

① a) We presume that the solutions of the time-independent Schrödinger equation with H_0 are known

$$H_0 \Psi_{nem_e} = E_n \Psi_{nem_e}$$

The solutions of the time-independent Schrödinger eq. with $H' = \lambda(\vec{S}_p \cdot \vec{S}_e)$ can be easily determined:

$$\vec{S}_p \cdot \vec{S}_e = \frac{1}{2} [\vec{S}^2 - \vec{S}_p^2 - \vec{S}_e^2] = \frac{\hbar^2}{2} [S(S+1) - S_p(S_p+1) - S_e(S_e+1)]$$

Here \vec{S} is the total spin of the proton and electron (both are spin $1/2$ particles)

$$S=0 \quad s=0, m_s=0$$

$$H' |s, m_s\rangle = \lambda \frac{\hbar^2}{2} \underbrace{[S(S+1) - \frac{3}{2}]}_{E_S} |s, m_s\rangle$$

$$S=1 \quad s=1, m_s=1, 0, -1$$

Now,

$$|s=0, m_s=0\rangle = \frac{1}{\sqrt{2}} (\chi_+^{(p)} \chi_-^{(e)} - \chi_-^{(p)} \chi_+^{(e)}) \quad E_0 = -\frac{3}{4} \lambda \hbar^2$$

$$|s=1, m_s=0\rangle = \frac{1}{\sqrt{2}} (\chi_+^{(p)} \chi_-^{(e)} + \chi_-^{(p)} \chi_+^{(e)}) \quad E_1 = \frac{1}{4} \lambda \hbar^2$$

We can see that our initial spin state $\chi_+^{(p)} \chi_-^{(e)}$ is a linear combination

$$\chi_+^{(p)} \chi_-^{(e)} = \frac{1}{\sqrt{2}} (|1,0\rangle + |0,0\rangle)$$

The general solution to the time-dependent Schrödinger equation with time-independent $H = H_0 + H'$ can be represented as

$$\Psi(t) = \sum_{n, m_e} \sum_{s, m_s} C_{nem_sms} \Psi_{nem_e} |s, m_s\rangle e^{-\frac{i}{\hbar}(E_n + E_S)t}$$

Knowing that $\Psi(0) = \Psi_{100} \frac{1}{\sqrt{2}} (|1,0\rangle + |0,0\rangle)$ we can determine the time-dependent wave function of the system:

$$\begin{aligned} \Psi(t) &= \frac{1}{\sqrt{2}} \Psi_{100} e^{-\frac{iE_1t}{\hbar}} \left[e^{-\frac{iE_0t}{\hbar}} |1,0\rangle + e^{-\frac{iE_0t}{\hbar}} |0,0\rangle \right] = \\ &= \frac{1}{\sqrt{2}} \Psi_{100} e^{-\frac{i}{\hbar}(E_1 + \frac{1}{4}\lambda\hbar^2)t} \left[|1,0\rangle + e^{-i\lambda\hbar t} |0,0\rangle \right] \end{aligned}$$

This wave function can also be written in terms of proton and electron spin eigenstates

$$\Psi(t) = \Psi_{100} e^{-\frac{i}{\hbar}(E_1 + \frac{1}{4}\lambda t^2)t} \frac{1}{2} \left[\chi_+^{(p)} \chi_-^{(e)} + \chi_-^{(p)} \chi_+^{(e)} + \chi_+^{(p)} \chi_-^{(e)} + \chi_-^{(p)} \chi_+^{(e)} \right]$$

$$+ e^{i\lambda t t} \chi_+^{(p)} \chi_-^{(e)} + e^{i\lambda t t} \chi_-^{(p)} \chi_+^{(e)} \right] =$$

$$= \Psi_{100} e^{-\frac{i}{\hbar}(E_1 - \frac{1}{4}\lambda t^2)t} \left[-\cos\left(\frac{\lambda t t}{2}\right) \chi_+^{(p)} \chi_-^{(e)} - i \sin\left(\frac{\lambda t t}{2}\right) \chi_-^{(p)} \chi_+^{(e)} \right]$$

b) Using the above expression for $\Psi(t)$ we can see that the probability of finding the spin of the proton pointing down is

$$P = \left| \langle \Psi_{100} \chi_-^{(p)} \chi_+^{(e)} | \Psi(t) \rangle \right|^2 = \sin^2\left(\frac{\lambda t t}{2}\right)$$

