Physics 3C26 - Solutions to Problem Set 4

March 27, 2006

1. **Quick questions [20]**

   (a) Perturbation theory allows us to compute changes in the eigenvalues and eigenvectors of a system when the Hamiltonian changes by a small amount. [2]

   (b) If the Hamiltonian for the system is $\hat{H} = \hat{H}_0 + \lambda \hat{V}$, where $\hat{H}_0 \phi_n = E_n \phi_n$ and $\hat{H}\psi_n = W_n \psi_n$, then

$$\begin{aligned} \psi_n &= \sum_{p=0}^{\infty} \lambda^p \psi_n^{(p)} \\ W_n &= \sum_{p=0}^{\infty} \lambda^p W_n^{(p)} \end{aligned}$$

   [2]

   (c) We use the unperturbed wavefunctions ϕ_n to expand the corrections to the wavefunction. [2]

   (d) The first order correction to the energy is $W_n^{(1)} = \int \phi_n^* \hat{V} \phi_n \, \mathrm{d}\tau$. [2]

   (e) The first order correction to the wavefunction is

$$\psi_n^{(1)} = \sum_{k(\neq n)} \frac{V_{kn}}{E_n - E_k} \phi_k$$

   where $V_{kn} = \int \phi_k^* \hat{V} \phi_n \, \mathrm{d}\tau$. [2]

   (f) The second order correction to the energy is

$$W_n^{(2)} = \sum_{k(\neq n)} \frac{|V_{kn}|^2}{E_n - E_k}$$

   [2]

   (g) Degenerate states need to be treated in a special way because the first order correction to the wavefunction contains terms that are zero in the denominator. [2]

   (h) The first order correction to the energy of degenerate states is given by the eigenvalues of the matrix V_{kn} where only the degenerate states are used to build the matrix. [2]

   (i) The linear Stark effect for hydrogen is given by degenerate perturbation theory. [2]

(j) The degeneracy in positronium is a result of the energy being independent of the orientation of the spins. [2]

2. **Degenerate perturbation theory [20]**

(a) We have

$$\begin{aligned}
\hat{s}_e \cdot \hat{s}_p &= \frac{1}{2}\left(\hat{s}_{e+}\hat{s}_{p-} + \hat{s}_{e-}\hat{s}_{p+}\right) + \hat{s}_{ez}\hat{s}_{pz} \\
&= \frac{1}{2}\left(\left(\hat{s}_{ex} + \mathrm{i}\hat{s}_{ey}\right)\left(\hat{s}_{px} - \mathrm{i}\hat{s}_{py}\right) + \left(\hat{s}_{ex} - \mathrm{i}\hat{s}_{ey}\right)\left(\hat{s}_{px} + \mathrm{i}\hat{s}_{py}\right)\right) \\
&= \hat{s}_{ex}\hat{s}_{px} + \hat{s}_{ey}\hat{s}_{py} + \hat{s}_{ez}\hat{s}_{pz}
\end{aligned}$$

[4]

(b) For one spin we have

$$\begin{aligned}
\langle m|\hat{s}_z|m'\rangle &= m\hbar\delta_{m,m'} \\
\langle m|\hat{s}_+|m'\rangle &= \hbar\delta_{m',-\frac{1}{2}}\delta_{m,\frac{1}{2}} \\
\langle m|\hat{s}_-|m'\rangle &= \hbar\delta_{m',\frac{1}{2}}\delta_{m,-\frac{1}{2}}
\end{aligned}$$

thus for two spins we get [10]

$$\begin{aligned}
\langle m_e m_p|\hat{s}_{ez}\hat{s}_{pz}|m_e' m_p'\rangle &= m_e\hbar\delta_{m_e m_e'} \times m_p\hbar\delta_{m_p m_p'} \\
\langle m_e m_p|\hat{s}_{e+}\hat{s}_{p-}|m_e' m_p'\rangle &= \hbar\delta_{m_e',-\frac{1}{2}}\delta_{m_e,\frac{1}{2}} \times \hbar\delta_{m_p',\frac{1}{2}}\delta_{m_p,-\frac{1}{2}} \\
\langle m_e m_p|\hat{s}_{e-}\hat{s}_{p+}|m_e' m_p'\rangle &= \hbar\delta_{m_e',\frac{1}{2}}\delta_{m_e,-\frac{1}{2}} \times \hbar\delta_{m_p',-\frac{1}{2}}\delta_{m_p,\frac{1}{2}}
\end{aligned}$$

Hence

$$\langle m_e m_p|\hat{s}_e \cdot \hat{s}_p|m_e' m_p'\rangle = \hbar^2 \begin{pmatrix} -1/4 & 1/2 & 0 & 0 \\ 1/2 & -1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix} \begin{array}{l} m_p = \frac{1}{2},\ m_e = -\frac{1}{2} \\ m_p = -\frac{1}{2}\ m_e = \frac{1}{2} \\ m_p = \frac{1}{2},\ m_e = \frac{1}{2} \\ m_p = -\frac{1}{2}\ m_e = -\frac{1}{2} \end{array}$$

