Física cuántica II - Examen final - 17 de junio de 2024 - Soluciones

1. [2 puntos] El hamiltoniano de un sistema formado dos partículas con espines $s_1 = \frac{3}{2}$ y $s_2 = \frac{1}{2}$ es

$$H = \frac{\omega}{\hbar}\, \vec{S}_1 \cdot \vec{S}_2 \,,$$

donde ω es una frecuencia angular constante y $\vec{S}_1$ y $\vec{S}_2$ son los operadores de espín de las partículas. Inicialmente el sistema se encuentra en el estado caracterizado por los números cuánticos de la componente z del espín de cada da partícula $m_1 = \frac{1}{2}$ y $m_2 = \frac{1}{2}$. Obtener la probabilidad de encontrar el sistema al cabo de un tiempo t en el estado caracterizado por los números cuánticos $m_1 = \frac{3}{2}$ y $m_2 = -\frac{1}{2}$.

In the coupled basis $\{\vec{S}_1^2,\, \vec{S}_2^2,\, \vec{S}^2,\, S_z\}$, with $\vec{S} = \vec{S}_1 + \vec{S}_2$ the total spin operator and S_z its third component, the Hamiltonian reads

$$H = \frac{\omega}{2\hbar}\, (\, \vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\,) \,.$$

Its eigenstates and eigenvalues are $|s_1 = \frac{3}{2},\, s_2 = \frac{1}{2},\, S,\, M\rangle$ and (0.25)

$$E_S = \frac{\hbar\omega}{2}\, \left[S(S+1) - \tfrac{9}{2}\right] \,.$$

From now on we will omit the quantum numbers s_1 and s_2 from the state labeling.

The initial state in the decoupled basis $\{\vec{S}_1^2,\, \vec{S}_2^2,\, S_{1z},\, S_{2z}\}$ is $|m_1 = \frac{1}{2},\, m_2 = \frac{1}{2}\rangle$, which using the Clebsch-Gordan tables can be written as (0.50)

$$|\psi(0)\rangle = |m_1 = \tfrac{1}{2},\, m_2 = \tfrac{1}{2}\rangle = \sqrt{\frac{3}{4}}\, |S=2,\, M=1\rangle - \sqrt{\frac{1}{4}}\, |S=1,\, M=1\rangle \,.$$

After time t the state has evolved into (0.50)

$$\begin{aligned} |\psi(t)\rangle &= \sqrt{\tfrac{3}{4}}\, e^{-\mathrm{i}E_2 t/\hbar}\, |S=2,\, M=1\rangle - \sqrt{\tfrac{1}{4}}\, e^{-\mathrm{i}E_1 t/\hbar}\, |S=1,\, M=1\rangle \\ &= \sqrt{\tfrac{3}{4}}\, e^{-3\mathrm{i}\omega t/4}\, |S=2,\, M=1\rangle - \sqrt{\tfrac{1}{4}}\, e^{\mathrm{i}5\omega t/4};|S=1,\, M=1\rangle \,, \end{aligned}$$

Using again the Clebsch-Gordan tables, this state can be written in the decoupled basis as (0.25)

$$\begin{aligned} |\psi(t)\rangle &= \sqrt{\tfrac{3}{4}}\, e^{-3\mathrm{i}\omega t/4} \left(\sqrt{\tfrac{1}{4}}\, |m_1 = \tfrac{3}{4},\, m_2 = -\tfrac{1}{2}\rangle + \sqrt{\tfrac{3}{4}}\, |m_1 = \tfrac{1}{2},\, m_2 = \tfrac{1}{2}\rangle\right) \\ &\quad - \sqrt{\tfrac{1}{4}}\, e^{5\mathrm{i}\omega t/4} \left(\sqrt{\tfrac{3}{4}}\, |m_1 = \tfrac{3}{2},\, m_2 = -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{4}}\, |m_1 = \tfrac{1}{2},\, m_2 = \tfrac{1}{2}\rangle\right) \\ &= \tfrac{\sqrt{3}}{4}\, \left(e^{-3\mathrm{i}\omega t/4} - e^{5\mathrm{i}\omega t/4}\right)\, |m_1 = \tfrac{3}{2},\, m_2 = -\tfrac{1}{2}\rangle + \tfrac{1}{4}\, \left(3\, e^{-3\mathrm{i}\omega t/4} + e^{5\mathrm{i}\omega t/4}\right)\, |m_1 = \tfrac{1}{2},\, m_2 = \tfrac{1}{2}\rangle \,. \end{aligned}$$

