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Física cuántica II - Examen final - 10 de enero de 2024

(Tiempo: 3 horas)

1 [2 puntos]. El hamiltoniano de un átomo de hidrógeno en un campo magnético constante de módulo B dirigido según el eje z es

$$H = -\frac{\hbar^2}{2\mu}\Delta + \frac{e^2}{4\pi\epsilon_0 r} + \omega S_z \qquad \omega = \frac{eB}{2\mu},$$

con S_z la tercera componente del operador de espín del electrón. El atomo se encuentrea en un estado del que se sabe:

i) su número cuántico radial es $n = 3$,

2i) es un autoestado del cuadrado $\mathbf{J}^2$ del momento angular total $\mathbf{J} = \mathbf{L} + \mathbf{S}$ con autovalor $\frac{15}{4}\hbar^2$.

3i) es un autoestado de la tercera componente J_z del momento angular total $\mathbf{J}$ con autovalor $\frac{3}{2}\hbar$.

4i) al medir el cuadrado $\mathbf{L}^2$ del momento angular orbital se obtiene $6\hbar^2$ con probabilidad $\frac{1}{2}$.

Se pregunta:

a) ¿Qué otros valores pueden obtenerse al medir $\mathbf{L}^2$ y con qué probabilidades?

b) Escribir el estado en las bases desacoplada $|n, \ell, s, m_\ell, m_s\rangle$ y acoplada $|n, \ell, s, j, m_j\rangle$.

c) Si se mide la energía, ¿qué valores pueden obtenerse y con qué probabilidades?

d) Se deja evolucionar el sisema y se mide $\mathbf{J}^2$ al cabo de un tiempo τ. ¿Cuál es la probabilidad de obtener $\frac{35}{4}\hbar^2$?

From the data we have

i) $n=3 \Rightarrow l = 0, 1, 2$

2i) $J(J+1) = \frac{15}{4} \Rightarrow J = \frac{3}{2}$

3i) $M_J = \frac{3}{2}$

Since $s = \frac{1}{2}$ and $\vec{J} = \vec{L} + \vec{S}$

$0 \times \frac{1}{2} = \frac{1}{2}$; $1 \times \frac{1}{2} = \frac{3}{2}, \frac{1}{2}$; $2 \times \frac{1}{2} = \frac{5}{2}, \frac{3}{2}$,

in the coupled basis $|n\, l\, s\, J\, M_J\rangle$ the atoms state is

$$|\psi(0)\rangle = a\,|n=3\;\; l=1\;\; s=\tfrac{1}{2}\;\; J=\tfrac{3}{2}\;\; M_J=\tfrac{3}{2}\rangle + b\,|n=3\;\; l=2\;\; s=\tfrac{1}{2}\;\; J=\tfrac{3}{2}\;\; M_J=\tfrac{3}{2}\rangle$$

with $|a|^2 + |b|^2 = 1$. If $\vec{L}^2$ is measured, only $2\hbar^2$ and $6\hbar^2$ can be obtained with probabilities

$$\text{Prob}(\vec{L}^2; 2\hbar^2) = |a|^2, \qquad \text{Prob}(\vec{L}^2; 6\hbar^2) = |b|^2 = 1 - |a|^2.$$

Data 4i) implies $|b|^2 = \frac{1}{2}$. Hence $|a|^2 = \frac{1}{2}$, so that

a) A measurement of $\vec{L}^2$, besides $6\hbar^2$, may give $2\hbar^2$ with probability $\frac{1}{2}$

b) Modulo an irrelevant global phase the atom's state is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(e^{i\theta}|n=3\ l=1\ s=\tfrac{1}{2}\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle + |n=3\ l=2\ s=\tfrac{1}{2}\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle\right),$$

with $e^{i\theta}$ an arbitrary local phase. Using the Clebsch-Gordan tables

$$|l=1\ s=\tfrac{1}{2}\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle = |l=1\ s=\tfrac{1}{2}\ m_l=1\ m_s=\tfrac{1}{2}\rangle \qquad (1)$$

$$|l=2\ s=\tfrac{1}{2}\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle = \frac{2}{\sqrt{5}}|l=2\ s=\tfrac{1}{2}\ m_l=2\ m_s=-\tfrac{1}{2}\rangle - \frac{1}{\sqrt{5}}|l=2\ s=\tfrac{1}{2}\ m_l=1\ m_s=\tfrac{1}{2}\rangle$$

