A Modern Approach to Quantum Mechanics by Townsend - Solutions

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11 Time-Independent Perturbations

11.1

a) **Show that the first-order shift in the energy is given by**

$$E_n^{(1)} = \frac{3\hbar^2 b}{4m^2\omega^2}(1 + 2n + 2n^2)$$

The 1st order correction to the energy is just the expectation value of the perturbing Hamiltonian in between the unperturbed states i.e.

$$E_n^{(1)} = \langle n| \hat{H}_1 |n\rangle \tag{1}$$

$$\begin{aligned} E_n^{(1)} &= \frac{b\hbar^2}{4m^2\omega^2} \langle n| [\hat{a} + \hat{a}^\dagger]^4 |n\rangle \\ &= \frac{b\hbar^2}{4m^2\omega^2} \langle n| 6\hat{a}\hat{a}^{\dagger 2} - 12\hat{a}\hat{a}^\dagger + 3 |n\rangle \\ &= \frac{3b\hbar^2}{4m^2\omega^2}(2n^2 + 2n + 1). \end{aligned}$$

b) **Argue that no matter how small b is, the perturbation will break down for some sufficiently large n. What is the physical reason?**

For convergence, the perturbation must be small relative to energy differences in $\hat{H}_0$ i.e.

$$\frac{E_n^{(1)}}{\Delta E_n^0} \sim \frac{b^2\hbar^2 n^2/m^2\omega^2}{\hbar\omega} \sim \frac{b^2\hbar n^2}{m^2\omega^3} \gg 1.$$

This assumption breaks down for some large n because the 1st order correction grows like n^2 and the unperturbed energy grows like n. No matter how small b is, the energy difference in $\hat{H}_0$ will be suppressed at large n.

11.2

$$e^{\frac{-iq|\boldsymbol{E}|\hat{p}_x}{m\omega^2\hbar}}|n\rangle \approx 1 - \frac{iq|\boldsymbol{E}|}{m\omega^2\hbar}\hat{p}_x + \left(\frac{q|\boldsymbol{E}|}{m\omega^2\hbar}\right)^2 \hat{p}_x^2$$

Higher order $\hat{p}_x$ terms go to zero

$$\begin{aligned}
|\Psi_n\rangle = e^{\frac{-iq|\boldsymbol{E}|\hat{p}_x}{m\omega^2\hbar}}|n\rangle &\approx |n\rangle - \frac{iq|\boldsymbol{E}|}{m\omega^2\hbar}\hat{p}_x|n\rangle \\
&= |n\rangle - \frac{iq|\boldsymbol{E}|}{m\omega^2\hbar}\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger)|n\rangle \\
&= |n\rangle - q|\boldsymbol{E}|\sqrt{\frac{n}{2m\hbar\omega^3}}|n-1\rangle + q|\boldsymbol{E}|\sqrt{\frac{n+1}{2m\hbar\omega^3}}|n+1\rangle
\end{aligned}$$

Perturbative results: Hamiltonian of an applied electric field $\hat{H}_1 = -q|E|\hat{x}$

$$\begin{aligned}
\hat{H}_1|n\rangle &= -q|E|\frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^\dagger)|n\rangle \\
&= -q|E|\frac{\hbar}{2m\omega}(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle)
\end{aligned}$$

When we calculated $\left\langle k|\hat{H}_1|n\middle|k|\hat{H}_1|n\right\rangle$ for equation (11.23), we are left with only $k = n-1$ and $k = n+1$.

$$k = n-1 \rightarrow \left\langle n-1|\hat{H}|n\middle|n-1|\hat{H}|n\right\rangle = -q|\boldsymbol{E}|\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n}$$

$$k = n+1 \rightarrow \left\langle n+1|\hat{H}|n\middle|n+1|\hat{H}|n\right\rangle = -q|\boldsymbol{E}|\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}$$

$$\begin{aligned}
E_n^{(0)} - E_k^{(0)} &= (n-k)\hbar\omega \\
E_n^{(0)} - E_{n-1}^{(0)} &= (n-n+1)\hbar\omega = \hbar\omega \\
E_n^{(0)} - E_{n+1}^{(0)} &= (n-n-1)\hbar\omega = -\hbar\omega
\end{aligned}$$

