

## Física cuántica II - Examen final - 19 de junio de 2023

(Tiempo: 3 horas)

**1 [3 puntos].** El hamiltoniano de un sistema formado por dos partículas con spines  $s_1 = 2$  y  $s_2 = 3/2$  es

$$H = \frac{a}{\hbar} (S_{1z} + S_{2z}) + \frac{b}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2,$$

en donde  $\mathbf{S}_i$  es el operador de spin de la partícula  $i = 1, 2$ , y  $a$  y  $b$  son constantes positivas con unidades de energía.

- a) Determinar los autovalores de  $H$ .
- b) El sistema se encuentra inicialmente en el estado  $|\psi_0\rangle = |m_{s_1} = 0, m_{s_2} = -\frac{3}{2}\rangle$ . Si se mide en  $t = 0$  el módulo al cuadrado del espín total  $\mathbf{S}^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2$  ¿qué valores pueden obtenerse y con qué probabilidades?
- c) Si en la medida anterior se ha obtenido el valor más alto y se mide después, al cabo de un tiempo  $t$ , la tercera componente del primer spin ¿qué valores pueden obtenerse y con qué probabilidades? ¿Cuál es el valor esperado de la tercera componente del primer spin en el tiempo  $t$ ?

a) To diagonalize the Hamiltonian it is convenient to write it in the coupled basis  $\{\mathbf{S}_1^2, \mathbf{S}_2^2, \mathbf{S}^2, S_z\}$ , with  $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$  the system total spin. This gives

$$H = \frac{a}{\hbar} S_z + \frac{a}{2\hbar^2} (\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2).$$

The Hamiltonian eigenstates are in this basis  $\{|S, M\rangle\} := \{|s_1 = 2, s_2 = \frac{3}{2}, S, M\rangle\}$ , where  $S$  may take values  $S = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}$  and, for a given  $S$ ,  $M$  may take the values  $M = -S, -S + 1, \dots, +S$  (0.25). The eigenenergy of the state  $|S, M\rangle$  is (0.25)

$$E_{SM} = aM + \frac{b}{2} [S(S+1) - s_1(s_1+1) - s_2(s_2+1)] = aM + \frac{b}{2} \left[ S(S+1) - \frac{39}{4} \right]$$

b) Using the  $2 \times \frac{3}{2}$  Clebsch-Gordan coefficients table, one writes the initial state  $|\psi_0\rangle$  in the coupled basis as (0.25)

$$\begin{aligned} |\psi_0\rangle &= |m_{s_1} = 0, m_{s_2} = -\frac{3}{2}\rangle \\ &= \sqrt{\frac{2}{7}} |S = \frac{7}{2}, M = -\frac{3}{2}\rangle + \sqrt{\frac{18}{35}} |S = \frac{5}{2}, M = -\frac{3}{2}\rangle + \sqrt{\frac{1}{5}} |S = \frac{3}{2}, M = -\frac{3}{2}\rangle, \end{aligned}$$

A measurement of  $\mathbf{S}^2$  has outcome  $S(S+1)\hbar^2$  with  $S = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$  and probability the absolute value squared of the corresponding Fourier coefficient. That is, (0.5)

$$\frac{63}{4}\hbar^2 \text{ with probability } \frac{2}{7}, \quad \frac{35}{4}\hbar^2 \text{ with probability } \frac{18}{35}, \quad \frac{15}{4}\hbar^2 \text{ with probability } \frac{1}{5}.$$

c) The highest value for the measurement of  $\mathbf{S}^2$  in b) is  $\frac{63}{4}\hbar^2$ . After a measurement with this outcome, the system collapses to state  $|S = \frac{7}{2}, M = -\frac{3}{2}\rangle$ , which from then on evolves in time stationarily with energy  $E_{\frac{7}{2}, -\frac{3}{2}}$ . Hence, after time  $t$ , the system is in state (0.5)

$$|\psi(t)\rangle = e^{-i\omega t} |S = \frac{7}{2}, M = -\frac{3}{2}\rangle \quad \omega = \frac{1}{\hbar} E_{\frac{7}{2}, -\frac{3}{2}} = \frac{3}{\hbar} \left( b - \frac{a}{2} \right).$$

Going back to the decoupled basis, one has (0.25)

$$|\psi(t)\rangle = e^{-i\omega t} \left[ \sqrt{\frac{2}{7}} |m_{s_1} = 0, m_{s_2} = -\frac{3}{2}\rangle + \sqrt{\frac{4}{7}} |m_{s_1} = -1, m_{s_2} = -\frac{1}{2}\rangle + \sqrt{\frac{1}{7}} |m_{s_1} = -2, m_{s_2} = +\frac{1}{2}\rangle \right].$$

