Physics 137B (Professor Shapiro) Spring 2010

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Homework 3 Solutions

1. The H_0 spectrum is non-degenerate so the first-order corrections are given by:

$$
\begin{aligned}
E_0^{(1)} &= <0|H'|0> \\
&= \int_{-\infty}^{\infty} \psi_0^* H' \psi_0 dx \\
&= \int_{-\infty}^{\infty} dx \lambda e^{-ax^2} \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2} dx \\
&= \frac{\lambda\alpha}{\sqrt{\pi}} \frac{\sqrt{\pi}}{\sqrt{a+\alpha^2}} \\
&= \frac{\lambda\alpha}{\sqrt{a+\alpha^2}} \\
E_1^{(1)} &= <1|H'|1> \\
&= \int_{-\infty}^{\infty} \psi_1^* H' \psi_1 dx \\
&= \int_{-\infty}^{\infty} dx \lambda e^{-ax^2} \frac{\alpha}{2\sqrt{\pi}} (2\alpha x)^2 e^{-\alpha^2 x^2} dx \\
&= \frac{\lambda\alpha}{2\sqrt{\pi}} (2\alpha)^2 \frac{\sqrt{\pi}}{2\sqrt{(a+\alpha^2)^3}} \\
&= \frac{\lambda\alpha^3}{\sqrt{(a+\alpha^2)^3}}
\end{aligned}
$$

In the above expressions $\alpha = (\frac{m\omega}{\hbar})^{1/2}$ (refer to equations 4.134 and 4.168 of the text).

2. H_0 is the hydrogenic Hamiltonian and so

$$\begin{aligned} H'(r) &= V(r) - (\frac{-Ze^2}{(4\pi\epsilon_0)r}) \\ &= \begin{cases} \frac{Ze^2}{(4\pi\epsilon_0)2R}(\frac{r^2}{R^2} - 3 + \frac{2R}{r}) & r \leq R \\ 0 & r > R \end{cases} \end{aligned}$$

(a) The H_0 energy spectrum is degenerate, with n^2 distinct values of l and m for each energy level. So we need to apply degenerate perturbation theory. Note that since H' only depends upon r (and not on angular variables), L^2 and L_z commute with H' and thus are still "good" operators for this perturbation. Therefore, if we choose a basis of L^2 and L_z eigenstates then H' will necessarily already be diagonal in each degenerate subspace. So, using this "good" basis, we can apply the usual formulae from non-degenerate perturbation theory. The first order energy shift for the state $|n, l, m>$ will be:

$$\begin{aligned} \Delta E &= <n, l, m|H'|n, l, m> \\ &= \int d^3r H'(r)|\psi_{nlm}(r, \theta, \phi)|^2 \\ &= \int_0^\infty drr^2 \int d\Omega H'(r)|R_{nl}(r)Y_{lm}(\theta, \phi)|^2 \\ &= \int_0^\infty drr^2 H'(r)|R_{nl}(r)|^2 \int d\Omega |Y_{lm}(\theta, \phi)|^2 \\ &= \int_0^\infty drr^2 H'(r)|R_{nl}(r)|^2 \qquad \text{(using equation 6.103 of text)} \\ &= \frac{Ze^2}{(4\pi\epsilon_0)2R} \int_0^R drr^2(\frac{r^2}{R^2} + \frac{2R}{r} - 3)(R_{nl}(r))^2 \end{aligned}$$