The probability of finding the system at time t in a state with $m_1 = 3/2$ and $m_2 = -1/2$ is (0.50)

$$\text{Prob}\left(t;\, m_1 = \tfrac{3}{2},\, m_2 = -\tfrac{1}{2}\right) = \frac{3}{16}\, \left|e^{-3\mathrm{i}\omega t/4} - e^{5\mathrm{i}\omega t/4}\right|^2 = \frac{3}{8}\, (1 - \cos 2\omega t) = \frac{3}{4}\, \sin^2 \omega t \,.$$

2 [2 puntos]. Un observable de un sistema cuántico de dos niveles está representado por el operador A, el cual tiene autovalores $a_1 = \sqrt{2}$ y $a_2 = -\sqrt{2}$ con autoestados normalizados $|a_1\rangle$ y $|a_2\rangle$. El hamiltoniano H del sistema actúa sobre los estados $|a_1\rangle$ y $|a_2\rangle$ de la siguiente forma:

$$H\,|a_1\rangle = |a_1\rangle + \frac{1+i}{\sqrt{2}}\,|a_2\rangle\,, \qquad H\,|a_2\rangle = \frac{1-i}{\sqrt{2}}\,|a_1\rangle + |a_2\rangle\,.$$

El sistema se encuentra en un estado sobre el que se mide el observable A obteniéndose el valor $-\sqrt{2}$. Inmediatamente después se realiza una medida de la energía. Calcular la probabilidad de que el estado tras la segunda medida sea el fundamental.

We need to find the eigenvalues and eigenstates of the Hamiltonian in the basis $\{|a_1\rangle, |a_2\rangle\}$ provided by the eigenstates of the operator A. The matrix form of the Hamiltonian is (0.50)

$$H = \begin{pmatrix} 1 & \frac{1+i}{\sqrt{2}} \\ \frac{1-i}{\sqrt{2}} & 1 \end{pmatrix}.$$

Its eigenvalues are the solutions E to the equation (0.50)

$$\det \begin{pmatrix} 1-E & \frac{1+i}{\sqrt{2}} \\ \frac{1-i}{\sqrt{2}} & 1-E \end{pmatrix} = 0 \quad \Rightarrow \quad (1-E)^2 - 1 = 0 \quad \Rightarrow \quad E = 0,\, 2 := E_0,\, E_2.$$

The corresponding eigenstates are (0.50)

$$|E_0\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1-i}{2} \end{pmatrix} = \tfrac{1}{\sqrt{2}}\,|a_1\rangle - \tfrac{1-i}{2}\,|a_2\rangle\,, \qquad |E_2\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1-i}{2} \end{pmatrix} = \tfrac{1}{\sqrt{2}}\,|a_1\rangle + \tfrac{1-i}{2}\,|a_2\rangle\,.$$

After the measurement of A the system is in state $|a_2\rangle$. The probability of obtaining the ground state energy E_0 in the measurement of the energy in the state $|a_2\rangle$ is (0.50)

$$\mathrm{Prob}_{|a_2\rangle}(E_0) = \left|\langle E_0|a_2\rangle\right|^2 = \left|\tfrac{1-i}{2}\right|^2 = \tfrac{1}{2}\,.$$

3 [2 puntos]. Un sistema está formado por dos partículas idénticas de espín $\frac{1}{2}$, siendo su hamiltoniano

$$H = \frac{P^2}{2\mu} + \frac{1}{2}\,\mu\omega^2 x^2 + \lambda\,\frac{\mu\omega^2}{\hbar^2}\,x^2\,\vec{S}_1\cdot\vec{S}_2\,.$$

donde $P = -\mathrm{i}\hbar\frac{d}{dx}$ es el operador momento para la coordenada relativa $x = x_1 - x_2$ de las partículas y $0 < \lambda \ll 1$ es un parámetro adimensional. Obtener las dos energías más bajas del sistema.