The state in the decoupled basis is (omitting $n=3$ and $s=1/2$ in the notation)

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\Big[e^{i\theta}|l=1\ m_l=1\ m_s=\tfrac{1}{2}\rangle + \frac{2}{\sqrt{5}}|l=2\ m_l=2\ m_s=-\tfrac{1}{2}\rangle - \frac{1}{\sqrt{5}}|l=2\ m_l=1\ m_s=\tfrac{1}{2}\rangle\Big]$$

c) The Hamiltonian eigenstates and eigenvalues are

$$|n\ l\ s\ m_l\ m_s\rangle, \qquad E_{n m_s} = -\frac{13.6}{n^2}\,eV + \hbar\omega\, m_s =: -\frac{E_0}{n^2} + \hbar\omega\, m_s$$

A measurement of the energy may give

$$E_{3,1/2} = -\frac{E_0}{9} + \frac{\hbar\omega}{2} \text{ with probability } = \left|\frac{e^{i\theta}}{\sqrt{2}}\right|^2 + \left|\frac{-1}{\sqrt{2}\sqrt{5}}\right|^2 = \frac{6}{10} = \frac{3}{5}$$

$$E_{3,-1/2} = -\frac{E_0}{9} - \frac{\hbar\omega}{2} \text{ with probability } = \left|\frac{1}{\sqrt{2}}\frac{2}{\sqrt{5}}\right|^2 = \frac{2}{5}$$

d) At time t the state is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\Big[e^{-iE_{3,1/2}t/\hbar}\Big(e^{i\theta}\,|l=1\ m_l=1\ m_s=\tfrac{1}{2}\rangle - \frac{1}{\sqrt{5}}\,|l=2\ m_l=1\ m_s=\tfrac{1}{2}\rangle\Big)$$

$$+\, e^{-iE_{3,-1/2}t/\hbar}\,\frac{2}{\sqrt{5}}\,|l=2\ m_l=2\ m_s=-\tfrac{1}{2}\rangle\Big]$$

= Go back to the coupled basis

$$= \frac{1}{\sqrt{2}}e^{iE_0t/a\hbar}\Big[e^{-i\omega t/2}\,e^{i\theta}\,|l=1\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle$$

$$-\frac{e^{-i\omega t/2}}{\sqrt{5}}\Big(\frac{2}{\sqrt{5}}|l=2\ J=\tfrac{5}{2}\ M_J=\tfrac{3}{2}\rangle - \frac{1}{\sqrt{5}}|l=2\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle\Big)$$

$$+\, e^{i\omega t/2}\frac{2}{\sqrt{5}}\Big(\frac{1}{\sqrt{5}}|l=2\ J=\tfrac{5}{2}\ M_J=\tfrac{3}{2}\rangle + \frac{2}{\sqrt{5}}|l=2\ J=\tfrac{3}{2}\ M_J=\tfrac{3}{2}\rangle\Big)\Big]$$

The probability of obtaining $\frac{35}{4}\hbar^2$ ($\Leftrightarrow J=\frac{5}{2}$) in a measurment of $\vec{L}^2$ is

$$\text{Prob}(\vec{L}^2, \tfrac{35}{4}\hbar^2) = \left|-\frac{\sqrt{2}}{5}e^{-i\omega t/2} + \frac{\sqrt{2}}{5}e^{i\omega t/2}\right|^2 = \frac{8}{25}\sin^2\!\left(\frac{\omega t}{2}\right)$$

2 [2 puntos]. Un sistema está formado por cuatro partículas idénticas de espín 1/2 que se encuentran en un pozo infinito unidimensional de anchura a centrado en el origen. Recordando que las autoenergías del pozo infinito son $E_n = \hbar^2\pi^2 n^2/2ma^2$ $(n = 1, 2, \ldots)$, llamando $\phi_n(x)$ a las autofunciones correspondientes y despreciando la interacción entre las partículas,

(a) Encontrar la función de ondas, la energía y la degeneración del estado fundamental del sistema.

