

假设在某四维Hilbert子空间中，体系Hamiltonian的矩阵表示为

$$\hat{H} = \hat{H}_0 + \hat{V} \to H_0 + V = \begin{pmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_1 & 0 & 0 \\ 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & a & d & 0 \\ a & 0 & b & 0 \\ d & b & 0 & c \\ 0 & 0 & c & 0 \end{pmatrix}$$

其中a, b, c, d均为实数小量（设它们同量级）. 求体系所有能量本征值（精确到二阶小量）.

观察H_0，我们发现两本征值E_1和E_2均为双重简并. 此时当然可以采用简并微扰论进行处理，但更直观的方法是通过对V的块对角化操作将其转化为非简并情形.

设题述矩阵表示是在正交完备基$\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$下写出的，则$E_1$和$E_2$各自简并子空间$\mathscr{H}_1$和$\mathscr{H}_2$的基分别是$\{|1\rangle, |2\rangle\}$和$\{|3\rangle, |4\rangle\}$. 下面，我们分别在$\mathscr{H}_1$和$\mathscr{H}_2$内对微扰项$\hat{V}$进行对角化.

- 对$V_{\mathscr{H}_1} = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}$作对角化，不难得到本征值和本征矢

$$\begin{cases} a \to |1'\rangle = \dfrac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \\ -a \to |2'\rangle = \dfrac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right) \end{cases} \tag{1.1}$$

- 对$V_{\mathscr{H}_2} = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}$作对角化，同理得到本征值和本征矢

$$\begin{cases} c \to |3'\rangle = \dfrac{1}{\sqrt{2}}\left(|3\rangle + |4\rangle\right) \\ -c \to |4'\rangle = \dfrac{1}{\sqrt{2}}\left(|3\rangle - |4\rangle\right) \end{cases} \tag{1.2}$$

因此，$\hat{V}$在$\{|1'\rangle, |2'\rangle, |3'\rangle, |4'\rangle\}$这组基下的矩阵表示可写为

$$V' = \begin{pmatrix} a & 0 & V'_{13} & V'_{14} \\ 0 & -a & V'_{23} & V'_{24} \\ V'_{31} & V'_{32} & c & 0 \\ V'_{41} & V'_{42} & 0 & -c \end{pmatrix} \tag{1.3}$$

由$\hat{V}$的Hermite性我们知道$V'_{ij} = V'^{*}_{ji}$，可只考虑右上角的四个矩阵元，即$i = 1, 2; j = 3, 4$. 有：

$$\begin{cases} V'_{13} = \left\langle 1' \middle| \hat{V} \middle| 3' \right\rangle = \dfrac{1}{2} \left(\langle 1| + \langle 2| \right) \hat{V} \left(|3\rangle + |4\rangle \right) = \dfrac{d+b}{2} \\ V'_{23} = \left\langle 2' \middle| \hat{V} \middle| 3' \right\rangle = \dfrac{1}{2} \left(\langle 1| - \langle 2| \right) \hat{V} \left(|3\rangle + |4\rangle \right) = \dfrac{d-b}{2} \\ V'_{14} = \left\langle 1' \middle| \hat{V} \middle| 4' \right\rangle = \dfrac{1}{2} \left(\langle 1| + \langle 2| \right) \hat{V} \left(|3\rangle - |4\rangle \right) = \dfrac{d+b}{2} \\ V'_{24} = \left\langle 2' \middle| \hat{V} \middle| 4' \right\rangle = \dfrac{1}{2} \left(\langle 1| - \langle 2| \right) \hat{V} \left(|3\rangle - |4\rangle \right) = \dfrac{d-b}{2} \end{cases} \tag{1.4}$$

