Lect 19 Pertubation theory (II) - degenerate case

If system has symmetry, it often leads to degenercay (say rotational symmetry lead to $2j+1$ fold degeneracy for each angular momentum sector).
In we impose a weak external field to break such a symmetry, then the degeneracy will be removed. In this case, we cannot use the formalism developed in the last lecture.

We consider a degenerate or nearly degenerate subspace D spanned by the $\underbrace{\text{unpertubated states}}_{\text{multiplet}}$ $\underbrace{|\alpha_i\rangle}_{(i=1\sim g)}$. The other unpertubated states $\{|\mu\rangle\}$ are distant from D, with $|\langle\alpha_i|H'|\mu\rangle| \ll |E_\alpha - E_\mu|$. Thus we have to consider the ~~states~~ in D separatly, but other states outside D pertubatively. We will derive a new effective Hamiltonian in the truncate Hilbert space D.

Now let us write $H = H_0 + H'$, and its eigenstates close to the subspace D are expressed as

$$|a\rangle = \sum_{\alpha_i} C_\alpha |\alpha_i\rangle + \sum_\mu d_\mu |\mu\rangle,$$

where C_α is at the order of 1, and d_μ is at the $\underbrace{\text{small}}$ order.

The eigen equation $(H - E_a)|a\rangle = 0. \Rightarrow$

$$\sum_{\alpha_i} C_\alpha (E_\alpha^{(0)} + H' - E_a)|\alpha_i\rangle + \sum_\mu d_\mu (E_\mu^{(0)} + H' - E_a)|\mu\rangle = 0$$

Projected into the subspace by doing the inner product $|\alpha_j\rangle$

$$\Rightarrow \; C_{\alpha_j}(E^{(0)}_{\alpha_j} - E_a) + \sum_{\alpha_i} C_{\alpha_i} \langle\alpha_j| H' |\alpha_i\rangle + \sum_{\mu} d_\mu \langle\alpha_j| H' |\mu\rangle = 0 \quad (*)$$

and for state $|\nu\rangle$ outsider the subspace

$$\sum_{\alpha_i} C_{\alpha_i} \langle\nu| H' |\alpha_i\rangle + d_\nu (E^0_\nu - E_a) + \sum_\mu d_\mu \langle\nu| H' |\mu\rangle = 0 \quad (**)$$

In $(**)$, since $\nu \neq \alpha_j$, d_ν and d_μ are small, and $\langle\nu| H' |\mu\rangle$ is also small, such that we neglect the last term in $(**)$. $\Rightarrow$

$$d_\nu \simeq \frac{1}{E_a - E^0_\nu} \sum_{\alpha_i} C_{\alpha_i} \langle\nu| H' |\alpha_i\rangle$$

. plug this into $(*)$

$$\Rightarrow \boxed{C_{\alpha_j}(E^{(0)}_{\alpha_j} - E_a) + \sum_{\alpha_i} C_{\alpha_i} \left\{ \langle\alpha_j| H' |\alpha_i\rangle + \sum_\mu \frac{\langle\alpha_j| H' |\mu\rangle\langle\mu| H' |\alpha_i\rangle}{E_a - E^0_\mu} \right\} = 0}$$

we can approximate E_a in the denominater with the unperterbated energy in the subspace D, $E^{(0)}_\alpha$. If these states are not exactly degenerate without perturbations, we replace E_a with the mean value of $E^{(0)}_\alpha$.

$$\rightarrow \boxed{C_{\alpha_j}(E^{(0)}_{\alpha_j} - E_a) + \sum_{\alpha_i} C_{\alpha_i} \left\{ \langle\alpha_j| H' |\alpha_i\rangle + \sum_\mu \frac{\langle\alpha_j| H' |\mu\rangle\langle\mu| H' |\alpha_i\rangle}{\overline{E}_\alpha - E^0_\mu} \right\} = 0}$$

This is the eigenvalue problem in the subspace D, with a new effective Hamiltonian $\boxed{H_{eff} = PH'P + PH' \frac{1-P}{\bar{E}-H_0} H'P}$,

where P is the projection operator, $\boxed{P = \sum_\alpha |\alpha\rangle\langle\alpha| .}$

Example: Stark effect of H-atom. — energy level splitting in the $\vec{E}$

The $n=2$ level of H-atom is 4-fold degenerate $|2lm\rangle$: $\boxed{|200\rangle, |211\rangle, |210\rangle, |21-1\rangle}$

let us consider to add an eletric field $\vec{E}$ along the z-axis, $\boxed{\begin{aligned} H' &= -eEz \\ &= -eEr\cos\theta . \end{aligned}}$

H' breaks the 3D rotation symmetry, but still maintain the L_z conserved. Let us stay in the lowest order to calculate $\boxed{H_{eff} = PH'P}$ in this $n=2$ subspace.