Ayuda. Permutar las coordenadas espaciales $x_1 \leftrightarrow x_2$ de las partículas equivale a $x \leftrightarrow -x$. Los autoestados $\phi_n(x)$ del oscilador armónico satisfacen $\phi_n(-x) = (-1)^n\phi_n(x)$ y tienen energías $E_n = \hbar\omega(n + \frac{1}{2})$.

The problem can be solved either exactly or perturbatively. Exact solution is preferred, but perturbative is accepted.

Exact solution. In the coupled basis $\{\vec{S}_1^2,\ \vec{S}_2^2,\ \vec{S}^2,\ S_z\}$, with $\vec{S} = \vec{S}_1 + \vec{S}_2$ the total spin operator and S_z its third component, the Hamiltonian reads

$$H = \frac{P^2}{2\mu} + \frac{1}{2}\,\mu\omega^2 x^2 + \lambda\,\frac{\mu\omega^2}{2\hbar^2}\,x^2\,\big(\,\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\,\big)$$

In this basis the spin states of the systems are $\{|S, M\rangle\}$ and there are only four of them, organized in a triplet and a singlet:

$$\begin{aligned} \text{triplet:}\ & |1, M\rangle,\ \text{ with } M = -1, 0, 1,\ \text{symmetric under } m_1 \leftrightarrow m_2\,,\\ \text{singletlet:}\ & |0, 0\rangle,\ \text{ antisymmetric under } m_1 \leftrightarrow m_2\,. \end{aligned}$$

The wave function will be then

$$\psi(1, 2) = \chi(x) \otimes |S, M\rangle\,.$$

where $\chi(x)$ is to be determined. Upon subsitution in the time-independent Schrödinger equation $H\psi(1, 2) = E\psi(1, 2)$ and using $s_1 = s_2 = \frac{1}{2}$, it follows that $\chi(x)$ satisfies

$$\left\{\frac{P^2}{2\mu} + \frac{1}{2}\,\mu\omega^2 x^2 + \frac{\lambda}{2}\,\mu\omega^2 x^2\left[\,S(S+1) - \frac{3}{2}\right]\right\}\chi(x) = E\chi(x)\,.$$

This is the time-independent Schrödinger equation of a harmonic oscillator with angular frequency ω_S given by

$$\omega_S^2 = \omega^2 + \lambda\omega^2\left[\,S(S+1) - \frac{3}{2}\right]$$

The solutions are

$$\chi_n(x) = \phi_{n,\omega_S}(x)\,,\quad E_{n,S} = \hbar\omega_S\big(n + \tfrac{1}{2}\,\big) = \hbar\omega\sqrt{1 + \lambda\big[S(S+1) - \tfrac{3}{2}\big]}\,\big(n + \frac{1}{2}\,\big)\quad n = 0, 1, 2, \ldots$$

The system's wave functions are

$$\psi(1, 2) = \phi_{n,\omega_S}(x) \otimes |S, M\rangle\,.$$

For $n=0$, the spatial part is symmetric, so the spin part must be antisymmetric, which selects $S=0$. For $n=1$, the space part is antisymmetric, in which case only $S=1$ is allowed. The four states with lower energies are then

$$\begin{aligned}
\text{Ground state:}\quad & \phi_{0,\omega_0}(x)\otimes|0,0\rangle\,, \qquad E_{0,0}=\frac{1}{2}\,\hbar\omega\sqrt{1-\tfrac{3\lambda}{2}}\,, \quad \text{non-degenerate}\,,\\
\text{First excited state:}\quad & \phi_{1,\omega_1}(x)\otimes|1,M\rangle\,, \qquad E_{1,1}=\frac{3}{2}\,\hbar\omega\sqrt{1+\tfrac{\lambda}{2}}\,, \quad \text{degeneracy=3}\ \ (M=-1,0,1)\,.
\end{aligned}$$