故体系Hamiltonian在新基下的矩阵表示是

$$\begin{aligned} H' = H_0 + V' &= \begin{pmatrix} E_1 + a & 0 & \frac{d+b}{2} & \frac{d+b}{2} \\ 0 & E_1 - a & \frac{d-b}{2} & \frac{d-b}{2} \\ \frac{d+b}{2} & \frac{d-b}{2} & E_2 + c & 0 \\ \frac{d+b}{2} & \frac{d-b}{2} & 0 & E_2 - c \end{pmatrix} \\ &= \begin{pmatrix} E_1 + a & 0 & 0 & 0 \\ 0 & E_1 - a & 0 & 0 \\ 0 & 0 & E_2 + c & 0 \\ 0 & 0 & 0 & E_2 - c \end{pmatrix} + \begin{pmatrix} 0 & 0 & \frac{d+b}{2} & \frac{d+b}{2} \\ 0 & 0 & \frac{d-b}{2} & \frac{d-b}{2} \\ \frac{d+b}{2} & \frac{d-b}{2} & 0 & 0 \\ \frac{d+b}{2} & \frac{d-b}{2} & 0 & 0 \end{pmatrix} \triangleq H''_0 + V'' \end{aligned} \tag{1.5}$$

若形象地视V''为对H''_0的微扰，则可利用非简并微扰论直接给出精确至二阶修正的本征能量

$$\begin{cases} \varepsilon_1^{\mathrm{II}} = E_1 + a + \dfrac{(d+b)^2/4}{(E_1+a) - (E_2+c)} + \dfrac{(d+b)^2/4}{(E_1+a) - (E_2-c)} \approx E_1 + a + \dfrac{(d+b)^2}{2(E_1 - E_2)} \\ \varepsilon_2^{\mathrm{II}} = E_1 - a + \dfrac{(d-b)^2/4}{(E_1-a) - (E_2+c)} + \dfrac{(d-b)^2/4}{(E_1-a) - (E_2-c)} \approx E_1 - a + \dfrac{(d-b)^2}{2(E_1 - E_2)} \\ \varepsilon_3^{\mathrm{II}} = E_2 + c + \dfrac{(d+b)^2/4}{(E_2+c) - (E_1+a)} + \dfrac{(d-b)^2/4}{(E_2+c) - (E_1-a)} \approx E_2 + c - \dfrac{d^2 + b^2}{2(E_1 - E_2)} \\ \varepsilon_4^{\mathrm{II}} = E_2 - c + \dfrac{(d+b)^2/4}{(E_2-c) - (E_1+a)} + \dfrac{(d-b)^2/4}{(E_2-c) - (E_1-a)} \approx E_2 - c - \dfrac{d^2 + b^2}{2(E_1 - E_2)} \end{cases} \tag{1.6}$$

2 第二题

设体系Hamiltonian为$\hat{H} = A\hat{\boldsymbol{L}}^2 + B\hat{L}_z + \lambda\hat{L}_y$，其中$\hat{\boldsymbol{L}}^2, \hat{L}_z, \hat{L}_y$为角动量算符及其分量，实参数$\lambda \ll A, B$. 试求体系能谱，精确到二阶小量（即精确到$\lambda^2$量级）.

2.1 法一：非简并微扰论

依题，可记$\hat{H}_0 = A\hat{\boldsymbol{L}}^2 + B\hat{L}_z$，微扰项$\hat{V} = \lambda\hat{L}_y$. 则微扰前的体系能谱为$E_{lm}^{(0)} = Al\left(l+1\right)\hbar^2 + Bm\hbar$.

我们考虑$\hat{L}_y = \dfrac{1}{2\mathrm{i}}\left(\hat{L}_+ - \hat{L}_-\right)$对$\hat{H}_0$本征态$|l,m\rangle$的作用情况($-l \le m \le l$)：

$$\hat{L}_y\left|l,m\right\rangle = \frac{\hbar}{2\mathrm{i}}\left[\sqrt{l\left(l+1\right)-m\left(m+1\right)}\left|l,m+1\right\rangle - \sqrt{l\left(l+1\right)-m\left(m-1\right)}\left|l,m-1\right\rangle\right] \tag{2.1}$$

故$\hat{L}_y$的非零矩阵元有且仅有

$$\begin{cases}\left\langle l,m+1\middle|\hat{L}_y\middle|l,m\right\rangle = \dfrac{\hbar}{2\mathrm{i}}\sqrt{l\left(l+1\right)-m\left(m+1\right)}\\ \left\langle l,m-1\middle|\hat{L}_y\middle|l,m\right\rangle = -\dfrac{\hbar}{2\mathrm{i}}\sqrt{l\left(l+1\right)-m\left(m-1\right)}\end{cases} \tag{2.2}$$

其对角元均为0，即能量的一阶修正为0.