(b) Encontrar las enrgías y las degeneraciones del primer y segundo estados excitados del sistema.

According to Pauli's principle there can be at most two electrons with the same n (one with $m_s = 1/2$ and the other one with $m_s = -1/2$). Noting that the system's energy is

$$E = \frac{\hbar^2\pi^2}{2ma^2}\left(n_1^2 + n_2^2 + n_3^2 + n_4^2\right)$$

we have that

- ground state has

$n_1 = 1$ $m_{s_1} = \frac{1}{2}$; $n_2 = 1$ $m_{s_2} = -\frac{1}{2}$; $n_3 = 2$ $m_{s_3} = \frac{1}{2}$; $n_4 = 2$ $m_{s_4} = -\frac{1}{2}$. Nondegenerate.

$$E = 10\,\frac{\hbar^2\pi^2}{2ma^2}$$

$$\phi(1,2,3,4) = \frac{1}{\sqrt{4!}}\det\begin{pmatrix} \phi_{1,\frac{1}{2}}(1) & \phi_{1,\frac{1}{2}}(2) & \phi_{1,\frac{1}{2}}(3) & \phi_{1,\frac{1}{2}}(4) \\ \phi_{1,-\frac{1}{2}}(1) & \phi_{1,-\frac{1}{2}}(2) & \phi_{1,-\frac{1}{2}}(3) & \phi_{1,-\frac{1}{2}}(4) \\ \phi_{2,\frac{1}{2}}(1) & \phi_{2,\frac{1}{2}}(2) & \phi_{2,\frac{1}{2}}(3) & \phi_{2,\frac{1}{2}}(4) \\ \phi_{2,-\frac{1}{2}}(1) & \phi_{2,-\frac{1}{2}}(2) & \phi_{2,-\frac{1}{2}}(3) & \phi_{2,-\frac{1}{2}}(4) \end{pmatrix}$$

- First excited state (second smallest value of E) is accomplished for

$n_1 = 1$ $m_{s_1} = \frac{1}{2}$; $n_2 = 1$ $m_{s_2} = -\frac{1}{2}$; $n_3 = 2$ $m_{s_3} = \frac{1}{2}$; $n_4 = 3$ $m_{s_4} = \pm\frac{1}{2}$. Degeneracy = 4

$$E = \frac{\hbar^2\pi^2}{2ma^2}\left(1 + 1 + 2^2 + 3^2\right) = \frac{15}{2}\,\frac{\hbar^2\pi^2}{ma^2}$$

- Second excited state (third smallest value of E) is obtained for

$n_1 = 1$ $m_{s_1} = \pm\frac{1}{2}$; $n_2 = 2$ $m_{s_2} = \frac{1}{2}$; $n_3 = 2$ $m_{s_3} = -\frac{1}{2}$; $n_4 = 3$ $m_{s_4} = \pm\frac{1}{2}$. Degeneracy = 4

$$E = 18\,\frac{\hbar^2\pi^2}{2ma^2}\;\left(1^2 + 2^2 + 2^2 + 3^2\right) = 9\,\frac{\hbar^2\pi^2}{ma^2}$$

3 [2 puntos]. El movimiento de una partícula de espín 1 está regido por el hamiltoniano efectivo

$$H = H_0 + H_I\,, \qquad H_0 = \frac{\omega}{\hbar}\left(\mathbf{S}^2 - S_y^2 - \hbar\, S_y\right), \qquad H_I = -\lambda\omega S_z\,,$$

donde el operador de espín $\mathbf{S} = (S_x, S_y, S_z)$ de la partícula está dado por las matrices

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}, \qquad S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -\mathrm{i} & 0\\ \mathrm{i} & 0 & -\mathrm{i}\\ 0 & \mathrm{i} & 0\end{pmatrix}, \qquad S_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix},$$

$\omega > 0$ es una frecuencia y $0 \ll \lambda \ll 1$ es un parmámetro adimensional.