Use these values to evaluate the shift to the harmonic oscillator state

$$
\begin{aligned}
|\Psi_n\rangle &= \left|\Psi_n^{(0)}\right\rangle + \lambda \left|\Psi_n^{(1)}\right\rangle + ... \\
&= \left|\Psi_n^{(0)}\right\rangle + \sum_{k\neq n} \left|\Psi_k^{(0)}\right\rangle \frac{\left\langle k|\hat{H}|n\right|k|\hat{H}|n\right\rangle}{E_n^{(0)} - E_k^{(0)}} \\
&= |n\rangle + \frac{\left\langle n-1|\hat{H}|n\right|n-1|\hat{H}|n\right\rangle}{E_n^{(0)} - E_{n-1}^{(0)}} |n-1\rangle + \frac{\left\langle n+1|\hat{H}|n\right|n+1|\hat{H}|n\right\rangle}{E_n^{(0)} - E_{n+1}^{(0)}} |n+1\rangle \\
&= |n\rangle - q|\boldsymbol{E}|\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\hbar\omega}\sqrt{n}\,|n-1\rangle + q|\boldsymbol{E}|\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\hbar\omega}\sqrt{n+1}\,|n+1\rangle \\
&= |n\rangle - q|\boldsymbol{E}|\sqrt{\frac{n}{2m\hbar\omega^3}}\,|n-1\rangle + q|\boldsymbol{E}|\sqrt{\frac{n+1}{2m\hbar\omega^3}}\,|n+1\rangle
\end{aligned}
$$

This agrees with the above result. Yay.

11.3

First Order

$$
\begin{aligned}
\hat{x} &= \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \\
\hat{x}^2 &= \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger^2}) \\
E_n^{(1)} &= \left\langle \Psi_n^{(0)}|\hat{H}_1|\Psi_n^{(0)}\right|\Psi_n^{(0)}|\hat{H}_1|\Psi_n^{(0)}\right\rangle = \frac{\hbar}{2m\omega}\frac{m\omega_1^2}{2}\left\langle n|(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger^2})|n\right|n|(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger^2})|n\right\rangle \\
&= \frac{\hbar\omega_1^2}{4\omega}\left((n+1) + n\right) = \frac{\hbar\omega_1^2}{4\omega}(2n+1)
\end{aligned}
$$

Second Order

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\left\langle \Psi_k^{(0)}|\hat{H}_1|\Psi_n^{(0)}\right\rangle\left\langle \Psi_k^{(0)}|\hat{H}_1|\Psi_n^{(0)}\right\rangle|^2}{E_n^0 - E_k^0} = \frac{m^2\omega_1^4}{4}\frac{\hbar^2}{4m^2\omega^2}\sum_{k\neq n}\frac{|\left\langle k|(\hat{a}^2+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a}+\hat{a}^{\dagger 2})|n\right\rangle k|(}{E_n^0 - E}$$

$$\left\langle k|\hat{H}_1|n\right\rangle k|\hat{H}_1|n\rangle = \sqrt{n}\sqrt{n-1}\,\langle k|n-2|k|n-2\rangle + (n+1)\,\langle k|n|k|n\rangle + n\,\langle k|n|k|n\rangle + \sqrt{n+1}\sqrt{n+2}\,\langle k|n+2|k|n$$

Only $k \neq n$ terms survive so

$$E_n^{(2)} = \left(\frac{\hbar\omega_1^2}{4\omega}\right)^2\left[\frac{|\sqrt{n}\sqrt{n-1}|^2}{\hbar\omega(n+\frac{1}{2}-n+2-\frac{1}{2}} + \frac{|\sqrt{n+1}\sqrt{n+2}|^2}{\hbar\omega(n+\frac{1}{2}-n-2-\frac{1}{2}}\right]$$

$$E_n^{(2)} = \left(\frac{\hbar\omega_1^2}{4\omega}\right)^2\left[\frac{n(n-1)}{\hbar\omega 2} - \frac{(n+1)(n+2)}{\hbar\omega 2}\right] = \frac{\omega_1^4\hbar}{16\omega^3}(-2n-1)$$

$$E = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = \hbar\omega(n+\frac{1}{2})\frac{\hbar\omega_1^2}{4\omega}(2n+1) - \frac{\hbar\omega_1^4}{16\omega^3}(2n+1)$$

$$= \left[\hbar\omega + \frac{\hbar\omega_1^2}{2\omega} - \frac{\hbar\omega_1^4}{8\omega^3}\right](n+\frac{1}{2})$$

Exact Solution

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m(\omega^2+\omega_1^2)\hat{x}^2$$

$$E_n = \hbar\sqrt{\omega_1^2+\omega^2}(n+\frac{1}{2})$$

11.4

a) **for the constant perturbation $\hat{H}_1 = V_1$ and**

The first order energy shift of the ground state is given by

$$E_1^{(1)} = \langle n|\,\hat{H}_1\,|n\rangle = \langle 1|\,\hat{V}_1\,|1\rangle$$

Which given the potential $V(x)$

$$E_1^{(1)} = \begin{cases} 0 & 0 < x < L \\ \infty & \text{elsewhere} \end{cases}$$