最终，我们得到精确至二阶修正的体系能谱

$$\begin{aligned}\varepsilon_{lm}^{\mathrm{II}} &= E_{lm}^{(0)} + 0 + \frac{\left|\lambda\left\langle l,m+1\middle|\hat{L}_y\middle|l,m\right\rangle\right|^2}{E_{lm}^{(0)} - E_{l,m+1}^{(0)}} + \frac{\left|\lambda\left\langle l,m-1\middle|\hat{L}_y\middle|l,m\right\rangle\right|^2}{E_{lm}^{(0)} - E_{l,m-1}^{(0)}}\\ &= Al\left(l+1\right)\hbar^2 + Bm\hbar + \frac{\lambda^2\hbar^2\left[l\left(l+1\right)-m\left(m+1\right)\right]}{-4B\hbar} + \frac{\lambda^2\hbar^2\left[l\left(l+1\right)-m\left(m-1\right)\right]}{4B\hbar}\\ &= Al\left(l+1\right)\hbar^2 + Bm\hbar + \frac{m\hbar}{2B}\lambda^2\end{aligned} \tag{2.3}$$

2.2 法二：Taylor展开

有心的同学可能已经发现，本体系的能谱原则上是可以精确求解的. 我们只需定义$\mathbb{R}^3$空间中的单位向量

$$\boldsymbol{n} = \left(0, \frac{\lambda}{\sqrt{B^2+\lambda^2}}, \frac{B}{\sqrt{B^2+\lambda^2}}\right) \tag{2.4}$$

即可将体系Hamiltonian重新写为

$$\hat{H} = A\hat{\boldsymbol{L}}^2 + \sqrt{B^2+\lambda^2}\,\hat{L}_n \tag{2.5}$$

因此，若选取$\left\{\hat{H}, \hat{\boldsymbol{L}}^2, \hat{L}_n\right\}$为一组新的CSCO，我们将得到体系精确的本征能量

$$E_{lm_n}^{(0)} = Al\left(l+1\right)\hbar^2 + \sqrt{B^2+\lambda^2}\,m_n\hbar \tag{2.6}$$

其中$-l \le m_n \le l$. 下面，再对式中右端的第二项关于小量λ作Taylor展开：

$$\sqrt{B^2+\lambda^2}\,m_n\hbar = Bm_n\hbar\sqrt{1+\left(\frac{\lambda}{B}\right)^2} \approx Bm_n\hbar\left(1+\frac{\lambda^2}{2B^2}\right) \tag{2.7}$$

并不失一般性地记$m_n = m$，我们同样能够得到精确至二阶修正的体系能谱2.3.

3 第三题

自旋1/2的三维各向同性谐振子处于基态. 求在微扰$\hat{V}=\lambda\hat{\sigma}_z\hat{x}^2$作用下的基态能量（精确到二阶小量，$\lambda$为实参数）.

微扰前，本征能量对自旋自由度有双重简并，即

$$\begin{cases}|n_x,n_y,n_z,\uparrow\rangle \\ |n_x,n_y,n_z,\downarrow\rangle\end{cases} \to E^{(0)}_{n_x,n_y,n_z}=\left(n_x+n_y+n_z+\frac{3}{2}\right)\hbar\omega \tag{3.1}$$

可以预见，加入微扰项后该简并将被消除.

引入升降算符$\{\hat{a}_x,\hat{a}_x^\dagger\}$和直积符号$|n_x,n_y,n_z,\text{spin}\rangle=|n_x,n_y,n_z\rangle\otimes|\text{spin}\rangle$，微扰项可改写为

$$\hat{V}=\lambda\hat{x}^2\otimes\hat{\sigma}_z=\lambda\frac{\hbar}{2m\omega}\left[\hat{a}_x^2+\left(\hat{a}_x^\dagger\right)^2+\hat{a}_x\hat{a}_x^\dagger+\hat{a}_x^\dagger\hat{a}_x\right]\otimes\hat{\sigma}_z\triangleq\frac{\lambda\hbar}{2m\omega}\hat{A}\otimes\hat{\sigma}_z \tag{3.2}$$