(c) The top left 2×2 block has eigenvalues λ given by

$$\begin{aligned}
\begin{vmatrix} -\frac{\hbar^2}{4} - \lambda & \frac{\hbar^2}{2} \\ \frac{\hbar^2}{2} & -\frac{\hbar^2}{4} - \lambda \end{vmatrix} &= 0 \\
\Rightarrow \left(-\frac{\hbar^2}{4} - \lambda\right)^2 - \left(\frac{\hbar^2}{2}\right)^2 &= 0 \\
\Rightarrow \lambda &= \frac{\hbar^2}{4} \text{ OR } -\frac{3\hbar^2}{4}
\end{aligned}$$

and the energies are $A\hbar^2/4$ and $-3A\hbar^2/4$. [6]

3. **Non-degenerate perturbation theory [20]**

(a) The first order change in energy for state n is

$$\begin{aligned}
\Delta\varepsilon_n^{(1)} &= \int_{-\infty}^{\infty} \psi_n(x) V(x) \psi_n(x)\,\mathrm{d}x \\
&= \frac{2}{L}\int_0^L V_0 \sin^2\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\,\mathrm{d}x \\
&= \frac{2V_0}{4L}\int_0^L \left[\sin\left(\frac{(2n-m)\pi x}{L}\right) + 2\sin\left(\frac{m\pi x}{L}\right) - \sin\left(\frac{(2n+m)\pi x}{L}\right)\right]\,\mathrm{d}x \\
&= \frac{V_0}{2L}\left[\frac{-L}{(2n-m)\pi}\cos\left(\frac{(2n-m)\pi x}{L}\right) - \frac{2L}{m\pi}\cos\left(\frac{m\pi x}{L}\right) + \frac{L}{(2n+m)\pi}\cos\left(\frac{(2n+m)\pi x}{L}\right)\right]_0^L \\
&= \frac{V_0}{2L}\left[\frac{-L}{(2n-m)\pi}\left((-1)^{(2n-m)}-1\right) - \frac{2L}{m\pi}\left((-1)^m-1\right) + \frac{L}{(2n+m)\pi}\left((-1)^{(2n+m)}-1\right)\right] \\
&= \frac{V_0}{2\pi}\left((-1)^m-1\right)\left[\frac{-1}{(2n-m)} - \frac{2}{m} + \frac{1}{(2n+m)}\right] \\
&= \frac{8V_0}{\pi}\frac{n^2}{m(4n^2-m^2)} \qquad (m\,\mathrm{is\,odd})
\end{aligned}$$

[7]

(b) Show that the matrix element $V_{nn'} = \int_{-\infty}^{\infty} \psi_n(x) V(x) \psi_{n'}(x)\,\mathrm{d}x$ is given by

$$\begin{aligned}
V_{nn'} &= \int_{-\infty}^{\infty} \psi_n(x) V(x) \psi_{n'}(x)\,\mathrm{d}x \\
&= \frac{2}{L}\int_0^L V_0 \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n'\pi x}{L}\right)\,\mathrm{d}x \\
&= \frac{2V_0}{4L}\int_0^L \left[\sin\left(\frac{(n+m-n')\pi x}{L}\right) + \sin\left(\frac{(n-m+n')\pi x}{L}\right)\right. \\
&\qquad \left. - \sin\left(\frac{(n+m+n')\pi x}{L}\right) - \sin\left(\frac{(n-m-n')\pi x}{L}\right)\right]\,\mathrm{d}x \\
&= -\frac{V_0}{2L}\left[\frac{L}{(n+m-n')\pi}\cos\left(\frac{(n+m-n')\pi x}{L}\right) + \frac{L}{(n-m+n')\pi}\cos\left(\frac{(n-m+n')\pi x}{L}\right)\right. \\
&\qquad \left. - \frac{L}{(n+m+n')\pi}\cos\left(\frac{(n+m+n')\pi x}{L}\right) - \frac{L}{(n-m-n')\pi}\cos\left(\frac{(n-m-n')\pi x}{L}\right)\right]_0^L \\
&= -\frac{V_0}{2\pi}\left[\frac{1}{(n+m-n')}\left((-1)^{(n+m-n')}-1\right) + \frac{1}{(n-m+n')}\left((-1)^{(n-m+n')}-1\right)\right. \\
&\qquad \left. - \frac{1}{(n+m+n')}\left((-1)^{(n+m+n')}-1\right) - \frac{1}{(n-m-n')}\left((-1)^{(n-m-n')}-1\right)\right] \\
&= \frac{V_0}{2\pi}\left((-1)^{(n-n')}+1\right)\left[\frac{1}{n+m-n'} + \frac{1}{n-m+n'} - \frac{1}{n-m-n'} - \frac{1}{n+m+n'}\right]
\end{aligned}$$

[9]

(c) The first order correction to the wave function ψ_n is

$$\begin{aligned}
\Delta\psi_n^{(1)} &= \sum_{p(\neq n)} \frac{V_{pn}}{E_n - E_p}\phi_p \\
&= \frac{V_0}{2\pi}\frac{2m}{\hbar^2}\left(\frac{L}{\pi}\right)^2\sqrt{\frac{2}{L}}\sum_{p\neq n}\frac{(-1)^{p-n}+1}{n^2-p^2}\left[\frac{1}{p+m-n}+\frac{1}{p-m+n}-\frac{1}{p-m-n}-\frac{1}{p+m+n}\right]\sin(\frac{p\pi x}{L})
\end{aligned}$$

[4]