课堂练习

练习1：写出三级能量修正的表达式

解：三级能量修正的表达式为$\Delta_n^{(3)}=\langle n^{(0)}|\hat{H}^{'}|n^{(2)}\rangle$，而态矢的二级修正为

$$
\begin{aligned}
|n^{(2)}\rangle &= (E_n^{(0)}-\hat{H}_0)^{-1}\hat{Q}_n(\hat{H}^{'}-\Delta_n^{(1)})|n^{(1)}\rangle \\
&= (E_n^{(0)}-\hat{H}_0)^{-1}\sum_{l\neq n}|l^{(0)}\rangle\langle l^{(0)}|(\hat{H}^{'}-H_{nn}^{'})\sum_{k\neq n}\frac{H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle \\
&= (E_n^{(0)}-\hat{H}_0)^{-1}\sum_{l,k\neq n}\frac{H_{lk}^{'}H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|l^{(0)}\rangle-(E_n^{(0)}-\hat{H}_0)^{-1}\sum_{l,k\neq n}\frac{\delta_{lk}H_{nn}^{'}H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|l^{(0)}\rangle \\
&= (E_n^{(0)}-\hat{H}_0)^{-1}\sum_{l,k\neq n}\frac{H_{lk}^{'}H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|l^{(0)}\rangle-(E_n^{(0)}-\hat{H}_0)^{-1}\sum_{k\neq n}\frac{H_{nn}^{'}H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle \\
&= \sum_{l,k\neq n}\frac{H_{lk}^{'}H_{kn}^{'}}{(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_k^{(0)})}|l^{(0)}\rangle-\sum_{k\neq n}\frac{H_{nn}^{'}H_{kn}^{'}}{(E_n^{(0)}-E_k^{(0)})^2}|k^{(0)}\rangle
\end{aligned}
$$

因此三级能量修正为

$$
\begin{aligned}
\Delta_n^{(3)} &= \langle n^{(0)}|\hat{H}^{'}|n^{(2)}\rangle=\langle n^{(0)}|\hat{H}^{'}\sum_{l,k\neq n}\frac{H_{lk}^{'}H_{kn}^{'}}{(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_k^{(0)})}|l^{(0)}\rangle-\langle n^{(0)}|\hat{H}^{'}\sum_{k\neq n}\frac{H_{nn}^{'}H_{kn}^{'}}{(E_n^{(0)}-E_k^{(0)})^2}|k^{(0)}\rangle \\
&= \sum_{l,k\neq n}\frac{H_{nl}^{'}H_{lk}^{'}H_{kn}^{'}}{(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_k^{(0)})}-\sum_{k\neq n}\frac{H_{nn}^{'}|H_{kn}^{'}|^2}{(E_n^{(0)}-E_k^{(0)})^2}
\end{aligned}
$$

练习2：在“谐振子在外电场下的极化”中，推导能量二级修正的表达式 $\Delta_n^{(2)}=-\frac{q^2\varepsilon^2}{2m\omega_0^2}$

解：体系的总哈密尔顿算符为$\hat{H}=\hat{H}_0+\hat{H}^{'}=(\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega_0^2\hat{x}^2)+(-q\varepsilon\hat{x})$，根据二级能量修正的表达式，得

$$
\begin{aligned}
\Delta_n^{(2)} &= \langle n^{(0)}|\hat{H}^{'}|n^{(1)}\rangle=\sum_{k\neq n}\frac{|H_{kn}^{'}|^2}{E_n^{(0)}-E_k^{(0)}}=\sum_{k\neq n}\frac{|-q\varepsilon\langle k^{(0)}|\hat{x}|n^{(0)}\rangle|^2}{(n+\frac{1}{2})\hbar\omega_0-(k+\frac{1}{2})\hbar\omega_0} \\
&= \frac{|-q\varepsilon\langle(n-1)^{(0)}|\hat{x}|n^{(0)}\rangle|^2}{(n+\frac{1}{2})\hbar\omega_0-(n-1+\frac{1}{2})\hbar\omega_0}+\frac{|-q\varepsilon\langle(n+1)^{(0)}|\hat{x}|n^{(0)}\rangle|^2}{(n+\frac{1}{2})\hbar\omega_0-(n+1+\frac{1}{2})\hbar\omega_0} \\
&= \frac{q^2\varepsilon^2}{\hbar\omega_0}(|\langle(n-1)^{(0)}|\hat{x}|n^{(0)}\rangle|^2-|\langle(n+1)^{(0)}|\hat{x}|n^{(0)}\rangle|^2) \\
&= \frac{q^2\varepsilon^2}{\hbar\omega_0}|\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}\delta_{n-1,n-1}+\sqrt{n+1}\delta_{n-1,n+1})|^2 \\
&\quad -\frac{q^2\varepsilon^2}{\hbar\omega_0}|\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}\delta_{n+1,n-1}+\sqrt{n+1}\delta_{n+1,n+1})|^2 \\
&= \frac{q^2\varepsilon^2}{\hbar\omega_0}[\frac{n\hbar}{2m\omega_0}-\frac{(n+1)\hbar}{2m\omega_0}]=-\frac{q^2\varepsilon^2}{2m\omega_0^2}
\end{aligned}
$$