$\langle 2lm | H' | 2l'm' \rangle$ where $H' \propto Y_{10}(\Omega)$. According to Wigner-Eckert theorem $\begin{cases} l = l' \pm 1, \text{ or } l' \\ m' = m \end{cases}$. Also, check parity property, l and l' has to one even and one odd, because H' is odd.

$\Rightarrow |21\pm1\rangle$ will not be mixed by other states, but remains unchanged.

i.e. $\langle 2lm | H' | 2l\, m=\pm 1 \rangle = 0$.

What do can be mixed is $\langle 200 | H' | 210 \rangle \neq 0$.

$|200\rangle$: $R_{20} = \frac{1}{\sqrt{2}\,a^{3/2}}\left(1-\frac{r}{2a}\right)e^{-r/2a}$ $\qquad Y_{00} = \frac{1}{\sqrt{4\pi}}$

$R_{21} = \frac{1}{2\sqrt{6}\,a^{3/2}}\,\frac{r}{a}\,e^{-r/2a}$ $\qquad Y_{10} = \frac{\sqrt{3}}{\sqrt{4\pi}}\cos\theta$

$$\Rightarrow \int_0^{+\infty} dr\, r^2\, R_{20}(r) R_{21}(r)\,(-eEr) \int d\Omega\; Y_{00}\cos\theta\, Y_{10}$$

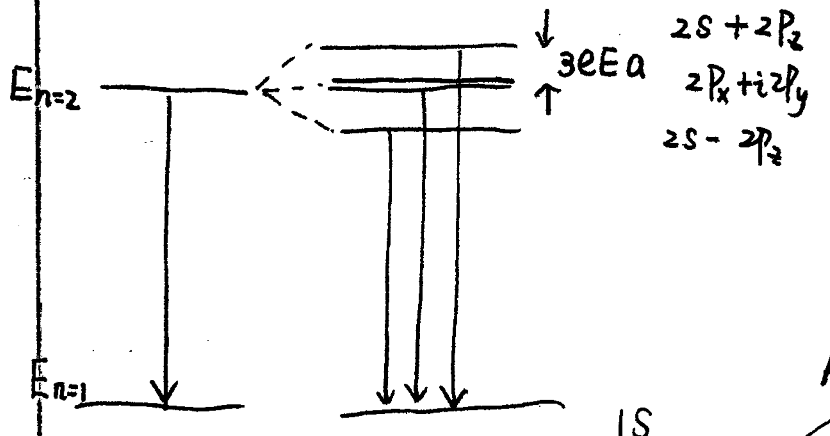
$$= \frac{-eEa}{2\sqrt{12}} \int_0^{+\infty} d\left(\frac{r}{a}\right)\left(\frac{r}{a}\right)^3 \left(1-\frac{r}{2a}\right)\left(\frac{r}{a}\right) e^{-r/a} \int \frac{d\Omega}{4\pi}\sqrt{3}\cos^2\theta$$

$$= \frac{-eEa}{12}\int_0^{+\infty} dx\; x^4\left(1-\frac{x}{2}\right)e^{-x} = \frac{-eEa}{12}\left[4! - \frac{5!}{2}\right] = -\frac{eEa}{12}(24-60)$$

$$= 3eEa$$

$$\Rightarrow \text{the} \begin{bmatrix} \langle 200|H'|200\rangle, & \langle 200|H'|210\rangle \\ \langle 210|H'|200\rangle, & \langle 210|H'|210\rangle \end{bmatrix} = -\frac{e^2}{2a}\cdot\frac{1}{4} + \begin{bmatrix} 0 & 3eEa \\ 3eEa & 0 \end{bmatrix}$$

$\Rightarrow$ splitting $\Delta E = \pm 3eEa$ with $\phi_\pm = \frac{1}{\sqrt{2}}\left[|200\rangle + |210\rangle\right]$

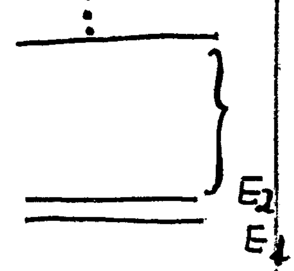


why the 2-fold degeneracy of $2P_{m=\pm1}$ are not removed?

A reflection symmetry protects it.