Similarly for the first excited state

$$E_2^{(1)} = \langle n|\,\hat{H}_1\,|n\rangle = \langle 2|\,\hat{V}_1\,|2\rangle$$

Which given the potential $V(x)$

$$E_2^{(1)} = \begin{cases} 0 & 0 < x < L \\ \infty & \text{elsewhere} \end{cases}$$

b) **for the linearly increasing perturbation $\hat{H}_1 = \varepsilon E_1^{(0)} \hat{x}/L$, where $E_1^{(0)}$ is the unperturbed energy of the ground state and $\varepsilon \ll 1$**

The first order energy shift of the ground state is given by

$$E_1^{(1)} = \langle n| \hat{H}_1 |n\rangle = \left\langle 1 \middle| \frac{\varepsilon E_1^{(0)} \hat{x}}{L} \middle| 1 \right\rangle = \frac{\varepsilon E_1^{(0)}}{L} \int_0^L \cos^2\left(\frac{\pi x}{L}\right) x \, dx = \frac{\varepsilon E_1^{(0)}}{L} \frac{L^2}{4}$$

where

$$E_1^{(0)} = \langle 1| H_0 |1\rangle = \frac{\hbar^2 \pi^2}{2mcL^2}$$

therefore

$$E_1^{(1)} = \begin{cases} \frac{\varepsilon}{4L} \frac{\hbar^2 \pi^2}{2mc} & 0 < x < L \\ \infty & \text{elsewhere} \end{cases}$$

The unperturbed energy outside the well is infinity because the potential will dominate its Hamiltonian

$$H = \frac{\hat{p}_x}{2m} + V(x)$$

Similarly for the first excited state

$$E_2^{(1)} = \left\langle 2 \middle| \frac{\varepsilon E_1^{(0)} \hat{x}}{L} \middle| 2 \right\rangle = \frac{\varepsilon E_1^{(0)}}{L} \int_0^L \sin^2\left(\frac{2\pi x}{L}\right) x \, dx = E_1^{(0)} \frac{\varepsilon}{2}$$

where

$$E_1^{(0)} = \langle 2| H_0 |2\rangle = \frac{\hbar^2 \pi^2 4}{2mcL^2}$$

therefore

$$E_1^{(1)} = \begin{cases} \frac{\varepsilon}{L} \frac{\hbar^2 \pi^2}{2mc} & 0 < x < L \\ \infty & \text{elsewhere} \end{cases}$$

11.5

a) Simply find the eigenvalues of the Hamiltonian given in part a)

$$\begin{aligned}
0 &= (E_0 + \mu_e|\vec{E}| - \lambda)(E_0 - \mu_e|\vec{E}| - \lambda) - A^2 \\
0 &= \lambda^2 - 2\lambda E_0 + E_0^2 - \mu_e^2|\vec{E}|^2 - A^2 \\
\lambda &= \frac{2E_0 \pm \sqrt{4E_0^2 - 4(E_0^2 - \mu_e^2|\vec{E}|^2 - A^2)}}{2} \\
&= E_0 \pm \sqrt{\mu_e^2|\vec{E}|^2 + A^2}
\end{aligned}$$

$\lambda_1 = E_0 + \sqrt{\mu_e^2|\vec{E}|^2 + A^2}$

$$|\lambda_1\rangle = \frac{1}{N_1}\left(\frac{-\mu_e|\vec{E}| - \sqrt{\mu_e^2|\vec{E}|^2 + A^2}}{A}|1\rangle + |2\rangle\right)$$

$$N_1 = \left(\left[\frac{-\mu_e|\vec{E}| - \sqrt{\mu_e^2|\vec{E}|^2 + A^2}}{A}\right]^2 + 1\right)$$

$\lambda_1 = E_0 - \sqrt{\mu_e^2|\vec{E}|^2 + A^2}$

$$|\lambda_2\rangle = \frac{1}{N_2}\left(\frac{-\mu_e|\vec{E}| + \sqrt{\mu_e^2|\vec{E}|^2 + A^2}}{A}|1\rangle + |2\rangle\right)$$

$$N_2 = \left(\left[\frac{-\mu_e|\vec{E}| + \sqrt{\mu_e^2|\vec{E}|^2 + A^2}}{A}\right]^2 + 1\right)$$

b) $\hat{H} = \hat{H}_0 + \hat{H}_1$

$$\hat{H} = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix} + \begin{bmatrix} \mu_e|\vec{E}| & 0 \\ 0 & -\mu_e|\vec{E}| \end{bmatrix}$$

Find eigenenergies and eigenvectors of $\hat{H}_0$.

$$|I\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \quad E_I = E_0 - A$$
$$|II\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \quad E_{II} = E_0 + A$$

Calculate first-order correction to the two above states using normal non-degenerate perturbation theory (because $E_I \neq E_{II}$).