Perturbative solution. The Hamiltonian can be written as the sum of an unperturbed part H_0 aned a perturbation H_I,

$$H+H_0=H_I, \quad H_0=\frac{P^2}{2\mu}+\frac{1}{2}\,\mu\omega^2x^2\,, \quad H_I=\lambda\,\frac{\mu\omega^2}{2\hbar^2}\,x^2\,\big(\,\vec{S}^2-\vec{S}_1^2-\vec{S}_2^2\,\big)\,,$$

where it has been used that $\vec{S}_1\cdot\vec{S}_2=\frac{1}{2}\big(\,\vec{S}^2-\vec{S}_1^2-\vec{S}_2^2\,\big)$. The unperturbed eigenstates are (0.50)

$$\psi_{n,S,M}=\phi_n(x)\otimes|S,M\rangle, \quad n=0,1,2,\ldots, \quad S=0,1, \quad M=-S,\ldots,M.$$

Antisymmetry under $1\leftrightarrow 2$ restricts them to (0.50)

$$\psi_{n=\text{even},0,0}=\phi_{n=\text{even}}(x)\otimes|0,0\rangle\,; \qquad \psi_{n=\text{odd},1,M}=\phi_{n=\text{odd}}(x)\otimes|1,M\rangle\,, \quad (M=-1,0,1).$$

In particular,

$$\begin{aligned}
\text{Ground state:}\quad & \psi^{(0)}_{0,0,0}=\phi_0(x)\otimes|0,0\rangle \qquad E^{(0)}_{0,0}=\frac{\hbar\omega}{2}\,, \quad \text{non-degenerate,}\\
\text{First excited state state:}\quad & \psi^{(0)}_{1,1,M}(1,2)=\phi_1(x)\otimes|1,M\rangle \quad E^{(0)}_{1,1}=\frac{\hbar\omega}{2} \quad \text{degeneracy=3.}
\end{aligned}$$

To compute the first order corrections to the ground and first excited state energies we use that

$$\begin{aligned}
\langle\psi^{(0)}_{n,S,M}\,|\,H_I\,|\,\psi^{(0)}_{n,S',M'}\rangle &= \langle\phi^{(0)}_n\,|\,\tfrac{1}{2}\mu\omega^2x^2\,|\,\phi^{(0)}_n\rangle\ \langle S,M\,|\,\frac{\lambda}{\hbar^2}\big(\,\vec{S}^2-\vec{S}_1^2-\vec{S}_2^2\big)\,|\,S',M'\rangle\\
&= \frac{\hbar\omega}{2}\,\big(n+\tfrac{1}{2}\big)\,\lambda\,\big[\,S(S+1)-\tfrac{3}{2}\,\big]\,\delta_{SS'}\,\delta_{MM'}\,.
\end{aligned}$$

This gives (1.00)

$$E^{(1)}_{0,0}=\langle\psi^{(0)}_0|H_I|\psi^{(0)}_0\rangle=-\frac{3\lambda}{4}\,\frac{\hbar\omega}{2}\,, \quad E^{(1)}_{1,1}=\langle\psi^{(0)}_1|H_I|\psi^{(0)}_0\rangle=\frac{\lambda}{8}\,\frac{3\hbar\omega}{2}\,,$$

These expressionas agree with the first order corrections that result from expanding in powers of λ the exact results.

4 [2 puntos]. Una partícula de carga q y masa m se encuentra en el estado fundamental de un oscilador armónico unidimensional en la dirección z con frecuencia angular ω_0. Para $t > 0$ se introduce una perturbación mediante un campo eléctrico débil oscilante en el tiempo pero uniforme en la dirección del eje z, dado por $\mathcal{E}_z(t) = \mathcal{E}_0 \cos(\omega t)\, e^{-t/\tau}$, donde la constante $\mathcal{E}_0$ tiene dimensiones de campo eléctrico, la constante ω es una frecuencia angular y la constante $\tau > 0$ representa una medida de la duración del pulso eleéctrico.