② In the case of the relativistic motion the connection between the total energy and momentum is

$$E^2 = m^2 c^4 + p^2 c^2$$

For the kinetic energy we then have

$$\begin{aligned} T = E - mc^2 &= \sqrt{m^2 c^4 + p^2 c^2} - mc^2 = mc^2 \left(\sqrt{1 + \frac{p^2}{m^2 c^2}} - 1 \right) \approx \\ &\approx mc^2 \left(1 + \frac{p^2}{2m^2 c^2} - \frac{p^4}{8m^4 c^4} + \dots - 1 \right) = \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} + \dots \end{aligned}$$

leading relativistic correction

While the total Hamiltonian is

$$H = \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} + \frac{mw^2 x^2}{2}$$

We can treat the $\frac{p^4}{8m^3 c^2}$ term as a perturbation, i.e.

$$H = H_0 + H' \quad \text{where} \quad H_0 = \frac{p^2}{2m} + \frac{mw^2 x^2}{2} \quad H' = -\frac{p^4}{8m^3 c^2}$$

The ground state wave function of H_0 is

$$\psi = \frac{\alpha^{1/4}}{\pi^{1/4}} e^{-\frac{\alpha x^2}{2}} \quad \text{where} \quad \alpha = \frac{mw^2}{\hbar^2}$$

In the first order of the perturbation theory the correction to the energy is given by

$$\begin{aligned} E^{(1)} &= \langle \psi | H' | \psi \rangle = -\frac{1}{8m^3 c^2} \frac{\alpha^{1/2}}{\pi^{1/2}} \int_{-\infty}^{+\infty} e^{-\frac{\alpha x^2}{2}} \left(-i\hbar \frac{\partial}{\partial x} \right)^4 e^{-\frac{\alpha x^2}{2}} dx = \\ &= -\frac{\alpha^{1/2} \hbar^4}{8m^3 c^2 \pi^{1/2}} \int_{-\infty}^{+\infty} e^{-\frac{\alpha x^2}{2}} (3\alpha^2 - 6\alpha^3 x^2 + \alpha^4 x^4) e^{-\frac{\alpha x^2}{2}} dx = \\ &= -\frac{\alpha^{5/2} \hbar^4}{8m^3 c^2 \pi^{1/2}} \int_{-\infty}^{+\infty} (3 - 6\alpha^2 x^2 + \alpha^4 x^4) e^{-\alpha x^2} dx = -\frac{\alpha^{5/2} \hbar^4}{8m^3 c^2 \pi^{1/2}} \left(3 \frac{\pi^{1/2}}{\alpha^{1/2}} - 3\alpha \frac{\pi^{1/2}}{\alpha^{3/2}} + \frac{3}{4} \alpha^2 \frac{\pi^{1/2}}{\alpha^{5/2}} \right) = \\ &= -\frac{3}{32} \frac{\alpha^2 \hbar^4}{m^3 c^2} = -\frac{3}{32} \frac{\hbar^2 w^2}{m c^2} \end{aligned}$$

③ H can be split into an unperturbed Hamiltonian H_0 and a perturbation H' :

$$H = H_0 + H'$$

where

$$H_0 = \epsilon \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

$$H' = \epsilon Y \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

The energy eigenvalues and the corresponding eigenvectors of H_0 are:

$$E_1 = 2\epsilon \quad \Psi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad E_2 = 0 \quad \Psi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} \quad E_3 = 2\epsilon \quad \Psi_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad E_4 = 0 \quad \Psi_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \end{pmatrix}$$

Clearly, we deal with a degenerate case here and need to find a proper basis in which H' is diagonal. That will also give us the first order corrections to the energy.