11.6

We can treat the j component of the magnetic field as a kind of perturbation, where

$$H_0 = -\frac{gq}{2mc}\hat{S}_z \cdot B_0$$
$$H_1 = -\frac{gq}{2mc}\hat{S}_y \cdot B_2$$

We will then write the zero and first order Hamiltonian with its matrix elements

$$\begin{bmatrix} \langle +|\hat{H}_0|+\rangle & \langle +|\hat{H}_0|-\rangle \\ \langle -|\hat{H}_0|+\rangle & \langle -|\hat{H}_0|-\rangle \end{bmatrix} = -\frac{gqB_0}{2mc}\begin{bmatrix} \langle +|\hat{S}_z|+\rangle & \langle +|\hat{S}_z|-\rangle \\ \langle -|\hat{S}_z|+\rangle & \langle -|\hat{S}_z|-\rangle \end{bmatrix}$$
$$= -\frac{gqB_0\hbar}{4mc}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$\begin{bmatrix} \langle +|\hat{H}_1|+\rangle & \langle +|\hat{H}_1|-\rangle \\ \langle -|\hat{H}_1|+\rangle & \langle -|\hat{H}_1|-\rangle \end{bmatrix} = -\frac{gqB_2}{2mc}\begin{bmatrix} \langle +|\hat{S}_y|+\rangle & \langle +|\hat{S}_y|-\rangle \\ \langle -|\hat{S}_y|+\rangle & \langle -|\hat{S}_y|-\rangle \end{bmatrix}$$
$$= -\frac{gqB_2\hbar}{4mc}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

The eigenvalues of this split Hamiltonian are

$$E_1^{(0)} = \frac{gqB_0\hbar}{4mc} \qquad E_2^{(0)} = -\frac{gqB_0\hbar}{4mc}$$
$$v_1 = |+\rangle \qquad v_2 = |-\rangle$$

And with the known representations of the perturbation orders, we find at first order that the contribution of the y-field component is negligible

$$E_1^{(1)} = \langle +|\hat{H}_1|+\rangle = \frac{gqB_2\hbar}{4mc}\begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$
$$E_2^{(1)} = \langle -|\hat{H}_1|-\rangle = -\frac{gqB_2\hbar}{4mc}\begin{bmatrix} 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$$

However at second-order we do find a non-negligible contribution

$$E_1^{(2)} = \frac{|\langle -|\hat{H}_1|+\rangle|^2}{E_1^{(0)} - E_2^{(0)}} = -\left(\frac{gqB_2\hbar}{4mc}\right)^2 \frac{1}{\frac{gqB_0\hbar}{4mc} + \frac{gq\hbar B_0}{4mc}} = \frac{gq\hbar}{4mc}\frac{B_2^2}{2B_0}$$
$$E_2^{(2)} = \frac{|\langle +|\hat{H}_2|-\rangle|^2}{E_2^{(0)} - E_1^{(0)}} = -\left(\frac{gqB_2\hbar}{4mc}\right)^2 \frac{-1}{\frac{gqB_0\hbar}{4mc} + \frac{gqB_0\hbar}{4mc}} = -\frac{gq\hbar}{4mc}\frac{B_2^2}{2B_0}$$

Therefore the perturbed energy is

$$E = \pm\frac{gqB_0\hbar}{4mc} \pm \frac{gq\hbar}{4mc}\frac{B_2^2}{2B_0}$$

But remember that technically the full Hamiltonian of the spin system is $H = H_0 + H_1$ and we are just treating it like a perturbation. The exact eigenvalues of the full spin system are solved by diagonalizing the full matrix

$$\begin{aligned}\det\left(\hat{H} - \lambda I\right) &= \det\begin{bmatrix} -\frac{gqB_0\hbar}{4mc} - \lambda & \frac{gqB_2\hbar}{4mc} \\ -\frac{gqB_2\hbar}{4mc} & \frac{gqB_0\hbar}{4mc} - \lambda \end{bmatrix} \\ &= \left(-\frac{gqB_0\hbar}{4mc} - \lambda\right)\left(\frac{gqB_0\hbar}{4mc} - \lambda\right) - \left(\frac{gqB_2\hbar}{4mc}\right)\left(-\frac{gqB_2\hbar}{4mc}\right) \\ &= -\left(\frac{gqB_0\hbar}{4mc}\right)^2 + \lambda^2 + \left(\frac{gqB_2\hbar}{4mc}\right)^2 = 0\end{aligned}$$

Therefore the exact eigenvalues are

$$E = \pm\sqrt{\left(\frac{gqB_0\hbar}{4mc}\right)^2 - \left(\frac{gqB_2\hbar}{4mc}\right)^2} = \pm\frac{gq\hbar}{4mc}\sqrt{B_0^2 - B_2^2} = \pm\frac{gq\hbar B_0}{4mc}\sqrt{1 - \left(\frac{B_2}{B_0}\right)^2}$$

