

① a) In our case $l=0$ $s=1/2$. The rules of addition of two angular momenta give us only one possibility: $j=1/2$

b) Here $s=1/2$ ($j=1/2$) and $i=3/2$. Adding two angular momenta gives two possibilities:

$$f=1 \quad f=2$$

c) The perturbing Hamiltonian can be written as

$$H_{hf} = A \vec{S} \cdot \vec{I} = \frac{A}{2} (F^2 - S^2 - I^2)$$

One could come up with these basis sets in this problem: $|l m_l s m_s i m_i\rangle$, $|l s j m_j i m_i\rangle$, $|l s j i f m_f\rangle$. Clearly the latter one is most convenient as it is composed of simultaneous eigenfunctions of F^2 , S^2 , and I^2 . An operator is diagonal in the basis of its eigenfunctions.

$$\begin{aligned} d) \langle l s j i f m_f | H_{hf} | l s j i f m_f \rangle &= \frac{A}{2} \langle l s j i f m_f | F^2 - S^2 - I^2 | l s j i f m_f \rangle = \\ &= \frac{A \hbar^2}{2} \left[f(f+1) - \underbrace{s(s+1)}_{3/4} - \underbrace{i(i+1)}_{15/4} \right] = \frac{A \hbar^2}{2} \left[f(f+1) - 9/2 \right] \end{aligned}$$

Given that f can take two values $f=1, 2$ we have:
the following shifts:

$$E_{f=1}^{(1)} = -\frac{5}{4} A \hbar^2 \quad \leftarrow \text{three-fold degenerate: } m_f = -1, 0, +1$$

$$E_{f=2}^{(1)} = \frac{3}{4} A \hbar^2 \quad \leftarrow \text{five-fold degenerate: } m_f = -2, -1, 0, +1, +2$$

② A particle of mass m has the following energy levels and wavefunctions in the box $0 \leq x \leq a$ $0 \leq y \leq a$ $0 \leq z \leq 2a$

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2ma^2} \left(n_x^2 + n_y^2 + \frac{n_z^2}{4} \right) \quad n_x = 1, 2, \dots \quad n_y = 1, 2, \dots \quad n_z = 1, 2, \dots$$

$$\Psi_{n_x, n_y, n_z} = \frac{2}{a^{3/2}} \sin \frac{\pi n_x x}{a} \sin \frac{\pi n_y y}{a} \sin \frac{\pi n_z z}{2a} = \phi_{n_x}(x) \phi_{n_y}(y) \psi_{n_z}(z)$$

The lowest energy levels are $(A \equiv \frac{\hbar^2 \pi^2}{2ma^2})$

n_x	n_y	n_z	
1	1	1	$E = 2.25A$
1	1	2	$E = 3A$
1	1	3	$E = 4.25A$
2	1	1	} $E = 5.25A$, two-fold degenerate
1	2	1	

So in the case of the fourth excited state we deal with two degenerate states:

$$|1\rangle \equiv |211\rangle$$

$$|2\rangle \equiv |121\rangle$$

The matrix elements of $V = \beta xyz$ in this basis are:

$$\langle 1|V|1\rangle = \beta \underbrace{\langle \phi_2(x)|x|\phi_2(x)\rangle}_{a/2} \underbrace{\langle \phi_1(y)|y|\phi_1(y)\rangle}_{a/2} \underbrace{\langle \psi_1(z)|z|\psi_1(z)\rangle}_a = \frac{a^3}{4}$$

$$\langle 2|V|1\rangle = \beta \underbrace{\langle \phi_2(x)|x|\phi_1(x)\rangle}_{-\frac{16a}{9\pi^2}} \underbrace{\langle \phi_1(y)|y|\phi_2(y)\rangle}_{-\frac{16a}{9\pi^2}} \underbrace{\langle \psi_1(z)|z|\psi_1(z)\rangle}_a = \frac{256}{81\pi^4} a^3$$

$$\langle 1|V|2\rangle = \langle 2|V|1\rangle \quad \langle 2|V|2\rangle = \langle 1|V|1\rangle$$

The perturbation matrix is then

$$W = \beta a^3 \begin{pmatrix} \frac{1}{4} & \frac{256}{81\pi^4} \\ \frac{256}{81\pi^4} & \frac{1}{4} \end{pmatrix}$$

The eigenvalues of this matrix give first-order corrections to the energy of the fourth excited state

$$E^{(1)} = \beta a^3 \left(\frac{1}{4} \pm \frac{256}{81\pi^4} \right)$$

③ In order to have discrete energy levels (bound states) the potential must be attractive. That is true only when $\alpha < 0$

To estimate the ground state energy the most obvious (and quite appropriate) trial wave function is the exponential one:

$$\psi(r) = e^{-\beta r} \quad \beta \text{ is an adjustable parameter}$$

it has a proper asymptotic behavior when $r \rightarrow \infty$.