For the two states corresponding to $E^{(0)} = 2\epsilon$ we have:

$$W = \begin{pmatrix} \langle \Psi_1 | H' | \Psi_1 \rangle & \langle \Psi_1 | H' | \Psi_3 \rangle \\ \langle \Psi_3 | H' | \Psi_1 \rangle & \langle \Psi_3 | H' | \Psi_3 \rangle \end{pmatrix} = \frac{\epsilon Y}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

problem $Wv = \lambda v$ yields

Solving the eigenvalue

$$\lambda_a = E_1^{(1)} = +\frac{\epsilon Y}{2} \quad v_a = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\text{so } \phi_1 = \frac{1}{\sqrt{2}} \Psi_1 + \frac{1}{\sqrt{2}} \Psi_3 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\lambda_b = E_3^{(1)} = -\frac{\epsilon Y}{2} \quad v_b = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{so } \phi_3 = \frac{1}{\sqrt{2}} \Psi_1 - \frac{1}{\sqrt{2}} \Psi_3 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

For the two states corresponding to $E^{(0)} = 0$ we have:

$$W = \begin{pmatrix} \langle \Psi_2 | H' | \Psi_2 \rangle & \langle \Psi_2 | H' | \Psi_4 \rangle \\ \langle \Psi_4 | H' | \Psi_2 \rangle & \langle \Psi_4 | H' | \Psi_4 \rangle \end{pmatrix} = -\frac{\epsilon Y}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$Wv = \lambda v$ yields

Solving the eigenvalue problem

$$\lambda_a = E_2^{(1)} = -\frac{\epsilon Y}{2} \quad v_a = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\text{so } \phi_2 = \frac{1}{\sqrt{2}} \Psi_2 + \frac{1}{\sqrt{2}} \Psi_4 = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

$$\lambda_a = E_4^{(1)} = \frac{\epsilon\gamma}{2} \quad V_6 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{so} \quad \Phi_4 = \frac{1}{\sqrt{2}} \Psi_2 - \frac{1}{\sqrt{2}} \Psi_4 = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}$$

Now in the second order of the perturbation theory we have the following formula:

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \Phi_m | H' | \Phi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

In our case it gives

$$E_1^{(2)} = \frac{|\langle \Phi_1 | H' | \Phi_2 \rangle|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|\langle \Phi_1 | H' | \Phi_4 \rangle|^2}{E_1^{(0)} - E_4^{(0)}} = \frac{(\frac{\epsilon\gamma}{2})^2}{-2\epsilon} + 0 = \frac{\epsilon\gamma^2}{8}$$

$$E_2^{(2)} = \frac{|\langle \Phi_2 | H' | \Phi_1 \rangle|^2}{E_2^{(0)} - E_1^{(0)}} + \frac{|\langle \Phi_2 | H' | \Phi_3 \rangle|^2}{E_2^{(0)} - E_3^{(0)}} = \frac{(\frac{\epsilon\gamma}{2})^2}{2\epsilon} + 0 = -\frac{\epsilon\gamma^2}{8}$$

$$E_3^{(2)} = \frac{|\langle \Phi_3 | H' | \Phi_2 \rangle|^2}{E_3^{(0)} - E_2^{(0)}} + \frac{|\langle \Phi_3 | H' | \Phi_4 \rangle|^2}{E_3^{(0)} - E_4^{(0)}} = 0 + \frac{(-\frac{\epsilon\gamma}{2})^2}{2\epsilon} = \frac{\epsilon\gamma^2}{8}$$

$$E_4^{(2)} = \frac{|\langle \Phi_4 | H' | \Phi_1 \rangle|^2}{E_4^{(0)} - E_1^{(0)}} + \frac{|\langle \Phi_4 | H' | \Phi_3 \rangle|^2}{E_4^{(0)} - E_3^{(0)}} = 0 + \frac{(-\frac{\epsilon\gamma}{2})^2}{-2\epsilon} = -\frac{\epsilon\gamma^2}{8}$$

So up to the second order in γ the energy levels of the system are:

$$E_1 = \epsilon \left(2 + \frac{\gamma}{2} + \frac{\gamma^2}{8} + \dots \right)$$

$$E_2 = \epsilon \left(0 - \frac{\gamma}{2} - \frac{\gamma^2}{8} + \dots \right)$$

$$E_3 = \epsilon \left(2 - \frac{\gamma}{2} + \frac{\gamma^2}{8} + \dots \right)$$

$$E_4 = \epsilon \left(0 + \frac{\gamma}{2} - \frac{\gamma^2}{8} + \dots \right)$$

④ In the Rayleigh-Ritz method the wave function is approximated by the linear combination

$$\psi(x) = \sum_{i=1}^N c_i \phi_i(x)$$

In our case $N=2$ and we have :

$$\psi = c_1 e^{-\gamma_1 x^2} + c_2 x e^{-\gamma_2 x^2}, \text{ where } \gamma_1 \text{ and } \gamma_2 \text{ are}$$

