Problem Set 5

PY 452

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Problem 6.23

The energy can be expressed as

$$E_{total} = E_{bohr} + E_{zeeman} + E_{fine\ structure}$$

where

$$E_{bohr} = \frac{-13.6\ eV}{n^2}$$

$$E_{zeeman} = \mu_B B_{ext} [m_\ell + 2m_s]$$

$$E_{fs} = \frac{(13.6\ eV)}{n^3} \alpha^2 \left\{ \frac{3}{4n} - \left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+\frac{1}{2})(\ell+1)} \right] \right\}$$

For this problem we only consider $n=2$. The other quantum numbers must obey...

$$\ell < n \Rightarrow \ell = 0, 1$$

$$|m_\ell| \leq \ell \Rightarrow m_\ell = 0 \quad \text{for } \ell = 0$$

$$m_\ell = -1, 0, 1 \quad \text{for } \ell = 1$$

$$|m_s| = \tfrac{1}{2} \Rightarrow m_s = -\tfrac{1}{2}, \tfrac{1}{2}$$

by plugging each of these 8 combinations into the above formula, the different energy levels are obtained.

Ignoring the fine structure correction, we see that the number of different energy levels only depends on the sum $m_\ell + 2m_s$. For $n=2$ there are

$\boxed{5}$ possible values of this

$$m_\ell + 2m_s = -2, -1, 0, 1, 2$$

Problem 6.27

a) Show $$I = \int_0^{2\pi}\int_0^{\pi} (\vec{a}\cdot\hat{r})(\vec{b}\cdot\hat{r})\sin\theta\, d\theta\, d\phi = \frac{4\pi}{3}(\vec{a}\cdot\vec{b})$$

There are multiple ways to solve this integral. Here is just one way:

notice ① I can take one of the constant vectors (say $\vec{a}$) out of the integral.

$$I = \vec{a}\cdot\int \hat{r}\,(\vec{b}\cdot\hat{r})\, d(\cos\theta)\, d\phi$$

② The integral is over the entire sphere so I can choose my axis any way I want. I choose axis so $\hat{z}$ is in the $\vec{b}$ direction, so $\vec{b}\cdot\hat{r} = |\vec{b}|\cos\theta$

$$I = \vec{a}\cdot\int \hat{r}\,|\vec{b}|\cos\theta\, d(\cos\theta)\, d\phi$$

Now I can expand $\hat{r}$ in the $\hat{x}, \hat{y}, \hat{z}$ directions so

$$I = \vec{a}\cdot\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\cdot|\vec{b}|\cos\theta\left[\cos\phi\sin\theta\,\hat{x} + \sin\phi\sin\theta\,\hat{y} + \cos\theta\,\hat{z}\right]$$

The ϕ integration makes the $\hat{x}$ and $\hat{y}$ terms vanish, leaving

$$I = \vec{a}\cdot 2\pi\int_{-1}^{1} d(\cos\theta)\cdot\cos^2\theta\cdot|\vec{b}|\,\hat{z}$$

recall, we chose our axis of integration so $\vec{b} = |\vec{b}|\hat{z}$, we can take this out of the integral. The integration is then simple, giving.

$$I = \frac{4\pi}{3}(\vec{a}\cdot\vec{b}) \quad \checkmark$$

b) for $\ell = 0$, the wavefunction depends only on r, not θ or ϕ. So the integral to determine the expectation value can be broken into radial and angular parts.

$$\left\langle \frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3} \right\rangle = \int_0^\infty |R(r)|^2 r^2 dr \; \frac{1}{4\pi}\int \left[3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e\right] \sin\theta \, d\theta \, d\phi$$

Using the previous result gives.

$$\langle \cdots \rangle = \frac{1}{4\pi}\int_0^\infty \frac{|R(r)|^2}{r^3} r^2 dr \cdot \left\{ 3\cdot\left(\frac{4\pi}{3}\vec{S}_p\cdot\vec{S}_e\right) - 4\pi\cdot\left(\vec{S}_p\cdot\vec{S}_e\right)\right\}$$

$$\boxed{\langle \cdots \rangle = 0} \quad \checkmark$$

Problem 6.30

The 3-D harmonic oscillator has

$$H = \frac{\vec{p}^2}{2m} + \frac{m\omega^2}{2} r^2 = \left(\frac{p_x^2}{2m} + \frac{m\omega^2}{2} x^2\right) + \left(\frac{p_y^2}{2m} + \frac{m\omega^2}{2} y^2\right) + \left(\frac{p_z^2}{2m} + \frac{m\omega^2}{2} z^2\right)$$

The solution is that of 3 decoupled harmonic oscillators (in the 3 directions).