If  $S_{1z}$  is measured, the following results can then be obtained (0.5)

$$0 \text{ with probability } \frac{2}{7}, \quad -\hbar \text{ with probability } \frac{4}{7}, \quad -2\hbar \text{ with probability } \frac{1}{7}.$$

d) The expectation value of  $S_{1z}$  is (0.5)

$$\langle S_{1z} \rangle_{\psi(t)} = \frac{2}{7} \cdot 0 + \frac{4}{7} \cdot (-\hbar) + \frac{1}{7} \cdot (-2\hbar) = -\frac{6}{7}\hbar.$$

**2 [2 puntos].** Un sistema está formado por dos electrones en un potencial coulombiano producido por una carga  $Ze$  en el origen. En este problema despreciaremos la repulsión coulombiana entre los electrones. El sistema se encuentra en un estado del que se sabe:

- (1) la energía del sistema está bien definida y vale  $E = E_1/2$ , siendo  $E_1$  la energía del estado fundamental de un átomo hidrogenoide; y
- (2) los cuadrados  $\mathbf{L}_1^2$  y  $\mathbf{L}_2^2$  de los momentos angulares de cada electrón y el cuadrado  $\mathbf{L}^2 = (\mathbf{L}_1 + \mathbf{L}_2)^2$  del momento angular total están bien definidos y todos ellos valen  $2\hbar^2$ .

Escribir los posibles estados del sistema en la base acoplada del momento angular orbital  $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ . Si se mide el cuadrado del spin total del sistema ¿qué valores pueden obtenerse y con qué probabilidades?

Ayuda. La energía de los estados propios de un átomo hidrogenoide es  $E = E_1/n^2$ , siendo  $n$  el número cuántico principal.

The total energy of the system is (0.25)

$$\frac{E_1}{2} = \frac{E_1}{n_1^2} + \frac{E_1}{n_2^2} \Rightarrow n_1 = n_2 = 2.$$

Since  $n_1$  and  $n_2$  may only take values  $0, 1, 2, \dots$ , the only solution to this equation is  $n_1 = n_2 = 2$ . Data (2) above implies that the orbital angular momentum quantum numbers  $\ell_1$  and  $\ell_2$  of the electrons are  $\ell_1 = \ell_2 = 1$ , and that the total orbital angular momentum quantum number  $L$  of the system is  $L = 1$  as well (0.25). The possible values for  $M_L$  associated to  $L_z$  are thus  $M_L = -1, 0, +1$ . The  $1 \times 1$  Clebsch-Gordan table shows that all the states  $|L = 1, M_L\rangle$  are linear combinations of states  $|m_{\ell_1}, m_{\ell_2}\rangle$  that are antisymmetric under  $m_{\ell_1} \leftrightarrow m_{\ell_2}$  (0.5). For the total wave function to be antisymmetric, the latter must then be symmetric under  $m_{s_1} \leftrightarrow m_{s_2}$  (0.25). 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 triplet for the spin part of the system state (0.5). Altogether, the system may be in any of the states

$$|n_1 = n_2 = 2, \ell_1 = \ell_2 = 1, L = 1, M_L\rangle \otimes |s_1 = s_2 = \frac{1}{2}, S = 1, M_S\rangle$$

in the coupled basis  $\{\mathbf{L}_1^2, \mathbf{L}_2^2, \mathbf{L}^2, L_z, \mathbf{S}_1^2, \mathbf{S}_2^2, \mathbf{S}^2, S_z\}$ . If  $\mathbf{S}^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2$  is measured, the only possible outcome is  $S(S = 1)\hbar^2 = 2\hbar^2$  with probability 1 (0.25).

**3 [3 puntos].** El hamiltoniano de un sistema formado por dos partículas distinguibles, ambas de spin  $1/2$ , es  $H = H_0 + H_I$ , con

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

$\lambda \ll 1$  un parámetro adimensional y  $\omega$  una frecuencia angular. En esta expresión  $S_z$  y  $S_x$  son las componentes  $z$  y  $x$  la del spin total del sistema.

- Encontrar las energías propias de  $H_0$  y sus degeneraciones.
- Determinar la corrección a la energía del estado fundamental hasta primer orden perturbativo.
- Calcular la corrección a la energía del primer estado excitado hasta segundo orden perturbativo.