If we expand this to second order about small ${}^{B_2}/_{B_0}$ using $(1+\epsilon)^\alpha \approx 1 + \alpha\epsilon$ we find agreement with the exact solution

$$E \approx \pm\frac{gq\hbar B_0}{4mc}\left(1 + \frac{1}{2}\left(\frac{B_2}{B_0}\right)^2\right) = \pm\frac{gqB_0\hbar}{4mc} \pm \frac{gq\hbar}{4mc}\frac{B_2^2}{2B_0}$$

11.7

11.8

$$\begin{aligned}\langle n, l', m'|\hat{z}|n, l, m|n, l', m'|\hat{z}|n, l, m\rangle &= \int_{-\infty}^{\infty}\int_0^{\pi}\int_0^{2\pi} Y^*_{l',m'}(\theta,\phi) z Y_{l',m'}(\theta,\phi)\sin\theta\, d\phi d\theta dz \\ &= \int_{-\infty}^{\infty} z\, dz \int_0^{\pi}\int_0^{2\pi} Y^*_{l',m'}(\theta,\phi) Y_{l',m'}(\theta,\phi)\sin\theta\, d\phi d\theta dz \\ &= \delta_{m,m'}\,\delta_{l,l'}\int_{-\infty}^{\infty} z\, dz\end{aligned}$$

If $m \neq m'$ then $\delta_{m,m'} = 0$, proving that $\langle n, l', m'|\hat{z}|n, l, m|n, l', m'|\hat{z}|n, l, m\rangle = 0$ for $m \neq m'$.

11.9

The ground state of the hydrogen atom is non-degenerate, therefore it's first order energy shift follows from non-degenerate perturbation theory

$$E_1^{(1)} = \langle n,l,m|\,\hat{H}_1\,|n,l,m\rangle = \langle 1,0,0|\,\hat{V}_1\,|1,0,0\rangle$$
$$= V_1 \int_0^{L/2} \frac{2}{L}\cos^2\left(\frac{\pi x}{L}\right)\,dx \int_0^{L/2} \frac{2}{L}\cos^2\left(\frac{\pi y}{L}\right)\,dy \int_0^{L} \frac{2}{L}\cos^2\left(\frac{\pi z}{L}\right)\,dz$$
$$= V_1 \frac{8}{L^3}\frac{L}{4}\frac{L}{4}\frac{L}{2} = \frac{V_1}{4}$$

Which given the potential $V(x)$

$$E_1^{(1)} = \begin{cases} V_1/4 & 0 < x < L/2,\ 0 < y < L/2,\ 0 < z < L \\ 0 & L/2 < x < L,\ L/2 < y < L \\ \infty & \text{elsewhere} \end{cases}$$

The excited states, however, have $n^2 = n_x^2 + n_y^2 + n_z^2 =$ 6-fold degeneracy. Ignoring analogous states makes this 3-fold. To find their energy shifts, we must follow degenerate perturbation theory and diagonalize the Hamiltonian in the basis of excited states of size $n^2 \times n^2$

$$E_2^{(1)} = \langle n,l,m|\,\hat{H}_1\,|n,l,m\rangle$$
$$= \begin{bmatrix} \langle 2,1,1|\,\hat{H}_1\,|2,1,1\rangle & \langle 2,1,1|\,\hat{H}_1\,|1,2,1\rangle & \langle 2,1,1|\,\hat{H}_1\,|1,1,2\rangle \\ \langle 1,2,1|\,\hat{H}_1\,|2,1,1\rangle & \langle 1,2,1|\,\hat{H}_1\,|1,2,1\rangle & \langle 1,2,1|\,\hat{H}_1\,|1,1,2\rangle \\ \langle 1,1,2|\,\hat{H}_1\,|2,1,1\rangle & \langle 1,1,2|\,\hat{H}_1\,|1,2,1\rangle & \langle 1,1,2|\,\hat{H}_1\,|1,1,2\rangle \end{bmatrix}$$

Matrix elements with symmetric states will follow the previous result. The perturbing Hamiltonian also has a symmetry about the z-axis, therefore matrix elements with differing z-axis wavefunctions will go to zero. The Hamiltonian is also Hermitian, so elements symmetric about the diagonal will be equivalent, and we only need to calculate one of remaining asymmetric possibilities to determine them both.

$$\langle 1,2,1|\,\hat{V}_1\,|2,1,1\rangle =$$
$$= V_1 \int_0^{L/2} \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\,dx$$
$$\int_0^{L/2} \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\,dy \int_0^{L} \frac{2}{L}\cos^2\left(\frac{\pi z}{L}\right)\,dz$$
$$= V_1 \frac{8}{L^3}\frac{2L}{3\pi}\frac{2L}{3\pi}\frac{L}{2} = \frac{16V_1}{9\pi^2}$$