基态的量子数$n_x=n_y=n_z=0$，因而不难得到$\hat{A}\otimes\hat{\sigma}_z$对零级基态的作用效果：

$$\begin{cases}\hat{A}\otimes\hat{\sigma}_z\,|000\uparrow\rangle=|000\uparrow\rangle+\sqrt{2}\,|200\uparrow\rangle \\ \hat{A}\otimes\hat{\sigma}_z\,|000\downarrow\rangle=-\,|000\downarrow\rangle-\sqrt{2}\,|200\downarrow\rangle\end{cases} \tag{3.3}$$

类似于课上例题，对基态而言，有用的非零$\hat{A}\otimes\hat{\sigma}_z$矩阵元仅有

$$\begin{cases}\left\langle 200\uparrow\middle|\hat{A}\otimes\hat{\sigma}_z\middle|000\uparrow\right\rangle=\sqrt{2} \\ \left\langle 000\uparrow\middle|\hat{A}\otimes\hat{\sigma}_z\middle|000\uparrow\right\rangle=1 \\ \left\langle 200\downarrow\middle|\hat{A}\otimes\hat{\sigma}_z\middle|000\downarrow\right\rangle=-\sqrt{2} \\ \left\langle 000\downarrow\middle|\hat{A}\otimes\hat{\sigma}_z\middle|000\downarrow\right\rangle=-1\end{cases} \tag{3.4}$$

由于本体系存在简并，因此将上述结果以矩阵表示可能更加形象：

$\hat{V}\Big/\frac{\lambda\hbar}{2m\omega}$	$000\uparrow$	$000\downarrow$	$200\uparrow$	$200\downarrow$
$000\uparrow$	1		$\sqrt{2}$	
$000\downarrow$		-1		$-\sqrt{2}$
$200\uparrow$	$\sqrt{2}$		$\times$	$\times$
$200\downarrow$		$-\sqrt{2}$	$\times$	$\times$

最终，我们得到精确至二阶修正的基态能量

$$\begin{cases}\varepsilon^{\text{II}}_{000\uparrow}=E^{(0)}_{000}+\left\langle 000\uparrow\middle|\hat{V}\middle|000\uparrow\right\rangle+\dfrac{\left|\left\langle 200\uparrow\middle|\hat{V}\middle|000\uparrow\right\rangle\right|^2}{E^{(0)}_{000}-E^{(0)}_{200}}=\dfrac{3}{2}\hbar\omega+\dfrac{\hbar}{2m\omega}\lambda-\dfrac{\hbar}{4m^2\omega^3}\lambda^2 \\ \varepsilon^{\text{II}}_{000\downarrow}=E^{(0)}_{000}+\left\langle 000\downarrow\middle|\hat{V}\middle|000\downarrow\right\rangle+\dfrac{\left|\left\langle 200\downarrow\middle|\hat{V}\middle|000\downarrow\right\rangle\right|^2}{E^{(0)}_{000}-E^{(0)}_{200}}=\dfrac{3}{2}\hbar\omega-\dfrac{\hbar}{2m\omega}\lambda-\dfrac{\hbar}{4m^2\omega^3}\lambda^2\end{cases} \tag{3.5}$$

需要注意，不少同学写出的矩阵表示形式是

$\hat{V} \Big/ \dfrac{\lambda\hbar}{2m\omega}$	$000\uparrow$	$000\downarrow$	$200\uparrow$	$200\downarrow$
$000\uparrow$		1		$\sqrt{2}$
$000\downarrow$	1		$\sqrt{2}$	
$200\uparrow$		$\sqrt{2}$	$\times$	$\times$
$200\downarrow$	$\sqrt{2}$		$\times$	$\times$

是因为将两自旋态$|\uparrow\rangle, |\downarrow\rangle$选取为了$\hat{\sigma}_x$的本征态. 该法不如取为$\hat{\sigma}_z$的本征态简洁. 并且，我们将看到写出第二种矩阵表示后还需将其对角化，得到的结果正是第一个矩阵，因而并不需舍近求远.