Since the Hamiltonian is written in terms of  $S_z$ , it is convenient to work in the coupled basis  $\{\mathbf{S}_1^2, \mathbf{S}_2^2, \mathbf{S}^2, S_z\}$ , in which the states are denoted by  $|S, M\rangle$ . In this basis, the eigenvalues of  $H_0$  are

$$E_{SM}^{(0)} = \hbar\omega M(M - 1) \quad S = -1, 0, = 1.$$

Noting that  $M = 0$  is compatible with  $S = 0$  and  $S = 1$  we have the following spectrum (0.50+0.25)

$$\begin{array}{lll} \text{ground state: } E_{0,0}^{(0)} = 0, & \text{degeneracy} = 3, & \text{eigenvectors : } |S = 0, M = 0\rangle, \\ & & |S = 1, M = 0\rangle, \\ & & |S = 1, M = 0\rangle. \\ \text{1st excited state: } E_{1,-1}^{(0)} = 2\hbar\omega, & \text{degeneracy} = 1, & \text{eigenvector : } |S = 1, M = 0\rangle. \end{array}$$

b) The first order corrections to the unperturbed ground state energy are the eigenvalues of the matrix

$$\mathbb{H}_I = \begin{pmatrix} \langle 0, 0 | H_I | 0, 0 \rangle & \langle 0, 0 | H_I | 1, 0 \rangle & \langle 0, 0 | H_I | 1, 1 \rangle \\ \langle 1, 0 | H_I | 0, 0 \rangle & \langle 1, 0 | H_I | 1, 0 \rangle & \langle 1, 0 | H_I | 1, 1 \rangle \\ \langle 1, 1 | H_I | 0, 0 \rangle & \langle 1, 1 | H_I | 1, 0 \rangle & \langle 1, 1 | H_I | 1, 1 \rangle \end{pmatrix}.$$

Using

$$S_x = \frac{1}{2}(S_+ + S_-), \quad S_{\pm}|S, M\rangle = \hbar\sqrt{S(S+1) - M(M \pm 1)}|S, M \pm 1\rangle$$

we have that the only nonvanishing matrix elements are

$$\langle 1, 0 | H_I | 1, 1 \rangle = \langle 1, 1 | H_I | 1, 0 \rangle = \frac{\lambda}{\sqrt{2}}\hbar\omega.$$

The matrix  $\mathbb{H}_I$  then becomes

$$\mathbb{H}_I = \frac{\lambda}{\sqrt{2}}\hbar\omega \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

whose eigenvalues are are

$$E^{(1)} = 0, \pm \frac{\lambda}{\sqrt{2}}\hbar\omega.$$

At first order in perturbation theory the unperturbed ground state energy completely breaks its degeneracy, splitting in three levels (1.25)

$$E = E^{(0)} + E^{(1)} = -\frac{\lambda}{\sqrt{2}}\hbar\omega, 0, \frac{\lambda}{\sqrt{2}}\hbar\omega.$$

b) The first excited state  $|1, -1\rangle$  is simple. At first perturbative order, the correction to its energy vanishes,

$$E_{1,-1}^{(1)} = \langle 1, -1 | H_I | 1, -1 \rangle = 0,$$

since  $\langle S, M | S_{\pm} | S, M \rangle = 0$ . At second order, the correction is given by

$$E_{1,-1}^{(2)} = \sum_{S, M; M \neq -1} \frac{|\langle S, M | H_I | 1, -1 \rangle|^2}{E_{1,-1}^{(0)} - E_M^{(0)}}.$$

To have a nonzero numerator in the sum,  $S$  must be 1 and  $M$  must be 0. Using that  $E_{1,0} = 0$ , it follows that

$$E_{1,-1}^{(2)} = \frac{\left(\frac{\lambda}{\sqrt{2}}\hbar\omega\right)^2}{2\hbar\omega} = \frac{\lambda^2}{4}\hbar\omega.$$

The energy up to second order in perturbation theory is (1.00)

$$E_{1,-1} = E_{1,-1}^{(0)} + E_{1,-1}^{(1)} + E_{1,-1}^{(2)} = 2\hbar\omega \left(1 + \frac{\lambda^2}{8}\right).$$

**4 [1 punto].** Para encontrar la energía del estado fundamental de un sistema con hamiltoniano  $H = H_0 + aH_I$ , siendo  $0 < a \ll 1$  un parámetro adimensional positivo y pequeño, se utiliza teoría de perturbaciones. A primer orden se obtiene  $E_{\text{pert}} = (4 + 2a) \text{ eV}$ . Por otro lado se aplica el método variacional usando  $|\psi(\lambda)\rangle$  como estados prueba, con  $\lambda$  un parámetro real. Para el valor esperado del Hamiltoniano en los estados prueba se obtiene

$$E(\lambda) = \langle \psi(\lambda) | H | \psi(\lambda) \rangle = (\lambda^2 - 2a\lambda + 4) \text{ eV}.$$

Discutir razonadamente cuál de los dos métodos, perturbativo hasta primer orden o variacional, proporciona un mejor resultado para la energía del estado fundamental.