Now that we have calculated each element we can diagonalize the Hamiltonian to find the energies

$$\det(H_1 - \lambda I) = \left| \begin{bmatrix} V_1/4 - \lambda & 16V_1/9\pi^2 & 0 \\ 16V_1/9\pi^2 & V_1/4 - \lambda & 0 \\ 0 & 0 & V_1/4 - \lambda \end{bmatrix} \right|$$
$$= \left(\frac{V_1}{4} - \lambda\right)\left(\left(\frac{V_1}{4} - \lambda\right)^2 - \left(\frac{16V_1}{9\pi^2}\right)^2\right) = 0$$

Which given the potential $V(x)$

$$E_2^{(1)} = \begin{cases} \frac{V_1}{4}, \frac{V_1}{4} + \frac{16V_1}{9\pi^2} & 0 < x < L/2,\ 0 < y < L/2,\ 0 < z < L \\ 0 & L/2 < x < L,\ L/2 < y < L \\ \infty & \text{elsewhere} \end{cases}$$

11.10

Begin with exact solution:

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \hat{S}_y = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \quad \hat{S}_z = \hbar\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\hat{S}_x^2 = \frac{\hbar^2}{2}\begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad \hat{S}_y^2 = \frac{\hbar^2}{2}\begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix} \quad \hat{S}_z^2 = \hbar^2\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\hat{H} = \frac{a}{\hbar^2}\hat{S}_x^2 + \frac{b}{\hbar^2}(\hat{S}_x^2 - \hat{S}_y^2)$$
$$\hat{H} = a\begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} + \frac{b}{2}\left(\begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix}\right)$$
$$\hat{H} = \begin{bmatrix} a & 0 & b \\ 0 & 0 & 0 \\ b & 0 & a \end{bmatrix}$$

Eigenenergies of $\hat{H}$ are $E_\pm = a \pm b$ and $E_0 = 0$
Perturbative solution:

$$\hat{H}_0 = \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a \end{bmatrix} \quad \text{and} \quad \hat{H}_1 = \begin{bmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{bmatrix}$$

Eigenvalues of $\hat{H}_0$ are a with a degeneracy of 2 and 0 with no degeneracy. Now we construct the perturbing Hamiltonian $\hat{H}_1$ in the subspace of the degenerate states. The eigenvectors associated with the degenerate states are $|1\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}$ and $|3\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix}$ so we construct an $\hat{H}_1$ given by

$$\begin{bmatrix}\left\langle 1|\hat{H}_1|1\right|1|\hat{H}_1|1\right\rangle & \left\langle 1|\hat{H}_1|3\right|1|\hat{H}_1|3\right\rangle \\ \left\langle 3|\hat{H}_1|1\right|3|\hat{H}_1|1\right\rangle & \left\langle 3|\hat{H}_1|3\right|3|\hat{H}_1|3\right\rangle\end{bmatrix} = \begin{bmatrix}0 & b\\ b & 0\end{bmatrix} \tag{2}$$

which has eigenenergies $E_\pm = \pm b$

These eigenenergies get added to the corresponding eigenenergies (the ones that were degenerate) of the unperturbed Hamiltonian, resulting in a total energy of $E_\pm = a \pm b$ which agrees with the exact solution. Recall, we also had an unperturbed energy E_0, but the perturbing Hamiltonian does not cause a shift in the state associated with this energy, $E_0 = E_0 + 0$.

11.11

This is a standard two dimensional isotropic harmonic oscillator, meaning that it can be separated into an $\hat{H}_x$ and $\hat{H}_y$ component because $[\hat{H}_x, \hat{H}_y] = 0$.

From this we can see that the total energy $E = E_x + E_y = \hbar\omega(n_x + \frac{1}{2}) + \hbar\omega(n_y + \frac{1}{2}) = \hbar\omega(n_x + n_y + 1)$, with $n_x, n_y = 0, 1, 2, 3, ...$, as explained in greater detail (for the three dimensional case) on pages 370 and 371 of the Townsend textbook. Also note that this means that $\hat{H}_x$ and $\hat{H}_y$ have simultaneous eigenstates (due to the fact that they commute) which are represented by the $|n_x, n_y\rangle$ ket.

$$E_n = \hbar\omega(n_x + n_y + 1) = \hbar\omega(n + 1),\ n = n_x + n_y = 0, 1, 2, 3, ...$$

The ground state, corresponding to the state with energy $E_{n=0} = \hbar\omega$, has no degeneracy because there is only one combination of n_x and n_y values that can result in $n = n_x + n_y = 0$, namely, $n_x = n_y = 0$. However, the first excited state, corresponding to the state with energy $E_{n=1} = 2\hbar\omega$, has a degeneracy of 2. This comes from the fact that there are two possible combinations of n_x and n_y values that can result in $n = n_x + n_y = 1$, namely, $n_x = 1$, $n_y = 0$ and $n_x = 0$, $n_y = 1$. Therefore we will use regular perturbation theory to find the first-order energy shifts for the ground state and degenerate perturbation theory to find the first-order energy shifts for the first excited states.

