Week 6 Discussion Session

2014.2.9

Homework #3

Problem 5.4, Sakurai

Solution:

(a) Ground state is $|0\rangle_x \otimes |0\rangle_y$, with energy $\hbar w$;

1^{st} excited states are $|0\rangle_x \otimes |1\rangle_y$ and $|1\rangle_x \otimes |0\rangle_y$, with energy $2\hbar w$.

(b) For ground state, $\langle 0|_x \otimes \langle 0|_y\, \delta m\, w^2 xy\, |0\rangle_x \otimes |0\rangle_y = 0$, hence 1^{st} order correction to energy vanishes.

For 1^{st} excited states, one should use degenerate perturbation theory. The appropriate matrix elements are

$$\langle 0|_x \otimes \langle 1|_y\, \delta m \cdot w^2 xy\, |0\rangle_x \otimes |1\rangle_y = 0$$

$$\langle 1|_x \otimes \langle 0|_y\, \delta m \cdot w^2 xy\, |1\rangle_x \otimes |0\rangle_y = 0$$

$$\langle 0|_x \otimes \langle 1|_y\, \delta m \cdot w^2 xy\, |1\rangle_x \otimes |0\rangle_y = \frac{1}{2}\frac{\delta m}{m}\hbar w$$

$$\langle 1|_x \otimes \langle 0|_y\, \delta m \cdot w^2 xy\, |0\rangle_x \otimes |1\rangle_y = \frac{1}{2}\frac{\delta m}{m}\hbar w$$

Then it is easy to get eigenvalues and eigenvectors of the 2×2 matrix $\begin{bmatrix} 0 & \frac{1}{2}\frac{\delta m}{m}\hbar w \\ \frac{1}{2}\frac{\delta m}{m}\hbar w & 0 \end{bmatrix}$ as follows:

Eigenvalue	Eigenvector
$\frac{1}{2}\frac{\delta m}{m}\hbar w$	$\frac{1}{\sqrt{2}}(|0\rangle_x \otimes |1\rangle_y + |1\rangle_x \otimes |0\rangle_y)$
$-\frac{1}{2}\frac{\delta m}{m}\hbar w$	$\frac{1}{\sqrt{2}}(|0\rangle_x \otimes |1\rangle_y - |1\rangle_x \otimes |0\rangle_y)$

(c) Now

$$H_0 + V = \frac{P_x^2}{2m} + \frac{P_y^2}{2m} + \frac{1}{2}mw^2 (x \quad y)\begin{bmatrix} 1 & \delta m/m \\ \delta m/m & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}.$$

One can use an orthogonal transformation to diagonalize the Hamiltonian:

$$H_0 + V = \frac{P_{x'}^2}{2m} + \frac{P_{y'}^2}{2m} + \frac{1}{2}mw^2 (x' \quad y')\begin{bmatrix} 1+\delta m/m & \\ & 1-\delta m/m \end{bmatrix}\begin{bmatrix} x' \\ y' \end{bmatrix}$$

where $\begin{bmatrix} x' \\ y' \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}$.

Hence the energies of the three lowest states are

$$\frac{1}{2}\hbar w\left(\sqrt{1+\delta m/m} + \sqrt{1-\delta m/m}\right) = \hbar w + O\left(\left(\frac{\delta m}{m}\right)^2\right)$$

$$\hbar w\left(\frac{1}{2}\sqrt{1+\delta m/m} + \frac{3}{2}\sqrt{1-\delta m/m}\right) = 2\hbar w - \frac{1}{2}\hbar w\frac{\delta m}{m} + O\left(\left(\frac{\delta m}{m}\right)^2\right)$$

$$\hbar w\left(\frac{3}{2}\sqrt{1+\delta m/m} + \frac{1}{2}\sqrt{1-\delta m/m}\right) = 2\hbar w + \frac{1}{2}\hbar w\frac{\delta m}{m} + O\left(\left(\frac{\delta m}{m}\right)^2\right),$$

in agreement with the perturbation results obtained in part (b).

Problem 5.11, Sakurai

Solution:

(a) $\mathcal{H} = \dfrac{E_1^0 + E_2^0}{2} I_2 + \dfrac{E_1^0 - E_2^0}{2} \sigma_3 + \lambda\Delta\,\sigma_1$

Hence eigenvalues are

$$\frac{E_1^0 + E_2^0}{2} \pm \sqrt{\left(\frac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2\Delta^2} \ .$$

Eigenfunctions are

for plus sign, $\dfrac{1}{N_+} \begin{bmatrix} -\lambda\Delta \\ \dfrac{E_1^0 - E_2^0}{2} - \sqrt{\left(\dfrac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2\Delta^2} \end{bmatrix}$,

for minus sign, $\dfrac{1}{N_-} \begin{bmatrix} -\lambda\Delta \\ \dfrac{E_1^0 - E_2^0}{2} + \sqrt{\left(\dfrac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2\Delta^2} \end{bmatrix}$.

where $N_\pm$ are appropriate normalization factors.