(b) Taking $|R_{nl}(r)|^2 \approx |R_{nl}(0)|^2 = \dfrac{4Z^3\delta_{l0}}{a_\mu^3 n^3}$ (see equation 7.145 of text), we have:

$$
\begin{aligned}
\Delta E &= \frac{Ze^2}{(4\pi\epsilon_0)2R}\int_0^R drr^2(\frac{r^2}{R^2}+\frac{2R}{r}-3)(\frac{4Z^3\delta_{l0}}{a_\mu^3 n^3}) \\
&= \frac{2Z^4e^2\delta_{l0}}{(4\pi\epsilon_0)a_\mu^3n^3R}\int_0^R dr(\frac{r^4}{R^2}+2Rr-3r^2) \\
&= \frac{2Z^4e^2\delta_{l0}}{(4\pi\epsilon_0)a_\mu^3n^3R}(\frac{R^5}{5R^2}+2R\frac{R^2}{2}-3\frac{R^3}{3}) \\
&= \frac{e^2}{(4\pi\epsilon_0)}\frac{2}{5}R^2\frac{Z^4}{a_\mu^3n^3}\delta_{l0}
\end{aligned}
$$

3. Let us first examine the H_0 energy spectrum. The energy levels with $n = p$ are all non-degenerate. The other energy levels with $n \neq p$ are doubly degenerate, with the $|n = m_1, p = m_2 >$ state having the same energy as the $|n = m_2, p = m_1 >$ state. In general we have:

$$
\begin{aligned}
< n,p|H'|r,s > &= 10^{-3}E_1(\frac{2}{L})^2\int_0^L dx\sin(\frac{n\pi x}{L})\sin(\frac{r\pi x}{L})\sin(\frac{\pi x}{L})\cdot \\
&\qquad \cdot\int_0^L dy\sin(\frac{p\pi y}{L})\sin(\frac{s\pi y}{L}) \\
&= 10^{-3}E_1(\frac{2}{L})\int_0^L dx\sin(\frac{n\pi x}{L})\frac{1}{2}[\cos(\frac{(r-1)\pi x}{L})-\cos(\frac{(r+1)\pi x}{L})]\delta_{s,p} \\
&= 10^{-3}E_1(\frac{2}{L})\int_0^L dx\frac{1}{4}[\sin(\frac{(n+r-1)\pi x}{L})+\sin(\frac{(n-r+1)\pi x}{L}) \\
&\qquad -\sin(\frac{(n+r+1)\pi x}{L})-\sin(\frac{(n-r-1)\pi x}{L})]\delta_{s,p}
\end{aligned}
$$

Therefore, for $n = r = m_1$ and $p = s = m_2$:

$$
\begin{aligned}
< m_1,m_2|H'|m_1,m_2 > &= 10^{-3}E_1(\frac{2}{L})\int_0^L dx\frac{1}{4}[\sin(\frac{(2m_1-1)\pi x}{L})+\sin(\frac{\pi x}{L}) \\
&\qquad -\sin(\frac{(2m_1+1)\pi x}{L})-\sin(\frac{-\pi x}{L})]\delta_{m_2,m_2} \\
&= 10^{-3}E_1(\frac{2}{L})\frac{L}{4\pi}[\frac{2}{(2m_1-1)}+2-\frac{2}{(2m_1+1)}+2] \\
&= 10^{-3}E_1\frac{2}{\pi}(\frac{1}{4m_1^2-1}+1)
\end{aligned}
$$

But when $n = s = m_1$ and $p = r = m_2$ for $m_1 \neq m_2$:

$$\begin{aligned} < m_1, m_2|H'|m_2, m_1 > &= 10^{-3}E_1(\frac{2}{L})\int_0^L dx \sin(\frac{m_1\pi x}{L})\sin(\frac{m_2\pi x}{L})\sin(\frac{\pi x}{L})\delta_{m_1,m_2} \\ &= 0 \end{aligned}$$

So the H' matrix block in the doubly degenerate subspace spanned by $\{|m_1, m_2>, |m_2, m_1>\}$ with $m_1 \neq m_2$ is:

$$\begin{aligned} H'|_{\text{deg. subspace}} &= \begin{pmatrix} < m_1, m_2|H'|m_1, m_2 > & < m_1, m_2|H'|m_2, m_1 > \\ < m_2, m_1|H'|m_1, m_2 > & < m_2, m_1|H'|m_2, m_1 > \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{4m_1^2-1} + 1 & 0 \\ 0 & \frac{1}{4m_2^2-1} + 1 \end{pmatrix} 10^{-3}E_1\frac{2}{\pi} \end{aligned}$$