Ground-state energy shift

$$\begin{aligned}
\hat{H}_1 &= b\hat{x}\hat{y} = \frac{\hbar b}{2m\omega}\left[(\hat{a}_x + \hat{a}_x^\dagger)(\hat{a}_y + \hat{a}_y^\dagger)\right] \\
E_0^{(1)} &= \left\langle n_x, n_y|\hat{H}_1|n_x, n_y\right|n_x, n_y|\hat{H}_1|n_x, n_y\Big\rangle \text{ for } n_x = n_y = 0 \\
&= \frac{\hbar b}{2m\omega}\left\langle 0,0|(\hat{a}_x\hat{a}_y + \hat{a}_x\hat{a}_y^\dagger + \hat{a}_x^\dagger\hat{a}_y + \hat{a}_x^\dagger\hat{a}_y^\dagger)|0,0\right|0,0|(\hat{a}_x\hat{a}_y + \hat{a}_x\hat{a}_y^\dagger + \hat{a}_x^\dagger\hat{a}_y + \hat{a}_x^\dagger\hat{a}_y^\dagger)|0,0\Big\rangle \\
&= 0 \\
E_0 &= E_0^{(0)} + E_0^{(1)} = \hbar\omega + 0
\end{aligned}$$

First-excited state energy shift, 2-fold degeneracy, define the perturbing Hamiltonian in the subspace of the degenerate states.

$$\begin{bmatrix}
\left\langle 1,0|\hat{H}_1|1,0\right|1,0|\hat{H}_1|1,0\Big\rangle & \left\langle 1,0|\hat{H}_1|0,1\right|1,0|\hat{H}_1|0,1\Big\rangle \\
\left\langle 0,1|\hat{H}_1|1,0\right|0,1|\hat{H}_1|1,0\Big\rangle & \left\langle 0,1|\hat{H}_1|0,1\right|0,1|\hat{H}_1|0,1\Big\rangle
\end{bmatrix} = \begin{bmatrix} 0 & \frac{\hbar b}{2m\omega} \\ \frac{\hbar b}{2m\omega} & 0 \end{bmatrix}$$

This has eigenenergies $E_\pm = \pm\frac{\hbar b}{2m\omega}$, leading to total first-excited state energy shift of

$$E_1 = E_1^{(0)} + E_1^{(1)} = 2\hbar\omega \pm \frac{\hbar b}{2m\omega}$$

11.12

11.13

When first determining the spin-orbit coupling we start with a classical argument where

$$\hat{H}_{S-O} = -\mu \cdot \mathbf{B}$$

here the spin of the electron is coupled to the procession, or orbit, about a magnetic field. To derive the desired form of this Hamiltonian, let us define the magnetic field as

$$\mathbf{B} = -\frac{\mathbf{v}}{c} \times \mathbf{E} = -\frac{\mathbf{v}}{c} \times (-\nabla V_{\mathbf{E}})$$

and the moment

$$\mu = \frac{ge}{2m_e c}\mathbf{S}$$

Therefore the coupling is

$$\hat{H}_{S-O} = -\left(\frac{ge}{2m_e c}\frac{1}{c}\right)\mathbf{S}\cdot\left(\mathbf{v}\times\left(-\frac{1}{r}\frac{dV(r)}{dr}\right)\right) = \frac{1}{2m_e c^2}\frac{1}{|\hat{\mathbf{r}}|}\frac{d\hat{V}}{dr}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}$$

Note that $\hat{\mathbf{S}}\cdot\hat{\mathbf{L}} = \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$, because the two operators act in different spaces and therefore commute. Also, for electrons $g_e = 2$ and we must include the relativistic factor of 1/2. Electric potential over a coulomb charge, e, is the potential energy.