练习3：在“谐振子在外电场下的极化”中，推导一级微扰下坐标的期望值 $\langle\hat{x}\rangle=\frac{q\varepsilon}{m\omega_0^2}$

解：由于一级微扰下的态矢为

$$
\begin{aligned}
|n\rangle &= |n^{(0)}\rangle + |n^{(1)}\rangle = |n^{(0)}\rangle + \sum_{k\neq n}\frac{H_{kn}^{'}}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle = |n^{(0)}\rangle + \sum_{k\neq n}\frac{-q\varepsilon\langle k^{(0)}|\hat{x}|n^{(0)}\rangle}{(n+\frac{1}{2})\hbar\omega_0-(k+\frac{1}{2})\hbar\omega_0}|k^{(0)}\rangle \\
&= |n^{(0)}\rangle + \frac{-q\varepsilon\langle (n-1)^{(0)}|\hat{x}|n^{(0)}\rangle}{(n+\frac{1}{2})\hbar\omega_0-(n-1+\frac{1}{2})\hbar\omega_0}|(n-1)^{(0)}\rangle + \frac{-q\varepsilon\langle (n+1)^{(0)}|\hat{x}|n^{(0)}\rangle}{(n+\frac{1}{2})\hbar\omega_0-(n+1+\frac{1}{2})\hbar\omega_0}|(n+1)^{(0)}\rangle \\
&= |n^{(0)}\rangle - \frac{q\varepsilon\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}\delta_{n-1,n-1}+\sqrt{n+1}\delta_{n-1,n+1})}{\hbar\omega_0}|(n-1)^{(0)}\rangle + \frac{q\varepsilon\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}\delta_{n+1,n-1}+\sqrt{n+1}\delta_{n+1,n+1})}{\hbar\omega_0}|(n+1)^{(0)}\rangle \\
&= |n^{(0)}\rangle - \frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}|(n-1)^{(0)}\rangle - \sqrt{n+1}|(n+1)^{(0)}\rangle)
\end{aligned}
$$

因此

$$
\begin{aligned}
\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\{ & (\sqrt{n}|(n-1)^{(0)}\rangle + \sqrt{n+1}|(n+1)^{(0)}\rangle) \\
& - \frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{\hbar}{2m\omega_0}}[\sqrt{n}(\sqrt{n-1}|(n-2)^{(0)}\rangle + \sqrt{n}|n^{(0)}\rangle) - \sqrt{n+1}(\sqrt{n+1}|n^{(0)}\rangle + \sqrt{n+2}|(n+2)^{(0)}\rangle)]\}
\end{aligned}
$$

从而有

$$
\langle n|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}[-\frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{\hbar}{2m\omega_0}}(n-n-1)] - \frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{\hbar}{2m\omega_0}}[\sqrt{\frac{\hbar}{2m\omega_0}}(n-n-1)] = \frac{q\varepsilon}{m\omega_0^2}
$$

$$
\langle n|n\rangle = 1 + (-\frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{n\hbar}{2m\omega_0}})^2 + (\frac{q\varepsilon}{\hbar\omega_0}\sqrt{\frac{(n+1)\hbar}{2m\omega_0}})^2 = 1 + \frac{q^2\varepsilon^2(2n+1)}{2m\hbar\omega_0^3}
$$

若一级微扰较小，则$\langle n|n\rangle \approx 1$，从而$\langle\hat{x}\rangle = \frac{\langle n|\hat{x}|n\rangle}{\langle n|n\rangle} \approx \langle n|\hat{x}|n\rangle = \frac{q\varepsilon}{m\omega_0^2}$，证毕