$\underbrace{}_{\phi_1} \quad \underbrace{}_{\phi_2}$

adjustable parameters. The resulting generalized eigenvalue problem takes the form :

$$\begin{pmatrix} \langle \phi_1 | -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^4 | \phi_1 \rangle & \langle \phi_1 | -\frac{\hbar^2}{2m} + \beta x^4 | \phi_2 \rangle \\ \langle \phi_2 | -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^4 | \phi_1 \rangle & \langle \phi_2 | -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^4 | \phi_2 \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} \langle \phi_1 | \phi_1 \rangle & \langle \phi_1 | \phi_2 \rangle \\ \langle \phi_2 | \phi_1 \rangle & \langle \phi_2 | \phi_2 \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

It is easy to see that because of the symmetry of ϕ_1 (even) and ϕ_2 (odd) the off-diagonal elements of both the Hamiltonian and overlap matrices vanish. Therefore for one solution (corresponding to the ground state) $c_2 = 0$, while for the other solution (corresponding to the excited state) $c_1 = 0$. Essentially the problem separates into two independent variational calculations

a) ground state with $\phi_1 = e^{-\gamma_1 x^2}$

b) first excited state with $\phi_2 = x e^{-\gamma_2 x^2}$

These can be easily done.

$$\text{a) } \langle \phi_1 | -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^4 | \phi_1 \rangle = \int_{-\infty}^{+\infty} \left[-\frac{\hbar^2}{2m} (-2\gamma_1 + 4\gamma_1 x^2) + \beta x^4 \right] e^{-2\gamma_1 x^2} dx =$$

$$= \sqrt{\frac{\pi}{2\gamma_1}} \left(\frac{\hbar^2}{2m} \gamma_1 + \frac{3}{16} \frac{\beta}{\gamma_1^2} \right)$$

$$\langle \phi_1 | \phi_1 \rangle = \int_{-\infty}^{+\infty} e^{-2\gamma_1 x^2} dx = \sqrt{\frac{\pi}{2\gamma_1}}$$

$$E = \frac{\hbar^2}{2m} \gamma_1 + \frac{3\beta}{16\gamma_1^2}$$

$$\frac{\partial E}{\partial \gamma_1} = \frac{\hbar^2}{2m} - \frac{3\beta}{8\gamma_1^3} = 0$$

$$\gamma_1 = \left(\frac{3}{4} \frac{\beta m}{\hbar^2} \right)^{1/3}$$

$$E_{\min} = \left(\frac{3\hbar}{4} \right)^{4/3} \frac{\beta^{1/3}}{m^{2/3}}$$

b) $\langle \phi_2 | -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^4 | \phi_2 \rangle = \int_{-\infty}^{+\infty} \left[-\frac{\hbar^2}{2m} (-6x\gamma_2 + 4x^3\gamma_2^2) + \beta x^4 \right] e^{-2\gamma_2 x^2} dx =$

$$= \sqrt{\frac{\pi}{2\gamma_2}} \left(\frac{3}{8} \frac{\hbar^2}{2m} + \frac{15}{64} \frac{\beta}{\gamma_2^3} \right)$$

$$\langle \phi_2 | \phi_2 \rangle = \sqrt{\frac{\pi}{2\gamma_2}} \frac{1}{4\gamma_2} \quad E = \frac{3}{2} \frac{\hbar^2}{2m} \gamma_2 + \frac{15}{16} \frac{\beta}{\gamma_2^2}$$

$$\frac{\partial E}{\partial \gamma_2} = \frac{3}{2} \frac{\hbar^2}{2m} - \frac{15}{8} \frac{\beta}{\gamma_2^3} = 0 \quad \gamma_2 = \left(\frac{5}{4} \frac{\beta m}{\hbar^2} \right)^{1/3}$$

$$E_{\min} = 9 \left(\frac{\hbar}{4} \right)^{4/3} \frac{5^{1/3} \beta^{1/3}}{m^{2/3}}$$

(5) The total wave function can be expanded in terms of partial waves

$$\psi(r, \theta) = A \left[e^{ikz} + \kappa \sum_{l=0}^{\infty} i^{l+1} (2l+1) a_e h_e^{(1)}(kr) P_l(\cos \theta) \right]$$