Example 2-energy level system $H = H_0 + H'$. There are two energy levels E_1 and E_2 very close to each other, and other levels very far away.

for the unperturbated H_0



$$H_0|\varphi_1\rangle = E_1|\varphi_1\rangle, \quad H_0|\varphi_2\rangle = E_2|\varphi_2\rangle.$$

In this 2D subspace, H is expressed as

$$H = \begin{bmatrix} E_1 & H'_{12} \\ H'_{21} & E_2 \end{bmatrix} \quad \text{where} \quad H'_{12} = \langle \varphi_1 | H' | \varphi_2 \rangle = H'^{*}_{21}$$

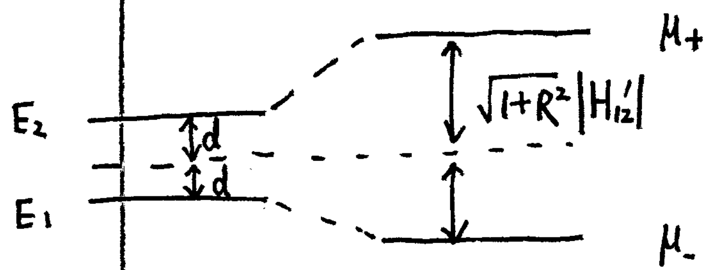
We can diagonalize the eigen-equation, $|\psi_\pm\rangle = C_1|\varphi_1\rangle + C_2|\varphi_2\rangle$ with eigenvalue $\mu_\pm$.

$$\begin{bmatrix} E_1 - \mu_\pm & -H'_{12} \\ -H'_{21} & E_2 - \mu_\pm \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = 0 \quad \Rightarrow \quad \mu_\pm = \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4|H'_{12}|^2} \right]$$

$$= E_c \pm |H'_{12}| \sqrt{1 + R^2}$$

where $E_c = \frac{E_1 + E_2}{2}$, $d = \frac{1}{2}(E_2 - E_1)$

$$R = \frac{d}{|H'_{12}|}.$$



For later convenience, we define $\tan\theta = 1/R$, $H'_{12} = |H'_{12}| e^{-i\gamma}$.

For the state μ_-, $$\frac{C_1}{C_2} = \frac{H'_{12}}{\mu_- - E_1} = \frac{|H'_{12}| e^{-i\gamma}}{-\sqrt{d^2 + |H'_{12}|^2} + d} = -\frac{e^{-i\gamma}}{\sqrt{R^2+1} - R}$$

$$= -\frac{\cos\theta/2}{\sin\theta/2} e^{-i\gamma}$$

$$\Rightarrow |\psi_-\rangle = \begin{bmatrix}\cos\frac{\theta}{2}\\ -\sin\frac{\theta}{2}\,e^{-i\gamma}\end{bmatrix}, \qquad \text{similarly} \Rightarrow |\psi_+\rangle = \begin{bmatrix}\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2}\,e^{-i\gamma}\end{bmatrix}.$$

- If $E_1 = E_2$, say, set $\gamma = \pi$. $\Rightarrow |\psi_\mp\rangle = \frac{1}{\sqrt{2}}(|\varphi_1\rangle \pm |\varphi_2\rangle)$

  The effect of H'_{12} is the strongest.

- If $R \gg 1$, then it reduces to non-degenerate perturbation.

$$|\psi_+\rangle \simeq |\varphi_2\rangle - \frac{1}{2R}|\varphi_1\rangle, \quad E_- \simeq E_c - d;$$
$$|\psi_-\rangle \simeq |\varphi_1\rangle + \frac{1}{2R}|\varphi_2\rangle, \quad E_+ \simeq E_c + d.$$

Example 3: Let us consider an eigen-value problem of 3-level system. In the unperturbated ground states $|1\rangle, |2\rangle$, and an excited state $|3\rangle$. The pertubation only has matrix elements between the ground and excited states

$$H_0 + H' = \begin{pmatrix} 0 & 0 & \lambda M \\ 0 & 0 & \lambda M \\ \lambda M & \lambda M & \Delta \end{pmatrix} \quad \text{and} \quad \left|\frac{\lambda M}{\Delta}\right| \ll 1.$$

We need to consider $P H' \frac{1-P}{E-H_0} H' P$ to lift the degeneracy.

$$\Rightarrow \langle i|H_{eff}|j\rangle = \frac{\langle i|H'|3\rangle\langle 3|H'|j\rangle}{-\Delta} = -\frac{(\lambda M)^2}{\Delta} \Rightarrow H_{eff} = -\frac{(\lambda M)^2}{\Delta}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}$$

for $|i\rangle\, |j\rangle = |1\rangle, |2\rangle$

$$\Rightarrow E_+ = 0 \quad \text{with } |\psi_+\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$
$$E_- = -2\frac{(\lambda M)^2}{\Delta} \quad \text{with } |\psi_-\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle).$$