a) Encontrar una conjunto de observables compatibles adecuado para diagonalizar H_0 y hallar los autoestados y autovalores de H_0 en la base asociada a dicho conjunto.

b) Calcular a primer orden en teoría de perturbaciones la corrección a la energía del estado fundamental de H_0 debida a H_I.

a) $[\vec{S}^2, S_y] = 0 \Rightarrow [H_0, \vec{S}^2] = [H_0, S_y] = 0 \Rightarrow \{H_0, \vec{S}^2, S_y\}$ have common eigenstates $|E_m, s=1, m\rangle$, with $m = -1, 0, 1$. They satisfy

$$\vec{S}^2 |E_m, 1, m\rangle = 2\hbar^2 |E_m, 1, m\rangle,$$

$$S_y |E_m, 1, m\rangle = m\hbar |E_m, 1, m\rangle \qquad (2)$$

$$H_0 |E_m, 1, m\rangle = E_m |E_m, 1, m\rangle, \quad E_m = (2 - m^2 - m)\hbar\omega$$

It is clear that

$|0, 1, 1\rangle \longrightarrow E_1 = 0 \longrightarrow$ ground state ; nondegenerate

$|0, 1, 0\rangle \longrightarrow E_0 = 2\hbar\omega$

$|0, 1, -1\rangle \longrightarrow E_{-1} = 2\hbar\omega$

Write

$$|0,1,1\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

Eq. (2) reads for $m=1$

$$\frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & i\\ 0 & i & 0\end{pmatrix}\begin{pmatrix}a\\ b\\ c\end{pmatrix} = \hbar\begin{pmatrix}a\\ b\\ c\end{pmatrix} \Rightarrow \begin{cases} -ib = \sqrt{2}a \\ i(a-c) = \sqrt{2}b \\ ib = \sqrt{2}c \end{cases} \Rightarrow$$

$$\Rightarrow |0,1,1\rangle = \frac{b}{\sqrt{2}}\begin{pmatrix}-i\\ \sqrt{2}\\ i\end{pmatrix} \qquad \Rightarrow \qquad |0,1,1\rangle = \frac{1}{2}\begin{pmatrix}-i\\ \sqrt{2}\\ i\end{pmatrix}$$

Normalization

$$\frac{|b|^2}{2}(1+2+1) = 1 \Rightarrow |b| = \frac{1}{\sqrt{2}}$$

The first order correction to its energy due to $H_I = \lambda\omega S_z$ is

$$E_1^{(1)} = \lambda\omega \langle 0,1,1|S_z|0,1,1\rangle = \frac{1}{\sqrt{2}}(i, \sqrt{2}, -i)\,\frac{\hbar}{\sqrt{2}}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}-i\\\sqrt{2}\\i\end{pmatrix} = 0$$

<u>Alternative solution</u>

$$H_0 = \frac{\omega}{\hbar}\left(S_x^2 + S_z^2 - \hbar S_y\right)$$

$$= \hbar\omega\left[\frac{1}{2}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}^2 + \frac{i}{2}\begin{pmatrix}0&\sqrt{2}&0\\-\sqrt{2}&0&\sqrt{2}\\0&-\sqrt{2}&0\end{pmatrix}\right] = \frac{\hbar\omega}{2}\begin{pmatrix}3&i\sqrt{2}&1\\-i\sqrt{2}&2&i\sqrt{2}\\1&-i\sqrt{2}&3\end{pmatrix}$$

Its eigenvalues are $E_0 = \frac{\hbar\omega}{2}\lambda$ with λ the solutions of

$$\det\begin{pmatrix}3-\lambda&i\sqrt{2}&1\\-i\sqrt{2}&2-\lambda&i\sqrt{2}\\1&-i\sqrt{2}&3-\lambda\end{pmatrix} = 0$$

$$(3-\lambda)^2(2-\lambda) - 2 - 2 - (2-\lambda) - 2(3-\lambda) - 2(3-\lambda) = 0$$

$$(9+\lambda^2-6\lambda)(2-\lambda) - 4 - 2 + \lambda - 12 + 4\lambda = 0$$

$$\cancel{18} - 9\lambda + 2\lambda^2 - \lambda^3 - 12\lambda + 6\lambda^2 - \cancel{18} + 5\lambda = 0$$

$$-\lambda^3 + 8\lambda^2 - 16\lambda = 0 \iff \lambda(\lambda^2 - 8\lambda + 16) = 0 \Rightarrow \lambda = 0, 4, 4$$