This is already diagonal so we are already working in a "good" basis. Therefore we can conclude that the change in the energy of state $|n, p>$ is:

$$E^{(1)}_{|n,p>} = 10^{-3}E_1\frac{2}{\pi}(\frac{1}{4n^2-1} + 1)$$

4. As shown on pages 290-292 of the text, the eigenstates of $H_0 = \dfrac{L^2}{2I}$ are the spherical harmonics $Y_{lm}(\theta, \phi)$, with $E_l = \dfrac{\hbar^2 l(l+1)}{2I}$. Choose a coordinate system so that the electric field lies along the z-axis. Then $H' = -d_z E = -qR_0\cos\theta E$, where $\cos\theta$ is the angle of the dipole from the z-axis. The matrix elements in each degenerate subspace (i.e. fixed l) must be calculated:

$$\begin{aligned} < l, m|H'|l, m' > &= \int d\Omega\ Y^*_{lm}(\theta, \phi)(-qER_0\cos\theta)Y_{lm'}(\theta, \phi) \\ &= (-qER_0)\int_{-1}^1 d(\cos\theta)\ \Theta^*_{lm}(\theta)\cos\theta\ \Theta_{lm'}(\theta)\int_0^{2\pi} d\phi\ \Phi^*_m(\phi)\Phi_{m'}(\phi) \\ &\qquad \text{(using the notation of section 6.3 of the text)} \\ &= (-qER_0)\int_{-1}^1 d(\cos\theta)\ \Theta^*_{lm}(\theta)\cos\theta\ \Theta_{lm'}(\theta)\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m'-m)\phi} \\ &= (-qER_0)\int_{-1}^1 d(\cos\theta)\ \Theta^*_{lm}(\theta)\cos\theta\ \Theta_{lm'}(\theta)\delta_{m,m'} \\ &= (-qER_0)\delta_{m,m'}\int_{-1}^1 d(\cos\theta)\ |\Theta_{lm}(\theta)|^2\cos\theta \end{aligned}$$

From equations 6.101 and 6.88 in the text, it is evident that $\Theta_{lm}(\theta)$ is either an even or odd function of $\cos\theta$. In either case, this implies that $|\Theta_{lm}(\theta)|^2$ is an even function of $\cos\theta$ and so the above integrand ($|\Theta_{lm}(\theta)|^2\cos\theta$) is an odd function of $\cos\theta$. Thus the integral vanishes (since integrating an odd function on a domain symmetric about the origin is zero). That is, $< l, m|H'|l, m' >= 0$. This means that the matrix elements of H' are zero in each degenerate subspace and thus H' does not separate the degeneracy at first order.

5. We are examining the degenerate $n = 2$ subspace of the hydrogen atom. We want to show that $H' = e\mathcal{E}z = e\mathcal{E}r\cos\theta$ is diagonal in this degenerate subspace when we choose the basis $\{\xi_1, \xi_2, \xi_3, \xi_4\}$, where:

$$\begin{aligned}
\xi_1 &= \psi_{211} \\
\xi_2 &= \tfrac{1}{\sqrt{2}}(\psi_{200} - \psi_{210}) \\
\xi_3 &= \tfrac{1}{\sqrt{2}}(\psi_{200} + \psi_{210}) \\
\xi_4 &= \psi_{21-1}
\end{aligned}$$