Let us now compute all necessary integrals

$$\langle \psi | \psi \rangle = 4\pi \int_0^\infty e^{-2\beta r} r^2 dr = \frac{\pi}{\beta^3}$$

$$\begin{aligned} \langle \psi | T | \psi \rangle &= -\frac{\hbar^2}{2m} 4\pi \int_0^\infty e^{-\beta r} \left(\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} e^{-\beta r} \right) dr = \\ &= -\frac{\hbar^2 \pi}{m} \int_0^\infty (\beta r^2 - 2\beta r) e^{-2\beta r} dr = \frac{\pi \hbar^2}{2m\beta} \end{aligned}$$

$$\langle \psi | V | \psi \rangle = -\alpha 4\pi \int_0^\infty e^{-\beta r} \frac{1}{\sqrt{r}} e^{-\beta r} r^2 dr = -4\pi \alpha \int_0^\infty r^{3/2} e^{-2\beta r} dr = -\frac{3\pi^{3/2}}{4\sqrt{2}} \frac{\alpha}{\beta^{5/2}}$$

(the last integral can be evaluated as $\int_0^\infty r^{3/2} e^{-\gamma r} dr \stackrel{y=r}{=} 2 \int_0^\infty y^4 e^{-\gamma y^2} dy = 2 \left(-\frac{\partial}{\partial \gamma} \right)^2 \sqrt{\frac{\pi}{\gamma}}$)

Our trial energy is then

$$E = \frac{\langle \psi | T | \psi \rangle + \langle \psi | V | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\hbar^2}{2m} \beta^2 - \frac{3\pi^{1/2}}{4\sqrt{2}} \alpha \beta^{1/2}$$

Finding the minimum with respect to β yields:

$$\frac{\partial E}{\partial \beta} = \frac{\hbar^2}{m} \beta - \frac{3\pi^{1/2}}{8\sqrt{2}} \alpha \frac{1}{\sqrt{\beta}} = 0 \quad \Rightarrow \quad \beta_{\min} = \left(\frac{3\sqrt{\pi} m \alpha}{8\sqrt{2} \hbar^2} \right)^{2/3}$$

$$\begin{aligned} E_{\min} &= \frac{\hbar^2}{2m} \left(\frac{3\sqrt{\pi} m \alpha}{8\sqrt{2} \hbar^2} \right)^{4/3} - \frac{3\sqrt{\pi}}{4\sqrt{2}} \alpha \left(\frac{3\sqrt{\pi} m \alpha}{8\sqrt{2} \hbar^2} \right)^{1/3} = \frac{3^{4/3} \pi^{2/3}}{4 \cdot 2^{11/3}} \frac{m^{1/3} \alpha^{4/3}}{\hbar^{2/3}} - \frac{3^{4/3} \pi^{2/3}}{2^{11/3}} \frac{m^{1/3} \alpha^{4/3}}{\hbar^{2/3}} = \\ &= -\frac{3^{7/3} \pi^{2/3}}{2^{7/3}} \frac{m^{1/3} \alpha^{4/3}}{\hbar^{2/3}} \end{aligned}$$

(4) First order corrections are given by

$$E_n^{(1)} = \langle \phi_n^{(0)} | H' | \phi_n^{(0)} \rangle = H'_{nn}$$

Second order corrections are given by

$$E_n^{(2)} = \sum_{k \neq n} \frac{|H'_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} \quad E_n^{(0)} = \hbar\omega \left(n + \frac{1}{2}\right)$$

Where $\phi_n^{(0)}$ are the wave functions of the harmonic oscillator. Matrix elements $H'_{nk} = \gamma \langle \phi_n^{(0)} | p^2 | \phi_k^{(0)} \rangle$ are given in the formula sheet (apart from multiplicative constant γ):

$$H'_{nk} = -\gamma \frac{m\hbar\omega}{2} \left[\sqrt{k(k-1)} \delta_{n,k-2} - (2k+1) \delta_{nk} + \sqrt{(k+1)(k+2)} \delta_{n,k+2} \right]$$

With that we have:

$$E_n^{(1)} = -\gamma m \hbar \omega \left(n + \frac{1}{2}\right) = \gamma m E_n^{(0)} \quad (\text{for the ground state we take } n=0)$$

$$E_0^{(2)} = \sum_{k \neq 0} \frac{\gamma^2 \frac{m^2 \hbar^2 \omega^2}{4} \left[\sqrt{k(k-1)} \delta_{0,k-2} - (2k+1) \delta_{0,k} + \sqrt{(k+1)(k+2)} \delta_{0,k+2} \right]^2}{-\hbar\omega k} =$$

$$= -\frac{\gamma^2 m^2 \hbar \omega [\sqrt{2}]^2}{8} = -\frac{\gamma^2 m^2}{4} \hbar \omega$$