Hence

$E_0^{(0)} = 0$ single, $\quad E_1^{(0)} = 2\hbar\omega$ doubly degenerate

The eigenstate of $E_0^{(0)} = 0$ is

$$H_0\begin{pmatrix}a\\b\\c\end{pmatrix} = 0 \iff \begin{pmatrix}3&i\sqrt{2}&1\\-i\sqrt{2}&2&i\sqrt{2}\\1&-i\sqrt{2}&3\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 0 \Rightarrow \begin{cases}3a + i\sqrt{2}b + c = 0 & (1)\\ -i\sqrt{2}a + 2b + i\sqrt{2}c = 0 & (2)\\ a - i\sqrt{2}b + 3c = 0 & (3)\end{cases}$$

$(1)+(3)$: $\quad 4a + 4c = 0 \Rightarrow c = -a$

$(1)-(3)$ $\quad 2a + 2i\sqrt{2}b - 2c = 0 \Rightarrow 4a + 2i\sqrt{2}b = 0 \Rightarrow b = -i\sqrt{2}a \quad \Rightarrow$

$$|\phi_0^{(0)}\rangle = \text{non-perturbed ground state} = \begin{pmatrix}a\\-i\sqrt{2}a\\-a\end{pmatrix} = \begin{pmatrix}1/2\\-i/\sqrt{2}\\-1/2\end{pmatrix}$$

normalization requires $4|a|^2 = 1$. We take $a = \frac{1}{2}$

The first order correction $E_0^{(1)}$ is

$$E_0^{(1)} = \langle \phi_0^{(0)} | H_I | \phi_0^{(0)} \rangle = -\lambda\hbar\omega \left(\frac{1}{2}, \frac{i}{\sqrt{2}}, -\frac{1}{2} \right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1/2 \\ -i/\sqrt{2} \\ -1/2 \end{pmatrix} = 0$$

4 [2 puntos]. Una partícula de masa m se mueve en un potencial unidimensional

$$V(x) = \begin{cases} \infty & \text{si } x \le 0\,, \\ V_0\, a^2 x^2 & \text{si } x > 0\,. \end{cases}$$

donde V_0 y a son constantes positivas con unidades de energía y (longitud)$^{-1}$ respectivamente. Para estimar la energía de su estado fundamental se usa el método variacional. Discutir cuáles de las siguientes funciones de onda prueba, con $\lambda > 0$, son adecuadas y usar aquellas que lo sean para estimarla:

$$(1)\;\; \psi_\lambda(x) = \begin{cases} 0 & \text{si } \; x < 0, \\ e^{-\lambda a^2 x^2} & \text{si } \; x \ge 0, \end{cases} \qquad (2)\;\; \psi_\lambda(x) = \begin{cases} 0 & \text{si } \; x < 0, \\ \sin(ax)\, e^{\lambda a^2 x^2} & \text{si } \; x \ge 0, \end{cases}$$

$$(3)\;\; \psi_\lambda(x) = \begin{cases} 0 & \text{si } \; x < 0, \\ x e^{-\lambda a^2 x^2} & \text{si } \; x \ge 0, \end{cases} \qquad (4)\;\; \psi_\lambda(x) = \begin{cases} 0 & \text{si } \; x < 0, \\ \cos(ax)\, e^{-\lambda a^2 x^2} & \text{si } \; x \ge 0. \end{cases}$$

Ayuda. Para $b > 0$ y $n = 0, 1, 2, \ldots$,

$$\int_0^\infty dx\, x^{2(n+1)}\, e^{-bx^2} = \frac{(2n+1)!!}{2\,(2b)^{n+1}} \sqrt{\frac{\pi}{b}}\,, \qquad \int_0^\infty dx\, x^{2n+1}\, e^{-bx^2} = \frac{n!}{2\, b^{n+1}}\,,$$

donde $(2n+1)!! = (2n+1)\cdot(2n-1)\,\cdots\,3\cdot 1$.