Denote the state ψ_{2lm} by $|l, m>$. Then:

$$\begin{aligned}
< l', m'|H'|l, m > &= \int d^3r\ \psi^*_{2l'm'}(r,\theta,\phi)\ (e\mathcal{E}r\cos\theta)\ \psi_{2lm}(r,\theta,\phi) \\
&= e\mathcal{E}\int_0^\infty dr\ r^2 R^*_{2l'}(r)R_{2l}(r)r\ \int d\Omega\ Y^*_{l'm'}(\theta,\phi)Y_{lm}(\theta,\phi)\cos\theta \\
&= e\mathcal{E}\int_0^\infty dr\ r^3 R^*_{2l'}(r)R_{2l}(r)\ \int_{-1}^1 d(\cos\theta)\ \Theta^*_{l'm'}(\theta)\Theta_{lm}(\theta)\cos\theta\ \cdot \\
&\qquad \cdot\int_0^{2\pi} d\phi\ \Phi^*_{m'}(\phi)\Phi_m(\phi) \\
&= e\mathcal{E}\int_0^\infty dr\ r^3 R^*_{2l'}(r)R_{2l}(r)\ \int_{-1}^1 d(\cos\theta)\ \Theta^*_{l'm'}(\theta)\Theta_{lm}(\theta)\cos\theta\ \delta_{m,m'}
\end{aligned}$$

The key term in the above expression is the $\delta_{m,m'}$ which allows us to conclude that any matrix element between states with different values of m is zero. Therefore:

$$\begin{aligned}
< \xi_1|H'|\xi_i > &= 0 \qquad \text{for i=2,3,4} \\
< \xi_2|H'|\xi_i > &= 0 \qquad \text{for i=1,4} \\
< \xi_3|H'|\xi_i > &= 0 \qquad \text{for i=1,4} \\
< \xi_4|H'|\xi_i > &= 0 \qquad \text{for i=1,2,3}
\end{aligned}$$

So the only possible non-zero off-diagonal terms are $<\xi_2|H'|\xi_3>$ and $<\xi_3|H'|\xi_2>$ which have $m=0$. In the $m=m'=0$ case we have:

$$\begin{aligned}
< l',0|H'|l,0> &= e\mathcal{E}\int_0^\infty dr\ r^3 R^*_{2l'}(r)R_{2l}(r)\ \int_{-1}^{1} d(\cos\theta)\ \Theta^*_{l'0}(\theta)\Theta_{l0}(\theta)\cos\theta \\
&= e\mathcal{E}\int_0^\infty dr\ r^3 R^*_{2l'}(r)R_{2l}(r)\cdot \\
&\qquad \cdot\int_{-1}^{1} d(\cos\theta)(l+\tfrac{1}{2})^{1/2}(l'+\tfrac{1}{2})^{1/2}P'_l(\cos\theta)P_l(\cos\theta)\cos\theta \\
&= K_{l,l'}\ \int_{-1}^{1} dw\ w\ P_{l'}(w)P_l(w) \qquad (\text{letting}\ \ w=\cos\theta)
\end{aligned}$$

where $K_{l,l'}$ is a real constant independent of w.

Note that P_l is an odd (even) polynomial when l is odd (even). So when $l=l'$ the integrand is an odd function of w and the integral is zero. Hence $<l,0|H'|l,0>=0$. Therefore:

$$\begin{aligned}
<\xi_2|H'|\xi_3> &= \tfrac{1}{\sqrt{2}}(<0,0|-<1,0|)H'\tfrac{1}{\sqrt{2}}(|0,0>+|1,0>) \\
&= \tfrac{1}{2}(<0,0|H'|0,0>+<0,0|H'|1,0>-<1,0|H'|0,0>-<1,0|H'|1,0>) \\
&= \tfrac{1}{2}(<0,0|H'|1,0>-<1,0|H'|0,0>) \\
&= \tfrac{1}{2}(<0,0|H'|1,0>-<0,0|H'|1,0>^*) \\
&= 0
\end{aligned}$$

because $<0,0|H'|1,0>$ is real (see the expression above).

Similarly $<\xi_3|H'|\xi_2>=<\xi_2|H'|\xi_3>^*=0$. So it has been shown that all off-diagonal elements are zero.