(b) We apply non-degenerate perturbation theory. Notice that 1st order energy correction vanishes.

For $\phi_1^{(0)}$, we have

$$\phi_1^{(1)} = \phi_2^{(0)} \cdot \frac{\langle \phi_2^{(0)} | H' | \phi_1^{(0)} \rangle}{E_1^0 - E_2^0}$$

$$= \frac{\lambda\Delta}{E_1^0 - E_2^0}\, \phi_2^{(0)}$$

$$\Delta E_1^{(2)} = \frac{|\langle \phi_2^{(0)} | H' | \phi_1^{(0)} \rangle|^2}{E_1^0 - E_2^0} = \frac{\lambda^2\Delta^2}{E_1^0 - E_2^0} \ .$$

Notice that from the exact results in (a), we have

$$\frac{E_1^0 + E_2^0}{2} + \sqrt{\left(\frac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2\Delta^2}$$

$$= \frac{E_1^0 + E_2^0}{2} + \frac{E_1^0 - E_2^0}{2}\left(1 + \frac{4\lambda^2\Delta^2}{E_1^0 - E_2^0}\right)^{\frac{1}{2}}$$

$$= E_1^0 + \frac{\lambda^2\Delta^2}{E_1^0 - E_2^0} + \mathcal{O}(\Delta^3)$$

$$\text{eigenfunction} = \frac{1}{N_+'} \begin{bmatrix} 1 \\ \dfrac{1}{\lambda\Delta}\left(\dfrac{E_1^0 - E_2^0}{2} - \sqrt{\left(\dfrac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2\Delta^2}\right) \end{bmatrix}$$

$$= \frac{1}{N_+'} \begin{bmatrix} 1 \\ \dfrac{\lambda\Delta}{E_1^0 - E_2^0} \end{bmatrix} + \mathcal{O}(\Delta^2)$$

and are consistent with perturbation results in part (a).

A similar analysis applied to $\phi_2^{(0)}$ gives

$$\phi_2^{(1)} = \frac{\lambda\Delta}{E_2^0 - E_1^0}\ \phi_1^{(0)}$$

$$\Delta E_2^{(2)} = \frac{\lambda^2\Delta^2}{E_2^0 - E_1^0}$$

(c) We apply degenerate perturbation theory with $\mathcal{H} = H_0 + H'$,
where $H_0 = \begin{bmatrix} E_1^0 & \\ & E_2^0 \end{bmatrix}$, $H' = \begin{bmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{bmatrix}$.

Zeroth order wave functions are

$\Psi_1^{(0)} = \frac{1}{\sqrt{2}}(\phi_1^{(0)} + \phi_2^{(0)})$, with energy shift $\lambda\Delta$;

$\Psi_2^{(0)} = \frac{1}{\sqrt{2}}(\phi_1^{(0)} - \phi_2^{(0)})$, with energy shift $-\lambda\Delta$.

It is direct to see that this agrees with part (a) when $E_1^0 = E_2^0$.

Problem 5.14, Sakurai

Solution :

Choose coordinate system such that the external electric field is along z-direction, then electric potential is

$$V(r) = -(-e)\vec{E}\cdot\vec{r} = eEz.$$

Since spin degree of freedom is still ~~degne~~ degenerate by assumption, we consider orbital part where there is a total of nine orbits $\{|3lm\rangle \,|\, 0\le l\le 2, -l\le m\le l\}$.

To apply degenerate perturbation theory, we need to calculate the following matrix elements : $\langle 3l'm'|V(r)|3lm\rangle$.

Notice that $V(r) = eEz$ is

a rank 1 irreducible tensor operator;

of eigenvalue zero under the action of taking commutator with L_z ;

odd under parity transformation.

Then by also noticing that $P\,Y_{lm} = (-1)^l Y_{lm}$, we have that $\langle 3l'm'|V(r)|3lm\rangle$ is not zero only when

$$\begin{cases} |l-1| \le l' \le l+1 \ ; \\ m' = m \ ; \\ (-1)^{l'} = (-1)\cdot(-1)^l \ , \end{cases}$$

i.e. only when $l' = l\pm 1$, $m' = m$.