Since $\psi(x)$ must vanish for $x<0$ $[V(x<0)=\infty]$ and $\psi(x)$ must be continuous at $x=0$, $\psi(x)$ must vanish at $x=0$. This discards (1) and (4). (2) is discarded because $\psi_\lambda(x) \to \infty$ at $x \to \infty$, so that $\psi_\lambda(x)$ is not square integrable. For (3) we have

$$\langle \psi_\lambda(x) | \psi_\lambda(x) \rangle = \int_0^\infty dx\; x^2 e^{-2\lambda a^2 x^2} = \frac{1}{8\lambda a^3}\sqrt{\frac{\pi}{2\lambda}} \qquad \frac{\sqrt{\pi}}{32 a^3 \lambda^{3/2}}$$

$$\langle \psi_\lambda(x) | H | \psi_\lambda(x) \rangle = \int_0^\infty dx\; x e^{-\lambda a^2 x^2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0 a x \right) x e^{-\lambda a^2 x^2}$$

$$\frac{d}{dx}\psi_\lambda(x) = e^{-\lambda a^2 x^2}\left(1 - 2\lambda a^2 x^2\right)$$

$$\frac{d^2}{dx^2}\psi_\lambda(x) = e^{-\lambda a^2 x^2}\left[-2\lambda a^2 x\left(1 - 2\lambda a^2 x^2\right) - 4\lambda a^2 x\right]$$

$$= e^{-\lambda a^2 x^2}\left(-6\lambda a^2 x + 4\lambda^2 a^4 x^3\right)$$

$$\langle \psi_\lambda(x) | H | \psi_\lambda(x) \rangle = \int_0^\infty dx \, e^{-2\lambda a^2 x^2} \left[-\frac{\hbar^2}{2m} \left(-6\lambda a^2 x^2 + 4\lambda^2 a^4 x^4 \right) + V_0 a^2 x^4 \right]$$

$$= -\frac{\hbar^2}{2m} \left(-\frac{3\sqrt{\pi}}{8a\sqrt{2\lambda}} \right) + \frac{3V_0\sqrt{\pi}}{32\sqrt{2}\, a^3 \lambda^{5/2}}$$

$$E(\lambda) = \frac{\langle \psi_\lambda(x) | H | \psi_\lambda(x) \rangle}{\langle \psi_\lambda(x) | \psi_\lambda(x) \rangle} = \frac{\dfrac{3\hbar^2\sqrt{\pi}}{16\, m a \sqrt{2\lambda}} + \dfrac{3V_0\sqrt{\pi}}{32\sqrt{2}\, a^3 \lambda^{5/2}}}{\dfrac{1}{8\lambda a^3}\sqrt{\dfrac{\pi}{2\lambda}}} = \frac{3\hbar^2 \lambda a^2}{2m} + \frac{3V_0}{4\lambda}$$

We must find the minimum of $E(\lambda)$:

$$\left.\frac{dE}{d\lambda}\right|_{\lambda_0} = 0 \iff \frac{3\hbar^2 a^2}{2m} - \frac{3V_0}{4\lambda_0^2} = 0 \iff \lambda_0^2 = \frac{V_0 m}{2\hbar^2 a^2}$$

$$\frac{d^2E}{d\lambda^2} = \frac{3V_0}{2\lambda^3} > 0 \text{ for all } \lambda > 0 \Rightarrow \lambda_0 \text{ is a minimum}$$

$$E(\lambda_0) = \frac{3\hbar^2 a^2}{2m}\left(\frac{V_0 m}{2\hbar^2 a^2}\right)^{1/2} + \frac{3V_0}{4}\left(\frac{2\hbar^2 a^2}{V_0 m}\right)^{1/2} = 3\hbar a\sqrt{\frac{V_0}{2m}}$$

} Variational estimate for ground state energy

5 [2 puntos]. Un átomo de hidrógeno se encuentra en el estado $|n,\ell,m\rangle = |3,0,0\rangle$. Se somete a un campo eléctrico exterior

