PHYS 487 Discussion 3 Solutions (Spring 2021)

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1. (a) Since the magnetic field components satisfy $B_x = B_y = 0$, we can simplify $\vec{s}\cdot\vec{B} = s_x B_x + s_y B_y + s_z B_z = s_z B_z$. Thus

$$H = -\gamma \vec{s} \cdot \vec{B} = -\gamma s_z B_z = -\gamma B_0 \cos(\omega t) s_z \tag{1}$$

(b) There are two ways to do this problem.

The first is the long way, which is also the most general way that one expresses the matrix of an operator in a particular basis. Given some operator A and an **orthonormal** basis of n kets $|j\rangle$ where $j = 1, \dots, n$, the matrix elements of A in this basis are given by (where A_{ij} is the entry in the i-th row and j-th column):

$$A_{ij} = \langle i|A|j\rangle$$

In this case, $n = 2$ and we fix $|1\rangle = |\uparrow\rangle$ and $|2\rangle = |\downarrow\rangle$, and one can calculate each of the $2 \times 2 = 4$ matrix elements H_{ij}. For instance,

$$H_{\uparrow\downarrow} = -\gamma B_z \langle \uparrow |s_z| \downarrow\rangle = \gamma B_z \frac{\hbar}{2} \langle \uparrow | \downarrow\rangle = 0$$

The second way, which is also the easy way, is to notice that we already know the matrix represntation of s_z in the $|\uparrow\rangle, |\downarrow\rangle$ basis. It's exactly the pauli matrix σ^z. Thus,

$$H_{ij} = -\gamma B_0 \cos(\omega t)(\sigma^z)_{ij} \tag{2}$$

(c) Because H is time-dependent, we cannot use the formula $|\psi(t)\rangle = \exp(-i\frac{H}{\hbar}t)|\psi(0)\rangle$, which is only valid when $\frac{\partial}{\partial t}H = 0$. We have to directly solve the Schrodinger equation. To do so, we first expand $|\psi(t)\rangle$ in the basis from (b):

$$|\psi(t)\rangle = a(t)|\uparrow\rangle + b(t)|\downarrow\rangle \tag{3}$$

$$\partial_t |\psi(t)\rangle = \dot{a}(t)|\uparrow\rangle + \dot{b}(t)|\downarrow\rangle \tag{4}$$

$$H|\psi(t)\rangle = -\gamma B_z(a(t)s_z|\uparrow\rangle + b(t)s_z|\downarrow\rangle) = -\gamma B_z \frac{\hbar}{2}(a(t)|\uparrow\rangle - b(t)|\downarrow\rangle) \tag{5}$$

where the dot over a, b indicates the time derivative. We are now equipped to solve the Schrodinger equation:

$$i\hbar\partial_t|\psi\rangle = H|\psi\rangle \implies \dot{a}(t)|\uparrow\rangle + \dot{b}(t)|\downarrow\rangle = \gamma B_z \frac{i}{2}(a(t)|\uparrow\rangle - b(t)|\downarrow\rangle) \tag{6}$$

Because $|\uparrow\rangle$ and $|\downarrow\rangle$ are independent of one another, this is really two separate equations:

$$\dot{a} = \frac{i\gamma B_z}{2} a$$
$$\dot{b} = \frac{-i\gamma B_z}{2} b$$

These are solved by separation of variable. For instance, solving for a,

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{i\gamma B_z}{2} a \implies \frac{\mathrm{d}a}{a} = \frac{i\gamma B_0}{2} \cos(\omega t)\,\mathrm{d}t \implies \log a = \frac{i\omega\gamma B_0}{2} \sin(\omega t) + C \tag{7}$$
$$\implies a = C \exp\left(\frac{i\omega\gamma B_0}{2} \sin(\omega t)\right) \tag{8}$$