To find the variational value for the ground state energy, we must minimize  $E(\lambda)$ :

$$\left. \frac{dE(\lambda)}{d\lambda} \right|_{\lambda_m} = 0 \Leftrightarrow 2\lambda_m - 2a = 0 \Leftrightarrow \lambda_m = a,$$

$$\left. \frac{d^2E(\lambda)}{d\lambda^2} \right|_{\lambda_m} = 2 > 0 \Rightarrow \lambda_m = a \text{ is a minimum, } E_{\text{var}} = E(\lambda_m) = (4 - a^2) \text{ eV}.$$

The best estimate for the ground state energy is the lowest among  $E_{\text{pert}}$  and  $E_{\text{var}}$ . Since

$$E_{\text{pert}} = 4 + 2a \geq E_{\text{var}} = 4 - a^2 \text{ for } 0 < a \ll 1.$$

we conclude that the variational method provides a better estimate (1.00).

**5 [1 punto].** Un átomo de hidrógeno se encuentra inicialmente en su estado fundamental. Se somete a un campo eléctrico exterior

$$\mathcal{E} = \begin{cases} 0 & \text{si } t \leq 0, \\ \mathcal{E}_0 e^{-t/\tau} & \text{si } t > 0, \end{cases}$$

dirigido según el eje  $z$ , con  $\mathcal{E}_0$  y  $\tau$  constantes. Calcular a primer orden en teoría de perturbaciones la probabilidad de que transite a un estado  $n = 2$ ,  $\ell = 1$ ,  $m_\ell$  en un tiempo  $t \rightarrow \infty$ .

Ayuda. El siguiente elemento de matriz es dato

$$\langle n = 2, \ell = 1, m_\ell | z | n = 1, \ell = 0, m_\ell = 0 \rangle = \frac{128\sqrt{2}}{243} a_0 \delta_{m_\ell, 0} \approx 0.745 a_0 \delta_{m_\ell, 0}.$$

The hamiltonian for the system is

$$H = H_0 + V(t), \quad H_0 = \text{Hydrogen atom Hamiltonian,}$$

$$V(t) = ze\mathcal{E}(t).$$

The transition probability from an initial state  $|i\rangle$  at time  $t = 0$  to a final state  $|f\rangle$  after a time  $t \rightarrow \infty$  is at first order in perturbation theory

$$P_{if}(0, \infty) = \frac{1}{\hbar^2} \left| \int_0^\infty dt e^{i\omega_{fi}t} V_{fi}(t) \right|^2, \quad \omega_{fi} = \frac{E_f - E_i}{\hbar}, \quad V_{fi}(t) = \langle f | V(t) | i \rangle.$$

In our case,

$$|i\rangle = |100\rangle, \quad E_i = -E_1; \quad |f\rangle = |21m_\ell\rangle, \quad E_f = -\frac{E_1}{4}; \quad E_1 = \frac{Z^2 e^2}{(4\pi\epsilon_0)2a_0},$$

hence  $\omega_{fi} = 3E_1/4\hbar =: \omega$ . It follows that

$$P_{if}(0, \infty) = \frac{1}{\hbar^2} |\langle 21 m_\ell | z | 100 \rangle|^2 \left| \int_0^\infty dt e^{i\omega t} \mathcal{E}(t) \right|^2.$$

Now,

$$\int_0^\infty dt e^{i\omega t} \mathcal{E}(t) = \mathcal{E}_0 \int_0^\infty dt e^{t[i\omega - (1/\tau)]} = \mathcal{E}_0 \left. \frac{e^{t[i\omega - (1/\tau)]}}{i\omega - \frac{1}{\tau}} \right]_{t=0}^{t \rightarrow \infty} = \frac{\mathcal{E}_0}{i\omega - \frac{1}{\tau}}$$

All in all, **(1.00, integration over  $t$  is important)**

$$P_{if}(0, \infty) = \frac{1}{\hbar^2} (0.745 a_0)^2 \delta_{m_\ell, 0} \frac{\mathcal{E}_0^2}{\omega^2 + (1/\tau^2)} = 0.555 \frac{a_0^2 \mathcal{E}_0^2}{\hbar^2} \frac{\delta_{m_\ell, 0}}{\omega^2 + (1/\tau^2)}.$$