Using the Rayleigh formula for the plane wave it can be rewritten as

$$\psi(r, \theta) = A \sum_{l=0}^{\infty} \left[j_e(kr) + \kappa i a_e h_e^{(1)}(kr) \right] i^l P_l(\cos \theta)$$

Because $\psi(a, \theta) = 0$ for any θ value it follows that

$$j_e(ka) + \kappa i a_e h_e^{(1)}(ka) = 0 \quad \text{and} \quad a_e = \frac{i j_e(ka)}{k h_e^{(1)}(ka)}$$

The total cross section in terms of the partial wave amplitudes is

$$\sigma_{\text{tot}} = 4\pi \sum_{l=0}^{\infty} (2l+1) |a_e|^2$$

$$\text{In our case it becomes } \sigma_{\text{tot}} = \frac{4\pi}{\kappa^2} \sum_{l=0}^{\infty} (2l+1) \left[\frac{j_e(ka)}{h_e^{(1)}(ka)} \right]^2$$

In the low energy limit $ka \ll 1$. Using the fact that $j_e(x) \rightarrow \frac{2^e e!}{(2e+1)!} x^e$ and $h_e \rightarrow -\frac{(2e)!}{2^e e!} x^{-e-1}$ for small x

we get

$$\frac{j_e(x)}{h_e^{(1)}(x)} = \frac{j_e(x)}{j_e(x) + i h_e(x)} \xrightarrow{x \gg 0} \frac{j_e(x)}{h_e(x)} \approx \frac{2^e e!}{(2e+1)!} x^{2e+1}$$

In the low energy limit we can restrict ourselves with the S-wave scattering ($l=0$). With that

$$\sigma_{\text{tot}} = \frac{4\pi}{\kappa^2} \sum_{e=0}^{\infty} (2e+1) \left[\frac{2^e e!}{(2e+1)!} ka^{2e+1} \right]^2 \approx \frac{4\pi}{\kappa^2} \kappa^2 a^2 = 4\pi a^2$$

In the context of this problem "low" energy means

$$ka = \frac{\sqrt{2mE} a}{\hbar} \ll 1 \quad \text{or} \quad E \ll \frac{\hbar^2}{2ma^2}$$

⑥ Since the Hamiltonian is time-independent
the time evolution of the wave function can be
determined as

$$\psi(t) = U(t, 0) \psi(0) = e^{-\frac{i}{\hbar} H t} \psi(0)$$

Then the survival probability of the initial state is

$$P = |\langle \psi(0) | \psi(t) \rangle|^2 = |\langle \psi_i | e^{-\frac{i}{\hbar} H t} | \psi_i \rangle|^2$$

Expanding the exponent in time we get

$$\begin{aligned} P &= \left(\langle \psi_i | 1 - \frac{i}{\hbar} H t - \frac{H^2 t^2}{2\hbar^2} + \frac{iH^3 t^3}{6\hbar^3} + \dots | \psi_i \rangle \right)^* \left(\langle \psi_i | 1 - \frac{i}{\hbar} H t - \frac{H^2 t^2}{2\hbar^2} + \frac{iH^3 t^3}{6\hbar^3} + \dots | \psi_i \rangle \right) = \\ &= 1 + \frac{t}{\hbar} \left[-i \langle H \rangle - i \langle H \rangle \right] + \frac{t^2}{\hbar^2} \left[-\frac{1}{2} \langle H^2 \rangle - \frac{1}{2} \langle H^2 \rangle + \langle H \rangle \langle H \rangle \right] \\ &\quad + \frac{t^3}{\hbar^3} \left[\frac{i}{6} \langle H^3 \rangle - \frac{i}{6} \langle H^3 \rangle - \frac{i}{2} \langle H^2 \rangle \langle H \rangle + \frac{i}{2} \langle H \rangle \langle H^2 \rangle \right] + O(t^4) = \\ &= 1 - \underbrace{\frac{t^2}{\hbar^2} [\langle H^2 \rangle - \langle H \rangle^2]}_{\Delta E^2} + O(t^4) = 1 - \frac{t^2}{\hbar^2} \Delta E^2 + O(t^4) \end{aligned}$$