So among all the $9^2 = 81$ matrix elements only the following 4 and their complex conjugate do not vanish:

$$\langle 300|V|310\rangle,\ \langle 310|V|320\rangle,\ \langle 311|V|321\rangle,\ \langle 31{-1}|V|32{-1}\rangle.$$

Notice that Wigner-Eckart theorem together with time reversal symmetry tells us that $\langle 311|V|321\rangle = \langle 31{-1}|V|32{-1}\rangle$.

Calculations give the following

$$\langle 311|V|321\rangle = -\frac{27}{2}eEa_0$$

$$\langle 310|V|320\rangle = -9\sqrt{3}\,eEa_0$$

$$\langle 300|V|310\rangle = -9\sqrt{6}\,eEa_0 .$$

This 9×9 matrix is block-diagonal in the following pattern:

$$\begin{array}{c} \\ 322 \\ 32{-2} \end{array}\!\!\begin{array}{c} \begin{array}{cc} 322 & 32{-2} \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \end{array}
\quad
\begin{array}{c} \\ 311 \\ 321 \end{array}\!\!\begin{array}{c} \begin{array}{cc} 311 & 321 \end{array} \\ \begin{bmatrix} 0 & -\frac{27}{2} \\ -\frac{27}{2} & 0 \end{bmatrix} \end{array}
\quad
\begin{array}{c} \\ 31{-1} \\ 32{-1} \end{array}\!\!\begin{array}{c} \begin{array}{cc} 31{-1} & 32{-1} \end{array} \\ \begin{bmatrix} 0 & -\frac{27}{2} \\ -\frac{27}{2} & \end{bmatrix} \end{array}
\quad
\begin{array}{c} \\ 300 \\ 310 \\ 320 \end{array}\!\!\begin{array}{c} \begin{array}{ccc} 300 & 310 & 320 \end{array} \\ \begin{bmatrix} 0 & -9\sqrt{6} & 0 \\ -9\sqrt{6} & 0 & -9\sqrt{3} \\ 0 & -9\sqrt{3} & 0 \end{bmatrix} \end{array}$$

$$(\times\, eEa_0)$$

It is easy to diagonalize the latter three blocks:

Energy $/ eEa_0$	0^{th} order wavefunction
$\frac{27}{2}$	$\begin{cases} \frac{1}{\sqrt{2}}(\lvert 311\rangle - \lvert 321\rangle) \\ \frac{1}{\sqrt{2}}(\lvert 31{-1}\rangle - \lvert 32{-1}\rangle) \end{cases}$
$-\frac{27}{2}$	$\begin{cases} \frac{1}{\sqrt{2}}(\lvert 311\rangle + \lvert 321\rangle) \\ \frac{1}{\sqrt{2}}(\lvert 31{-1}\rangle + \lvert 32{-1}\rangle) \end{cases}$
0	$\frac{1}{\sqrt{3}}(\lvert 300\rangle - \sqrt{2}\lvert 320\rangle)$
27	$\frac{1}{\sqrt{6}}(\sqrt{2}\lvert 300\rangle - \sqrt{3}\lvert 310\rangle + \lvert 320\rangle)$
-27	$\frac{1}{\sqrt{6}}(\sqrt{2}\lvert 300\rangle + \sqrt{3}\lvert 310\rangle + \lvert 320\rangle)$

We see that a 1^{st} order degenerate perturbation theory does not break the degeneracy in $\{\lvert 322\rangle, \lvert 32{-2}\rangle\}$ sector. One has to go to 2^{nd} degenerate perturbation to get the 0^{th} order wavefunction.

This turns to an eigen-problem of the following 2×2 matrix

$$P_0 V P_1 \frac{1}{E^{(0)} - H_0} P_1 V P_0 .$$

where

$$P_0 = \lvert 322\rangle\langle 322\rvert + \lvert 32{-2}\rangle\langle 32{-2}\rvert$$

$$P_1 = \mathbb{1} - P_0$$

To obtain this matrix, one has to perform an infinite sum over all levels, and also an integration over scattering states, and is a very difficult problem. Hence we will be satisfied by just the above order E' results.

Problem 5.15 Sakurai

Solution:

For Na atom ($Z=11$), $n=1$ and $n=2$ levels accomodate a total of $2\times(1^2+2^2)=10$ electrons, and the 11^{th} electron is in the $3s$ level ($n=3$, $\ell=0$) for ground state, as due to Coulumb screening, different ℓ's with same n now have different energies.

Since there is electric field $\vec{E}=-\frac{1}{e}\frac{dV_c}{dr}\hat{r}$ inside the atom produced by the ion core, the presumed electric dipole moment can couple with this internal electric field yielding a term $-\vec{\mu}_{el}\cdot\vec{E}=\frac{1}{e}\mu_{el}\frac{dV_c}{dr}\vec{\sigma}\cdot\hat{r}$ in the Hamiltonian, where we have set the coefficient between $\vec{\mu}_{el}$ and $\vec{\sigma}$ to be μ_{el}.

