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Physics 115 - Seminar 1

Shankar 17.2.2 Consider a spin-1/2 particle with gyromagnetic ratio γ in a magnetic field $\mathbf{B} = B\mathbf{i} + B_o\mathbf{k}$. Treating B as a perturbation, calculate the first- and second-order shifts in energy and first-order shift in wave function for the ground state. Then compare the exact answers expanded to the corresponding orders.

The Hamiltonian for a particle in a magnetic field $\mathbf{B}$ is

$$\hat{H} = -\mu \cdot \mathbf{B} = -\gamma \mathbf{S} \cdot \mathbf{B} = -\frac{\gamma\hbar}{2}\sigma \cdot \mathbf{B}. \tag{1}$$

So in this case,

$$\hat{H} = \hat{H}^0 + \hat{H}^1 = -\frac{\gamma\hbar}{2}\left(\sigma_z B_0 + \sigma_x B\right). \tag{2}$$

We must first calculate the unperturbed energies and eigenstates. To solve the Schrödinger equation,

$$\hat{H}^0 |n\rangle = E_n^0 |n\rangle\,, \tag{3}$$

we must find the eigenvalues of

$$\hat{H}^0 = -\frac{\gamma\hbar}{2}B_0 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4}$$

Letting $E_n^0 = \lambda\gamma\hbar B_0/2$, we have

$$0 = -\frac{\gamma\hbar}{2}B_0 \begin{vmatrix} 1+\lambda & 0 \\ 0 & 1-\lambda \end{vmatrix}, \tag{5}$$

so $\lambda = \pm 1$. This gives eigenvalues $E_-^0 = -\frac{\gamma\hbar}{2}B_0$ and $E_+^0 = \frac{\gamma\hbar}{2}B_0$. To find the wave functions for the unperturbed state, we insert these eigenvalues into Eq. (3) to find

$$|-^0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |+^0\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{6}$$

Now we find the change in energy and wave function for the ground state ($n = -$) due to the perturbing Hamiltonian,

$$\hat{H}^1 = -\frac{\gamma\hbar}{2}B \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{7}$$

We first calculate the first-order shift in the ground state energy from Shankar Eq. (17.1.7):

$$E_-^1 = \left\langle -^0 \middle| \hat{H}^1 \middle| -^0 \right\rangle = -\frac{\gamma\hbar}{2}B_0 \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0. \tag{8}$$

There is thus *no* first-order shift in the ground state energy. Shankar Eq. (17.1.14) gives the perturbed wave function with the first-order correction,

$$|-\rangle = |-^0\rangle + \frac{|+^0\rangle \left\langle +^0 \middle| \hat{H}^1 \middle| -^0 \right\rangle}{E_-^0 - E_+^0} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{\begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \left(-\frac{\gamma\hbar}{2}B \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{-\frac{\gamma\hbar}{2}B_0 - \frac{\gamma\hbar}{2}B_0} = |-^0\rangle + \frac{B}{2B_0}|+^0\rangle \tag{9}$$

To properly normalize this state vector, we would divide it by $[1 + B^2/(2B_0^2)]^{1/2}$, but this equals 1 to first order. Using this perturbed wave function, the second-order energy shift can be found by using Shankar Eq. (17.1.16):

$$E_-^2 = \left\langle -^0 \middle| \hat{H}^1 \middle| -^1 \right\rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \left(-\frac{\gamma\hbar}{2}B \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{B}{2B_0}\begin{bmatrix} 0 \\ 1 \end{bmatrix}\right) = -\frac{\gamma\hbar B^2}{4B_0}. \tag{10}$$

The perturbed energy, to second order, is thus

$$E_- = E_-^0 + E_-^1 + E_-^2 = -\frac{\gamma\hbar B_0}{2} - \frac{\gamma\hbar B^2}{4B_0^2} \tag{11}$$

To compare these results to the exact answers, we solve Eq. (3) for

$$\hat{H} = -\frac{\gamma\hbar}{2}\left[\begin{array}{cc} B_0 & B \\ B & -B_0 \end{array}\right] = -\frac{\gamma\hbar}{2}B_0\left[\begin{array}{cc} 1 & \frac{B}{B_0} \\ \frac{B}{B_0} & -1 \end{array}\right]. \tag{12}$$

Again letting $E_n^0 = \lambda\gamma\hbar B_0/2$, we find our eigenvalues from

$$\left|\begin{array}{cc} 1+\lambda & \frac{B}{B_0} \\ \frac{B}{B_0} & -1+\lambda \end{array}\right| = 0, \tag{13}$$

which gives $\lambda = \pm\left(1 + B^2/B_0^2\right)^{1/2}$, or

$$E_- = -\frac{\gamma\hbar B_0}{2}\left(1 + \frac{B^2}{B_0^2}\right)^{\frac{1}{2}} = -\frac{\gamma\hbar B_0}{2}\left(1 + \frac{B^2}{2B_0^2} + \cdots\right) = -\frac{\gamma\hbar B_0}{2} - \frac{\gamma\hbar B^2}{4B_0^2}, \tag{14}$$

where we can expand the radical in a Taylor series to second order since $B \ll B_0$. Note that this is idential to the perturbed energy to second order shown in Eq. (11). Now, to find the wave function for the ground state, we solve

$$\frac{\gamma\hbar B_0}{2}\left[\begin{array}{cc} -\frac{B^2}{2B_0^2} & \frac{B}{B_0} \\ \frac{B}{B_0} & -2-\frac{B^2}{2B_0^2} \end{array}\right]\left[\begin{array}{c} x \\ y \end{array}\right] = \left[\begin{array}{c} 0 \\ 0 \end{array}\right] \tag{15}$$

to find the ratio $y/x = B/(2B_0)$. This gives an eigenvector of

$$|-\rangle = \left[\begin{array}{c} 1 \\ \frac{B}{2B_0} \end{array}\right] = \left|-^0\right\rangle + \frac{B}{2B_0}\left|+^0\right\rangle, \tag{16}$$

which is equivalent to the result obtained with perturbation theory, Eq. (9).