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

dirigido según el eje z, con $\mathcal{E}_0$ y τ constantes. Discutir cuáles de las siguientes transiciones están permitidas y calcular la probabilidad de que ocurran en un tiempo $t_f \gg \tau$:

$$|3,0,0\rangle \to |2,1,1\rangle\,, \qquad |3,0,0\rangle \to |2,1,0\rangle\,.$$

Ayuda. Se sabe que

$$\int_0^\infty r^2 dr\, R_{21}(r)\, r\, R_{30}(r) = k\, a_0\,, \qquad \text{con} \qquad k = \text{const.}$$

The Hamiltonian is

$H = H_0 + V(t)$ $\qquad$ H_0 = Hamiltonian Hydrogen atom

$V = -e\,\mathcal{E}(t)\, z$

The transition probability at first order is

$$P_{if}(0,t_f) = \frac{1}{\hbar^2}\left|\int_0^{t_f} dt'\, e^{i\omega_{fi}t'}\, V_{fi}(t')\right|^2$$

with

$$V_{fi}(t') = \langle n\ell m|V(t')|300\rangle = -e\,\mathcal{E}(t)\,\langle n\ell m|z|300\rangle$$

It follows that

$$P_{if} = \frac{e^2\mathcal{E}_0^2}{\hbar^2}\,|\langle n\ell m|z|300\rangle|^2\left|\int_0^{t_f} dt'\, e^{t'(i\omega_{fi}-1/\tau)}\right|$$

The state $|300\rangle$ has $\ell_1=0$ and $m_1=0$. Since $|z\rangle$ has $\ell_2=1$ and $m_2=0$, $z|300\rangle$ has $L=1$ and $M=0$. For $\langle n\ell m|z|300\rangle$ to be nonzero, ℓ and m must be $\ell=L=1$ and $m=M=0$. This implies that out of the two transitions given, only $|300\rangle \to |110\rangle$ is possible at first order:

$|300\rangle \longrightarrow |211\rangle$ not permitted $\qquad$ $|300\rangle \longrightarrow |210\rangle$ is possible

Using that

$$\int_0^{t_f} dt' \, e^{t'(i\omega_{fi} - 1/\tau)} = \left.\frac{e^{t'(i\omega_{fi} - \frac{1}{\tau})}}{i\omega_{fi} - \frac{1}{\tau}}\right|_0^{t_f} = \frac{e^{i t_f \omega_{fi}} e^{-t_f/\tau} - 1}{i\omega_{fi} - \frac{1}{\tau}}$$

$$= \left\{ e^{-t_f/\tau} \to 0 \text{ for } t_f \gg \tau \right\} = -\frac{1}{i\omega_{fi} - \frac{1}{\tau}}$$

and

$$\langle 210 | z | 300 \rangle = \underbrace{\int_0^\infty r^2 dr \, R_{21}(r) \, r \, R_{30}(r)}_{ka_0} \int_0^{2\pi} d\phi \int_0^\pi \sin d\theta \, \underbrace{Y_1^0(\theta,\phi) \cos\theta \, Y_0^0(\theta,\phi)}_{\frac{\sqrt{3}}{4\pi}\cos^2\theta}$$

$$= ka_0 \frac{\sqrt{3}}{2} \int_0^\pi \cos^2\theta \sin\theta \, d\theta = \frac{ka_0}{\sqrt{3}}$$

we obtain for the probability of the allowed transitions

$$P_{300 \to 110}(0, t_f) = \frac{e^2 \mathcal{E}_0}{\hbar^2} \frac{k^2 a_0^2}{3} \left| \frac{\tau}{1 - i\omega_{23}\tau} \right|^2 = \frac{e^2 \mathcal{E}_0^2}{3\hbar^2} \frac{k^2 a_0^2 \tau^2}{1 + \omega_{23}\tau^2}$$

$$\omega_{23} = \frac{1}{\hbar}(E_2 - E_3) = \frac{1}{\hbar} \frac{Ze^2}{8\pi\varepsilon_0 a_0} \left(\frac{1}{4} - \frac{1}{9} \right) = \frac{5}{36\hbar} \frac{Ze^2}{8\pi\varepsilon_0 a_0}$$