We now analyze the effect of this additional term on ~~energies~~ energy levels treating it as a perturbation. First notice that $\vec{\sigma}\cdot\hat{r}$ commutes with total angular momentum $\vec{J}=\vec{L}+\vec{S}$, so (j,j_z) is good quantum number after this perturbation term is introduced. We denote new energy eigenstates as $\Psi_{n\ell}^{jj_z}$. This is not to say that ℓ is still a good quantum number now. It is only a reminder that this new eigenstate is very close to an unperturbed state with orbital angular momentum quantum number ℓ. More precisely, we are labeling new eigenstates via their zeroth order part, $\Psi_{n\ell}^{(0)jj_z}(\vec{r})=R_{n\ell}(r)\,\mathcal{Y}_{\ell}^{jj_z}(\hat{r})$, in which $j=\ell\pm1/2$ and $\mathcal{Y}_{\ell}^{jj_z}$ is the spin-angular function.

We are now prepared for a discussion of perturbation effect. First order energy correction $\langle\Psi_{n\ell}^{(0)jj_z}|-\vec{\mu}_{el}\cdot\vec{E}|\Psi_{n\ell}^{(0)jj_z}\rangle=0$ by selection rule: $\langle Y_{\ell'm'}|\vec{r}|Y_{\ell m}\rangle\neq0$ only when $\Delta\ell=\pm1$ (notice that $\Psi_{n\ell}^{(0)jj_z}$ consists of $Y_{\ell m}$ and $|S_z\rangle$ with fixed ℓ, and hence selection rule applies). The lowest non-vanishing energy correction has to be of 2^{nd} order. As to mixing, $\Psi_{n\ell}^{jj_z}=\sum_{n'\ell'}A_{n'\ell'}\Psi_{n'\ell'}^{(0)jj_z}$ with a peak of $A_{n'\ell'}$ at $(n',\ell')=(n,\ell)$, so different (n',ℓ') states got mixed (with same jj_z) where $|\ell'-\ell|=1$.

Let's consider the perturbation effect to lowest level state $n=3$, $\ell=0$, i.e. $\Psi_{30}^{(0)\frac{1}{2}j_z}$ as an illustration. We should use 2^{nd} order nondegenerate perturbation to get the lowest order energy correction. Then

$$E^{(2)}=\sum_{n'\ell}\frac{1}{E_{30}^{(0)\frac{1}{2}j_z}-E_{n\ell}^{(0)\frac{1}{2}j_z}}\left|\langle\Psi_{n\ell}^{(0)\frac{1}{2}j_z}|-\vec{\mu}_{el}\cdot\vec{E}|\Psi_{30}^{(0)\frac{1}{2}j_z}\rangle\right|^2$$

$$=\sum_{n\geq3}\frac{1}{E_{30}^{(0)}-E_{n1}^{(0)}}\left|\langle\Psi_{n1}^{(0)\frac{1}{2}j_z}|-\vec{\mu}_{el}\cdot\vec{E}|\Psi_{30}^{(0)\frac{1}{2}j_z}\rangle\right|^2.$$

Since for $n\geq4$,

$$|E_{30}^{(0)}-E_{n1}^{(0)}|\gg|E_{30}^{(0)}-E_{31}^{(0)}|,$$

we ignore the $n\geq4$ terms and only keep that of $n=3$. Then

$$E^{(2)} \doteq \frac{1}{E^{(0)}_{30} - E^{(0)}_{31}} \left| \langle \Psi^{(0)\frac{1}{2}j_z}_{31} \,|\, -\vec{\mu}_{el} \cdot \vec{E} \,|\, \Psi^{(0)\frac{1}{2}j_z}_{30} \rangle \right|^2$$

$$= \frac{1}{E^{(0)}_{30} - E^{(0)}_{31}} \left(\frac{\mu_{el}}{e}\right)^2 \left(\int R^*_{31}(r) R_{30}(r) r^2 \frac{dV_c}{dr}\, dr\right)^2 \cdot \left| \langle \mathcal{Y}^{\frac{1}{2}j_z}_{1} \,|\, \vec{\sigma}\cdot\hat{r} \,|\, \mathcal{Y}^{\frac{1}{2}j_z}_{0} \rangle \right|^2$$

in which one can express $\mathcal{Y}^{\frac{1}{2}j_z}_{1\,(\text{or }0)}$ in terms of $Y_{\ell m} \otimes |S_z\rangle$ and evaluate the inner product in the above expression.

A graphical illustration of this 2nd order correction is depicted as follows: