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## Quantum physics II - Final exam - January 20th, 2023 (Time: 3 horas)

**1** [3 points]. The Hamiltonian of a particle with spin s = 1 is

$$H = \frac{A}{\hbar^2} \mathbf{L} \cdot \mathbf{S} + \frac{B}{\hbar} \left( L_z + S_z \right),$$

where  $\mathbf{L}$  and  $\mathbf{S}$  are the particle's orbital angular momentum and spin operators, and A and B are constants with units of energy.

- (a) Find the energy levels and the allowed values for the quantum numbers on which the energies depend.
- (b) The system is initially in a state characterized by the quantum numbers  $\ell = 2, m_{\ell} = 0, m_s = 0$ . Find the state of the system at time t.
- (c) If the initial state of the system is as in (b), calculate the probability to obtain  $+\hbar$  in a measurement of the third component of the orbital angular momentum performed at t = T.

In terms of the total angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  the Hamiltonian reads

$$H = \frac{A}{2\hbar^2} \left( \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 \right) + \frac{B}{\hbar} J_z$$

In the coupled basis  $\{\mathbf{L}^2, \mathbf{S}^2, \mathbf{J}^2, J_z\}$  the energy levels are for s = 1

$$E_{\ell JM} = \frac{A}{2} \left[ J(J+1) - \ell(\ell+1) - 2 \right] + BM$$

where  $\ell$ , J and M may take the following values

i) 
$$\ell = 0, 1, 2, ...$$
  
2i)  $J = \ell + 1, \ell, \ell - 1$  for  $\ell = 1, 2, ...,$  and  $J = 1$  for  $\ell = 0$   
3i)  $M = -J, -J + 1, ..., J - 1, J.$ 

The system's initial state is

$$\begin{split} |\psi(0)\rangle &= |\ell = 2, \, s = 1, \, m_{\ell} = 0, \, m_s = 0\rangle = \{ \text{ use } 2 \times 1 \text{ Clebsch-Gordan coefficients table} \} \\ &= \sqrt{\frac{3}{5}} \, |\ell = 2, \, s = 1, \, J = 3, \, M = 0\rangle - \sqrt{\frac{2}{5}} \, |\ell = 2, \, s = 1, \, J = 1, \, M = 0\rangle \,. \end{split}$$

From now on we omit from the notation the quantum numbers  $\ell = 2$ , s = 1. The sates  $|J, M\rangle$  on the second line in the equation above are eigenstates of H, so their time evolution is stationary with energies

 $E_{230} = 2A$  and  $E_{210} = -3A$ . At time t the system is then in state

$$|\psi(t)\rangle = \sqrt{\frac{3}{5}} e^{-2iAt/\hbar} |J=3, M=0\rangle - \sqrt{\frac{2}{5}} e^{3iAt/\hbar} |J=1, M=0\rangle.$$

To calculate the probability of obtaining a given value when measuring  $L_z$  it is best to go back to the decoupled basis  $\{\mathbf{L}^2, \mathbf{S}^2, L_z, S_z\}$ . To do that, we again use the 2×1 table:

$$\begin{split} |\psi(t)\rangle &= \sqrt{\frac{3}{5}} \ e^{-2\mathrm{i}At/\hbar} \left[ \sqrt{\frac{1}{5}} \ |m_{\ell} = +1, \ m_{s} = -1 \rangle + \sqrt{\frac{3}{5}} \ |m_{\ell} = 0, \ m_{s} = 0 \rangle + \sqrt{\frac{1}{5}} \ |m_{\ell} = -1, \ m_{s} = +1 \rangle \right] \\ &- \sqrt{\frac{2}{5}} \ e^{3\mathrm{i}At/\hbar} \left[ \sqrt{\frac{3}{10}} \ |m_{\ell} = +1, \ m_{s} = -1 \rangle - \sqrt{\frac{2}{5}} \ |m_{\ell} = 0, \ m_{s} = 0 \rangle + \sqrt{\frac{3}{10}} \ |m_{\ell} = -1, \ m_{s} = +1 \rangle \right] \\ &= \frac{\sqrt{3}}{5} \ \left( e^{-2\mathrm{i}At/\hbar} - e^{3\mathrm{i}At/\hbar} \right) \ \left( \ |m_{\ell} = +1, \ m_{s} = -1 \rangle + \ |m_{\ell} = -1, \ m_{s} = +1 \rangle \right) \\ &+ \left( \frac{3}{5} \ e^{-2\mathrm{i}At/\hbar} + \frac{2}{5} \ e^{3\mathrm{i}At/\hbar} \right) \ |m_{\ell} = 0, \ m_{s} = 0 \rangle \,. \end{split}$$

The probability to obtain  $+\hbar$  for  $L_z$  at time t = T is then

$$P_{\psi(T)}(L_z, +\hbar) = \left| \frac{\sqrt{3}}{5} \left( e^{-2iAT/\hbar} - e^{3iAT/\hbar} \right) \right|^2 = \frac{3}{25} \left| e^{-5iAT/2\hbar} - e^{5iAT/2\hbar} \right|^2 = \frac{12}{25} \sin^2\left(\frac{5AT}{2\hbar}\right)$$

**2** [2 points]. A system is formed by two non-interacting electrons in a Coulomb potential produced by a charge Ze at the origin. The system is in a state of which the following is known:

(1) Its energy is  $E = E_1/2$ , with  $E_1$  the ground sate energy of an Hydrogen-like atom.

(2) The orbital angular momentum squared of the system is  $6\hbar^2$ .

Find the states in which the the system may be in the basis of the total orbital angular momentum  $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ . Determine the total spin of the system and its third component. Ayuda. The eigenenergies of an Hydrogen-like atom are  $E = E_1/n^2$ .

In accordance with (1), the quantum numbers  $n_1$  and  $n_2$  are given by

$$\frac{1}{2} = \frac{1}{n_1^2} + \frac{1}{n_2^2} \quad \Rightarrow \quad n_1 = n_2 = 2 \,.$$

The orbital angular momentum quantum numbers  $\ell_1$  and  $\ell_2$  of the electrons may then be 0 or 1. From condition (2) we have that the system's total orbital angular momentum number L is such that L(L+1) = 6. This gives L = 2 and implies that the system is in a total orbital angular momentum state  $|L = 2, M_L\rangle$  with  $M_L = -2, -1, 0, +1, +2$  as possibles values for its third component. Since L = 2, both  $\ell_1$  and  $\ell_2$  must be equal to 1. The 1×1 Clebsch-Gordan table shows that the all the states  $|L = 2, M_L\rangle$  are linear combinations of states  $|m_{\ell_1}, m_{\ell_2}\rangle$  that are symmetric under  $m_{\ell_1} \leftrightarrow m_{\ell_2}$ . For the total wave function to be antisymmetric, the latter must then be antisymmetric under  $m_{s_1} \leftrightarrow m_{s_2}$ . Now, the composition of two spins  $s_1 = s_2 = \frac{1}{2}$  gives a triplet  $|S = 1, M_S\rangle$ , whose three states  $M_S = -1, 0, +1$  are symmetric under  $m_{s_1} \leftrightarrow m_{s_2}$ , and a singlet  $|S = 0, M_S = 0\rangle$ , which is antisymmetric. This selects the singlet

$$|S=0, M_S=0\rangle = \frac{1}{\sqrt{2}} \left( |m_{s_1}=+\frac{1}{2}, m_{s_2}=-\frac{1}{2}\rangle - |m_{s_1}=-\frac{1}{2}, m_{s_2}=+\frac{1}{2}\rangle \right),$$

so the system may be in any of the states

$$|L = 2, M_L\rangle |S = 0, M_S = 0\rangle, M_L = -2, -1, 0, +1, +2,$$

with total spin S = 0 and total spin's thrid component  $M_S = 0$ .

**3** [3 points]. The Hamiltonian of a particle with spin 3/2 is  $H = H_0 + H_I$ , with

$$H_0 = \frac{\omega}{\hbar} (S_z^2 - 2\hbar S_z), \qquad H_I = \lambda \omega S_x, \qquad \lambda \ll 1$$

and  $\omega$  an angular frequency.

- i) Find the eigenenergies  $H_0$ , their degeneracies and their eigenvectors.
- 2i) Find the ground state energy of H up to first order in perturbation theory (that is, unperturbed energy plus first order correction).
- 3i) Find the first excited state energy of H up to second order.

The eigenvectors and eigenvalues of the unperturbed Hamiltonian  $H_0$  are

$$E_m^{(0)} = \hbar\omega \left(m^2 - 2m\right), \qquad |\phi_m^{(0)}\rangle = |s\,m\rangle =: |m\rangle, \qquad m = \frac{3}{2}, \, \frac{1}{2}, \, \frac{1}{2}, \, -\frac{3}{2}.$$

Hence

ground state: 
$$E_{3/2}^{(0)} = E_{1/2}^{(0)} = -\frac{3}{4}\hbar\omega$$
, degeneracy = 2, eigenvectors =  $|\frac{3}{2}\rangle$ ,  $|\frac{1}{2}\rangle$ ;  
1st excited state:  $E_{-1/2}^{(0)} = \frac{5}{4}\hbar\omega$ , degeneracy = 1, eigenvectors =  $|-\frac{1}{2}\rangle$ ;  
2nd excited state:  $E_{-3/2}^{(0)} = \frac{21}{4}\hbar\omega$ , degeneracy = 1, eigenvectors =  $|-\frac{3}{2}\rangle$ .

The unperturbed state is doubly degenerate. The first order corrections in perturbation theory produced by  $H_I$  are the eigenvalues of the matrix

$$\mathbb{H}_{I} = \begin{pmatrix} \langle \frac{3}{2} \mid H_{I} \mid \frac{3}{2} \rangle & \langle \frac{3}{2} \mid H_{I} \mid \frac{1}{2} \rangle \\ \langle \frac{1}{2} \mid H_{I} \mid \frac{3}{2} \rangle & \langle \frac{1}{2} \mid H_{I} \mid \frac{1}{2} \rangle \end{pmatrix}.$$

Using  $S_x = \frac{1}{2} \left( S_+ + S_- \right)$  and  $S_{\pm} |s, m\rangle = \hbar \sqrt{s(s+1) - m(m\pm 1)} |s, m\pm 1\rangle$ , we have

$$\mathbb{H}_{I} = \frac{\sqrt{3}}{2} \lambda \hbar \omega \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Its eigenvalues are  $E_{3/2}^{(1)} = \mp \lambda \hbar \omega \sqrt{3}/2$ , so the ground state energy splits then in two energy levels

$$E_{3/2,\pm} = -\frac{3}{4} \hbar \omega \left[ 1 \pm \frac{2}{\sqrt{3}} \lambda + O(\lambda^2) \right].$$

The first unpeturbed excited state is nondegenerate. Its first order correction due to  $H_I$  is

$$E_{-1/2}^{(1)} = \langle -\frac{1}{2} | H_I | -\frac{1}{2} \rangle = 0.$$

At second order the energy correction is given by

$$E_{-1/2}^{(2)} = \sum_{m \neq -\frac{1}{2}} \frac{\left| \langle m | H_I | -\frac{1}{2} \rangle \right|^2}{E_{-1/2}^{(0)} - E_m^{(0)}} = \left\{ \text{only } m = \frac{1}{2}, -\frac{3}{2} \text{ contribute } \right\} = \lambda^2 \hbar \omega \left( \frac{1}{2} - \frac{3}{16} \right) = \frac{5}{16} \lambda^2 \hbar \omega$$

The first excited state enegy up to second order corrections is thus

$$E_{-1/2} = E_{-1/2}^{(0)} + E_{-1/2}^{(1)} + E_{-1/2}^{(2)} + \dots = \frac{5}{4} \hbar \omega \left[ 1 + \frac{1}{4} \lambda^2 + O(\lambda^3) \right].$$

**4** [1 points]. The variational method is used to estimate the ground state energy of a system with Hamiltonian H. Two different trial wave functions  $\psi_1(\lambda)$  and  $\psi_2(\lambda)$  with the same parameter  $\lambda$  are used. The resulting values are  $E_1 = \min_{\lambda} \langle \psi_1(\lambda) | H | \psi_1(\lambda) \rangle = 3 eV$  and  $E_2 = \min_{\lambda} \langle \psi_2(\lambda) | H | \psi_2(\lambda) \rangle = 1 eV$ . Which one approximates most to the exact value? Why?

Since the variational method provides an upper bound to the ground state energy, the closest value to the exact value is the smallest one, namely  $E_2$ .

**5** [2 points]. A system has Hamiltonian  $H_0$ , eigenenergies  $E_{jm}$  and eigensates  $|j,m\rangle$ , where j and m are the quantum numbers labelling the eigenvalues of the operators  $\mathbf{J}^2$  and  $J_z$  of an angular mmomentum  $\mathbf{J}$ . At an initial time  $t_i = 0$  a perturbation  $V(t) = J_x f(t)$  is introduced, with f(t) a function of time. Find at first order in perturbation theory the final states  $|j_f m_f\rangle$  to which the system may have transited after a time  $t = t_f$  as a result of the perturbation if the system was initially in state

(a) 
$$|j_i = 2, , m_i = 2\rangle$$
,

(b) 
$$|j_i = 0, , m_i = 0\rangle$$
.

To first order the transistion probability to a state  $|j, f m_f \rangle$  in a time t is

$$P_{if}(0,t) = \frac{1}{\hbar^2} \left| \langle j_f \, m_f | J_x | j_i \, m_i \rangle \int_o^t dt' \, e^{\mathbf{i}\omega_{fi}t'} f(t') \right|^2$$

For this to be nonzero we need  $\langle j_f, m_f | J_x | j_i, m_i \rangle \neq 0$ . Using

$$J_x = \frac{1}{2} \left( J_+ + J_- \right), \qquad J_\pm |j_i, m_i\rangle = \hbar \sqrt{j_i(j_i + 1) - m_i(m_i \pm 1)} |j_i, m_i \pm 1\rangle,$$

we have that the final state quantum numbers must be  $j_f = j_i$  and either  $m_f = m_i + 1$  or  $m_f = m_i - 1$ . This gives for the cases that we are interested in

- a)  $|j_f = 2, m_f = 1\rangle$ , since  $m_f = 3$  is not compatible with  $j_f = 2$ , and
- b) There is no transition at first order since there are no states with  $j_f = 0$  and  $m_f = \pm 1$ .