11.14

$$2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} \to \hbar^2\begin{bmatrix} m & \sqrt{l(l+1)-m(m+1)} \\ \sqrt{l(l+1)-m(m+1)} & -(m+1)\end{bmatrix}$$

$$2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}\,|\lambda\rangle = \lambda\hbar^2\,|\lambda\rangle$$

The two eigenvalues are $\lambda = l$ and $\lambda = -(l+1)$. This problem gives you the eigenvalues and the matrix on page 403 of the Townsend textbook. The task is simply to do the math to find the eigenvectors given in (11.92a) and (11.92b). First we will find the eigenvectors associated with an eigenvalue and we will then normalize it. Lets start with $\lambda = l$:

$$\begin{bmatrix} m-l & \sqrt{l(l+1)-m(m+1)} \\ \sqrt{l(l+1)-m(m+1)} & -(m+1)-l\end{bmatrix}\begin{bmatrix} a \\ b\end{bmatrix} = 0$$

$$(m-l)a + b\sqrt{l(l+1)-m(m+1)} = 0,\ \to b = 1,\ a = \frac{\sqrt{l(l+1)-m(m+1)}}{(l-m)}$$

$$|\lambda_i\rangle = \begin{bmatrix} \frac{\sqrt{l(l+1)-m(m+1)}}{(l-m)} \\ 1\end{bmatrix}$$

Normalize the eigenvector, requiring $||\vec{\lambda}_i|| = 1$

$$1 = \sqrt{1+\frac{l(l+1)-m(m+1)}{(l-m)^2}} = \sqrt{\frac{2l+1}{l-m}},\ \text{meaning that}$$

$$b = \sqrt{\frac{l-m}{2l+1}}$$

$$a = \sqrt{\frac{l+m+1}{2l+1}}$$

$$|\lambda_i\rangle = \sqrt{\frac{l+m+1}{2l+1}}\,|l,m,+\boldsymbol{z}\rangle + \sqrt{\frac{l-m}{2l+1}}\,|l,m+1,-\boldsymbol{z}\rangle$$

Now do $\lambda = -(l+1)$

$$\begin{bmatrix} m+l+1 & \sqrt{l(l+1)-m(m+1)} \\ \sqrt{l(l+1)-m(m+1)} & l-m \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

$$\sqrt{l(l+1)-m(m+1)}a + (l-m)b = 0, \ \rightarrow a = 1, \ b = -\frac{\sqrt{l(l+1)-m(m+1)}}{(l-m)}$$

Normalize the eigenvector, following the same process described for the previous one, finding.

$$|\lambda_i\rangle = \sqrt{\frac{l-m}{2l+1}}\,|l, m, +\boldsymbol{z}\rangle - \sqrt{\frac{l+m+1}{2l+1}}\,|l, m+1, -\boldsymbol{z}\rangle$$

11.15

11.16

a) **First show that the exact eigenvalues are given by**

$$E_n = -\frac{\mu(Ze^2-\gamma)^2}{2\hbar^2 n^2}$$

The Hamiltonian for a hydrogen atom, with an additional perturbation is

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2\mu} - \frac{Ze^2}{r} - \frac{\gamma}{r} = \frac{\hat{\mathbf{p}}^2}{2\mu} - \frac{Z'e^2}{r}$$

where $Z' = Z - \gamma/e^2$. If we *exactly* follow the Frobenius method for solving the hydrogen atom (Townsend Eq 10.14-10.32), we arrive at the result

$$E_n = -\frac{\mu(Z'e^2)^2}{2\hbar^2 n^2} = -\frac{\mu((Z-\gamma/e^2)e^2)^2}{2\hbar^2 n^2} = -\frac{\mu(Ze^2-\gamma)^2}{2\hbar^2 n^2} \qquad n = 1, 2, 3, \ldots$$

b) **Since $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$, we can obtain $E_n^{(1)}$ either by explicitly finding the contribution to E_n that is linear in γ, or more generally, noting that**

$$E_n^{(1)} = \gamma \left(\frac{dE_n}{d\gamma}\right)_{\gamma=0}$$

Since $E_n^{(0)}$ is of course independent of γ and the higher order terms in the expansion are at least of order γ^2. In this way show that

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \frac{\mu Z e^2}{\hbar^2 n^2} = \frac{Z \mu c \alpha}{\hbar n^2} = \frac{Z}{a_0 n^2}$$

If

$$E_n^{(1)} = \left\langle \frac{\gamma}{r} \right\rangle_{n,l,m} = \gamma \left(\frac{dE_n}{d\gamma} \right)_{\gamma=0}$$

Then, including the result from the previous problem

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \left(\frac{dE_n}{d\gamma} \right)_{\gamma=0} = \frac{\mu(Ze^2 - (0))}{\hbar n}$$

The fine structure constant (α) is defined as ${}^{e^2}/_{\hbar c}$ and the bohr radius (a_0) is ${}^{\hbar}/_{\mu c \alpha}$, therefore

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \frac{\mu Z e^2}{\hbar^2 n^2} = \frac{Z \mu c \alpha}{\hbar n^2} = \frac{Z}{a_0 n^2}$$

11.17

11.18

11.19