Obtener a primer orden en teoría de perturtbaciones la probabilidad de que al cabo de un tiempo $t \gg \tau$ la partícula haya transitado a un estado del oscilador armónico de número cu antico k.

The sytem's Hamiltonian is

$$H = H_0 + V(t)\,, \qquad H_0 = \text{harmonic oscillator Hamiltonian}\,,$$
$$V(t) = zq\mathcal{E}(t) = q\mathcal{E}_0 z\cos(\omega t)\, e^{-t/\tau}.$$

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

$$P_{if}(0,t) = \frac{1}{\hbar^2}\left|\int_0^t dt' e^{\mathrm{i}\omega_{fi}t'}\, V_{if}(t')\right|^2, \qquad \omega_{if} = \frac{E_f - E_i}{\hbar}\,, \qquad V_{fi}(t) = \langle f|V(t)|i\rangle\,.$$

In our case,

$$|i\rangle = |0\rangle\,, \quad E_i = E_0 = \frac{\hbar\omega_0}{2}\,; \qquad |f\rangle = |k\rangle\,, \quad E_f = E_k = \hbar\omega_0\left(k + \frac{1}{2}\right); \qquad \omega_{fi} = k\omega_0$$

and

$$V_{fi}(t') = \langle k|V(t')|0\rangle = q\mathcal{E}_0\cos(\omega t')\, e^{-t'/\tau}\,\langle k|z|0\rangle\,.$$

Using

$$\langle k|z|0\rangle = \frac{\delta_{k1}}{\sqrt{2}\alpha}\,, \quad \alpha = \sqrt{\frac{m\omega_0}{\hbar}}\,,$$

we have

$$P_{0k}(0,t) = \delta_{k1}\,\frac{q^2\mathcal{E}_0^2}{2m\hbar\omega_0}\left|\int_0^t dt' e^{\mathrm{i}\omega_0 t'}\cos(\omega t')\, e^{-t'/\tau}\right|^2.$$

The integral over t' can be easily performed

$$\int_0^t dt' e^{\mathrm{i}k\omega_0 t'}\cos(\omega t')\, e^{-t'/\tau} = \frac{1}{2}\left[\frac{e^{\mathrm{i}(\omega_0+\omega)t - \frac{t}{\tau}} - 1}{\mathrm{i}(\omega_0+\omega) - \frac{1}{\tau}} + \frac{e^{\mathrm{i}(\omega_0-\omega)t - \frac{t}{\tau}} - 1}{\mathrm{i}(\omega_0-\omega) - \frac{1}{\tau}}\right]$$
$$= (\text{for } t \gg \tau) = -\frac{1}{2}\left[\frac{1}{\mathrm{i}(\omega_0+\omega) - \frac{1}{\tau}} + \frac{1}{\mathrm{i}(\omega_0-\omega) - \frac{1}{\tau}}\right] = -\frac{\mathrm{i}\omega_0 - \frac{1}{\tau}}{(\mathrm{i}\omega_0 - \frac{1}{\tau})^2 + \omega^2}$$

The probability is then

$$\mathrm{Prob}_{0k}(t \gg \tau) = \delta_{k1}\,\frac{q^2\mathcal{E}_0^2}{2m\hbar\omega_0}\,\frac{(\omega_0^2 + \frac{1}{\tau})^2}{\left(\omega_0^2 + \omega^2 + \frac{1}{\tau^2}\right)^2}\,.$$

5 [2 puntos]. Elegir una y sólo una de las siguientes dos opciones.

Opción (A). Un sistema tiene espacio de Hilbert $\mathbb{C}^2$ y base ortonormal $\{|1\rangle, |2\rangle\}$. Discutir si el operador

$$\varrho = \frac{3}{4}\,|1\rangle\langle 1| + \frac{1}{4}\,|2\rangle\langle 2|$$

puede representar un estado del sistema y, en caso afirmativo, determinar qué tipo de estado es.