The constant C is fixed by the fact that $a(0) = C = \frac{1}{\sqrt{2}}$. The final answer is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{\frac{i\omega\gamma B_0}{2} \sin(\omega t)} |\uparrow\rangle + e^{\frac{-i\omega\gamma B_0}{2} \sin(\omega t)} |\downarrow\rangle \right) \tag{9}$$

2. It is important to note that $[s_j, l_k] = 0$ for any $j, l = 1, 2, 3$. This is a consequence of the definitions: the spin operators s_j act on "internal" states of the electron that are distinct from the electron's motion (or, more precisely, spatial wavefunction), while the orbital operators l_k act on the spatial part of the wavefunction. They are both types of angular momentum because they satisfy the same commmutation relations (the same "algebra," in physics parlance) but they are independent of one another. That algebra is

$$[l_i, l_j] = i\hbar\epsilon_{ijk} l_k \qquad [s_i, s_j] = i\hbar\epsilon_{ijk} s_k \tag{10}$$

Also, we should review some commutator identities. The commutator is linear, so that $[A + B, C] = [A, C] + [B, C]$. Moreover, **if A and C commute**, we have that $[AB, C] = A[B, C]$ (there is a more general formula that you can either derive for yourself or find on Wikipedia).

(a) I'll do the calculation for l_3 only; the one for s_3 is identical.

$$[H, l_3] = [H_0 + \beta\vec{l} \cdot \vec{s}, l_3] = \underbrace{[H_0, l_3]}_{=0} + \beta[\vec{l} \cdot \vec{s}, l_3] = \beta[l_1 s_1 + l_2 s_2 + l_3 s_3, l_3] \tag{11}$$

Now, l_3 commutes with all the s_j and also with itself. Thus we get

$$[H, l_3] = \beta(s_1[l_1, l_3] + s_2[l_2, l_3]) = i\hbar\beta(-s_1 l_2 + s_2 l_1) \neq 0 \tag{12}$$

(b) We will use index notation $v \cdot w = v_j w_j$ in this problem. Thus $l^2 = l_k l_k$.

$$[H, l^2] = \beta[\vec{l} \cdot \vec{s}, l^2] = \beta[l_j s_j, l_k l_k] = \beta s_j [l_j, l_k l_k] = 0 \tag{13}$$

where the final equal sign follows from the fact that $[l_j, l^2] = 0$ for any $j = 1, 2, 3$.

3. The quantities m_l and m_s are not good quantum numbers, as the operators they are associated with (respectively, l_3 and s_3) do not commute with the Hamiltonian.

4. Note that $j^2 = l^2 + s^2 + l_j s_j + s_j l_j = l^2 + s^2 + 2l_j s_j$, all of which commute with the original Hamiltonian H_0. We can then calculate

$$[H, j^2] = \beta[l_j s_j, j^2 + s^2 + 2l_k s_k] = \beta(0 + 0 + 2[l_j s_j, l_k s_k]) = 0 \tag{14}$$

The first two terms are zero by part (b), and the last term is zero because it is the commutator of an operator with itself.

Now, for the second operator $j_3 = l_3 + s_3$, we also can see that $[H_0, j_3] = 0$. Thus,

$$[H, j_3] = \beta[l_j s_j, l_3 + s_3] = \beta(s_j[l_j, l_3] + l_j[s_j, s_3]) = i\hbar\beta(\epsilon_{j3k} s_j l_k + \epsilon_{j3k} l_j s_k) \tag{15}$$

$$= i\hbar\beta(\epsilon_{j3k} s_j l_k - \epsilon_{k3j} s_k l_j) \tag{16}$$

$$= i\hbar\beta(\epsilon_{j3k} s_j l_k - \epsilon_{j3k} s_j l_k) = 0 \tag{17}$$

In going from line (15) to line (16), we used the antisymmetry of the ϵ symbol to switch the j and k indices in the second term, introducing a minus sign. Going from (16) to (17), we relabeled the dummy indices in the second term (any index that is summed over is a so-called "dummy" index because it doesn't matter what symbol you assign it, as long as you don't assign it to two different sums in the same term).