The general wavefunction can be written as

$$|\psi\rangle = |n_x, n_y, n_z\rangle = |n_x\rangle|n_y\rangle|n_z\rangle$$ where $|n_x\rangle$ is solution to 1-D harmonic oscillator in x direction, and n_x^{th} energy level.

The ground state is

$$|\psi_0\rangle = |0\rangle|0\rangle|0\rangle$$

The 1st order correction for perterbation $H' = \lambda x^2 y z$ is

$$E_0^1 = \langle\psi_0| H' |\psi_0\rangle = \lambda \langle 0|x^2|0\rangle \langle 0|y|0\rangle \langle 0|z|0\rangle$$

$\langle 0|y|0\rangle = 0$ and $\langle 0|z|0\rangle = 0$

so

$$\boxed{E_0^1 = 0}$$

There's no 1st order correction to the ground state.

The 1st excited states are triple degenerate. I can choose them to be

$$|\Psi_1\rangle = \begin{cases} |A\rangle = |n_x=0\rangle |n_y=0\rangle |n_z=1\rangle \\ |B\rangle = |n_x=0\rangle |n_y=1\rangle |n_z=0\rangle \\ |C\rangle = |n_x=1\rangle |n_y=0\rangle |n_z=0\rangle \end{cases}$$

The perturbation Matrix (after calculation) $W_{i,j} = \langle i|H'|j\rangle$; $i,j = A,B,C$ is

$$W = \frac{\lambda\hbar^2}{4m^2\omega^2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The eigenvalues are the 1st order corrections. They are

$$\boxed{E_1' = 0, \pm \frac{\lambda\hbar^2}{4m^2\omega^2}}$$

Problem 6.36

$$H_s' = eE_{ext} z = eE_{ext} r\cos\theta$$

a) The ground state is $\psi_{nem} = \psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$; $a \equiv$ bohr radius.

The 1st order correction is

$$E_1' = \langle \psi_{100} | H_s' | \psi_{100} \rangle = \int \frac{e^{-2r/a}}{\pi a^3} \cdot eE_{ext} r\cos\theta \, d^3\vec{r} = 0$$

The θ integral is zero.

$E_1' = 0$, the ground state is unaffected to 1st order

b) The four 1st excited states are

$$|1\rangle = \psi_{200} = \frac{1}{\sqrt{2\pi a}} \cdot \frac{1}{2a}\left(1 - \frac{r}{2a}\right) e^{-r/2a}$$

$$|2\rangle = \psi_{211} = -\frac{1}{\sqrt{\pi a}} \frac{1}{8a} re^{-r/2a} \sin\theta e^{i\phi}$$

$$|3\rangle = \psi_{210} = \frac{1}{\sqrt{2\pi a}} \frac{1}{4a^2} re^{-r/2a} \cos\theta$$

$$|4\rangle = \psi_{21-1} = \frac{1}{\sqrt{\pi a}} \frac{1}{8a^2} re^{-r/2a} \sin\theta e^{-i\phi}$$

Creating the Perturbation matrix, $W_{ij} = \langle i | H_s' | j \rangle$ involves a bit of work. remembering the $W_{ij} = W_{ji}^*$ eliminates some work. For the rest, there are symmetry arguments for why many elements are zero. In the end, we find

$$W = -3aeE_{ext} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The eigenvalues are the 1st order energy corrections. We find

$$E_2^1 = 0, 0, 3aeE_{ext}, -3aeE_{ext}$$

The 4-fold degenerate state broke into 3 different energy states, one of which is 2-fold degenerate.

c) Diagonalizing W gives the "good" eigenstates:

eigenvalue / 1st order energy correction	eigenvector / "good" eigenstates
0	$\|A\rangle \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \|2\rangle = \psi_{211}$
0	$\|B\rangle \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \|4\rangle = \psi_{21-1}$
$3aeE_{ext}$	$\|C\rangle \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(\|1\rangle + \|3\rangle) = \frac{1}{\sqrt{2}}(\psi_{200} + \psi_{210})$
$-3aeE_{ext}$	$\|D\rangle \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(\|1\rangle - \|3\rangle) = \frac{1}{\sqrt{2}}(\psi_{200} - \psi_{210})$

Calculating $\langle \vec{p}_e \rangle = -e\langle \vec{r} \rangle$ involves integrals over these "good" quantum states.

after integration, we find.

$\langle \vec{p}_e \rangle_A = 0$

$\langle \vec{p}_e \rangle_B = 0$

$\langle \vec{p}_e \rangle_C = 3ae\,\hat{z}$

$\langle \vec{p}_e \rangle_D = -3ae\,\hat{z}$

A useful relation for solving all these integrals is this.

$$\int_0^\infty r^n e^{-\lambda r} dr = \frac{n!}{\lambda^{n+1}} \quad ; \; n = 0, 1, 3 \ldots \quad \lambda > 0$$