Opción (B). El hamiltoniano de un sistema es $H = H_0 + \mu H_I$, con $0 < \mu \ll 1$ un parámetro adimensional. Para encontrar la energía del estado fundamental se usa, por un lado, teoría de perturbaciones a primer orden, con resultado $(94 - 5\mu)$ eV. Y por otro lado, se utiliza el método variacional con una familia de funciones de onda prueba que depende de un parámetro c real, obteniéndose para el valor esperado del hamiltoniano la expresión $E(c) = (c^2 - 2c\mu + 100)$ eV.

¿Cuál de dos métodos (perturbativo o variacional) se aproxima más a la energía del estado fundamental del sistema.

Option (A). In matrix form ϱ can be written as

$$\varrho = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} .$$

It is trivial that ϱ satisfies the three conditions for it to describe a physical state, namely:

(1) $\mathrm{tr}\varrho = \frac{3}{4} + \frac{1}{4} = 1$ (0.50).

(2) ϱ is self-adjoint ($\varrho^+ = \varrho$ (0.50).

(3) ϱ is semipositive definite, since its eigenvalues, $\frac{3}{4}$ and $\frac{1}{4}$, are non-negative (0.50).

For ϱ to describe a pure state, it must satisfy $\varrho^2 = \varrho$. It is trivial that this condition is not met, since (0.50)

$$\varrho^2 = \begin{pmatrix} \frac{9}{16} & 0 \\ 0 & \frac{1}{16} \end{pmatrix} \neq \varrho\,.$$

All inall, ϱ describes a mixed state.

Option (B). The ground state energy computed with the variational method is the minimum of $E(c) = (c^2 - 2c\mu + 100)$. The minimum is located at c_0 given by (1.00)

$$\frac{dE}{dc}\,(c)\Big|_{c=c_0} = 0 \quad \Rightarrow \quad c_0 = \mu\,,$$

$$\frac{d^2E}{dc^2}\,(c)\Big|_{c=c_0} = 2 > 0 \quad \Rightarrow \quad c_0 \text{ is a minimum, and } \quad E_{\mathrm{var}} = E(c_0) = 100 - \mu^2\,.$$

E_{var} must be compared with the perturbative result

$$E_{\mathrm{pert}} = 94 - 5\mu\,.$$

In the range $0 < \mu \ll 1$, in which perturtbation theory makes sense, the minimum of the two values provides a better approximation to the true ground state energy. Since $E_{\rm pert} < E_{\rm var}$ in that range, the perturbative method provides a better result. (1.00)

Note. From the variational method we know that the expectation value $\langle E\rangle = \langle\psi|H|\psi\rangle$ of the Hamiltonian $H + H_0 = H_I$ in any normalized state $|\psi\rangle$ of the Hilbert space is an upper bound of the exact ground state energy $E_0^{\rm exact}$,

$$\langle E\rangle = \langle\psi|H|\psi\rangle \geq E_0^{\rm exact}\,.$$

Assume for generality that the gound state has degeneracy N with energy $E_n^{(0)}$. Let $\{|\phi_{ni}^{(0)}\rangle\}_{i=1\cdots N}$ be a basis of eigenstates of the Hilbert subspace $\mathcal{H}_n$ associated to $E_n^{(0)}$ such that the restriction of H_I to $\mathcal{H}_n$ is diagonal, *i. e.* $\langle\phi_{ni}^{(0)}|H_I|\psi_{nj}^{(0)}\rangle = E_{ni}^{(1)}\delta_{ij}$. Take now $|\psi\rangle = |\phi_{ni}^{(0)}\rangle$, for any $i = 1,\ldots,N$. Then

$$\langle E\rangle = E_n^{(0)} + E_{ni}^{(1)} \geq E_0^{\rm exact} \qquad (i = 1,\ldots,N)\,,$$

so that first order perturbation theory also provides an upper bound for the exact ground state energy.