(1) a) A particle on a ring is described by the following Hamiltonian when $V(\phi) = 0$:

$$H = \frac{L_z^2}{2I} = \frac{L_z^2}{2mR^2} = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\phi^2}$$

The corresponding Schrödinger equation is

$$\frac{d^2\Psi}{d\phi^2} = -\frac{2mR^2}{\hbar^2}E\Psi \quad \text{or} \quad \Psi'' + k^2\Psi = 0 \quad \text{where } k = \frac{R}{\hbar}\sqrt{2mE}$$

The general solution of this differential equation is

$$\Psi = Ae^{ik\phi} + Be^{-ik\phi}$$

Now we must impose the boundary condition

$$\Psi(\phi + 2\pi) = \Psi(\phi)$$

which yields

$$k = n \qquad n = 0, \pm 1, \pm 2, \ldots$$

Thus the allowed energies are

$$\frac{R}{\hbar}\sqrt{2mE} = n \quad \Rightarrow \quad E_n = \frac{n^2\hbar^2}{2mR^2}$$

The corresponding wave functions are (each energy level, except $n=0$, is two-fold degenerate and the wave functions correspond to clockwise and counterclockwise motion)

$$\Psi_n = Ae^{in\phi} \qquad n = 0, \pm 1, \pm 2, \ldots$$

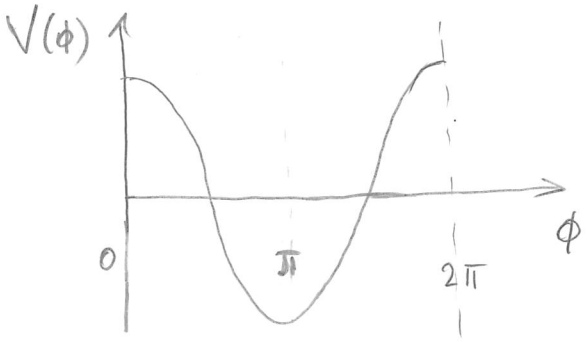
or, if we normalize them according to $\int_0^{2\pi} |\Psi_n|^2 d\phi = 1$

$$\Psi_n = \frac{1}{\sqrt{2\pi}}e^{in\phi}$$

Note that the ground state wave function is a constant :

$$\Psi_0 = \frac{1}{\sqrt{2\pi}}$$

b) Now $V = q\mathcal{E}x = q\mathcal{E}R\cos\phi$



A good trial wave function for the ground state should have the following properties:

i) Is periodic (with a period 2π)

ii) Is smooth, including the point $\phi = 0, 2\pi$

iii) Is flexible enough to become a non-zero constant (upon proper adjustment of the tunable parameter). This is because it should be able to describe a partial case $V = 0$ for which we know the exact solution is a constant

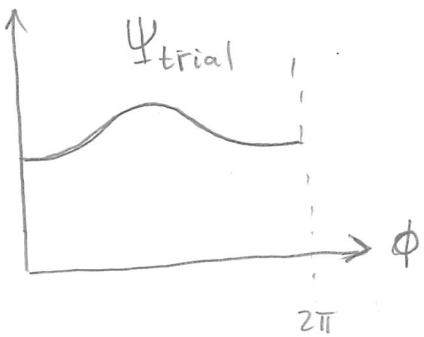
iv) Is simple enough so that the evaluation of the Hamiltonian expectation value can be done analytically

v) Should have a minimum at $\phi = 2\pi$ and maximum at $\phi = 0, 2\pi$

A trial wave function that has all these properties is

$$\Psi_{trial} = C\left(1 + \alpha \sin^2\frac{\phi}{2}\right)$$

$$= C\left(1 + \frac{\alpha}{2}\left[1 - \cos\phi\right]\right)$$



In this function C is a normalization constant and α is a tunable parameter

(2) The Hamiltonian can be written as a sum of the unperturbed Hamiltonian H_0 and a small perturbation H':

$$H = H_0 + H' \qquad H_0 = \epsilon \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad H' = \alpha\epsilon \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

The eigenvalues and normalized eigenvectors of H_0 are:

$$E_1^{(0)} = 2\epsilon \qquad E_2^{(0)} = 2\epsilon \qquad E_3^{(0)} = 0$$

$$\psi_1^{(0)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad \psi_2^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \psi_3^{(0)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

State 3 is non-degenerate. Therefore the first order correction to its energy is simply

$$E_3^{(1)} = \langle \psi_3^{(0)} | H' | \psi_3^{(0)} \rangle = \alpha\epsilon \frac{1}{2} (1 \; -1 \; 0) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = 0$$

States 1 and 2 are degenerate, so we must use the degenerate perturbation theory. Let us compute and diagonalize W matrix.

$$W_{ij} \equiv \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle \qquad i,j = 1,2$$

$$W_{11} = \alpha\epsilon \frac{1}{2} (1 \; 1 \; 0) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$W_{12} = W_{21} = \alpha\epsilon \frac{1}{\sqrt{2}} (1 \; 1 \; 0) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \sqrt{2}\alpha\epsilon$$

$$W_{22} = \alpha\epsilon (0 \; 0 \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$$W = \sqrt{2}\alpha\epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The eigenvalues and eigenvectors of W are:

$$\lambda_1 = \sqrt{2}\alpha\epsilon \qquad \lambda_2 = -\sqrt{2}\alpha\epsilon$$

$$\chi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \chi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Eigenvalues λ_1 and λ_2 give first order corrections to the energies:

$$E_1^{(1)} = \sqrt{2}\alpha\epsilon \qquad E_2^{(1)} = -\sqrt{2}\alpha\epsilon$$

The proper basis is then:

$$\Phi_1^{(0)} = \frac{1}{\sqrt{2}}\left(\Psi_1^{(0)} + \Psi_2^{(0)}\right) = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\Phi_2^{(0)} = \frac{1}{\sqrt{2}}\left(\Psi_1^{(0)} - \Psi_2^{(0)}\right) = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\Phi_3^{(0)} = \Psi_3^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

The off-diagonal matrix elements of H' in this basis (only off-diagonal elements appear in the formulae for the first order corrections to the wave functions) are:

$$\langle \Phi_1^{(0)} | H' | \Phi_2^{(0)} \rangle = \langle \Phi_2^{(0)} | H' | \Phi_1^{(0)} \rangle = 0 \quad \text{(by construct)}$$

$$\langle \Phi_1^{(0)} | H' | \Phi_3^{(0)} \rangle = \langle \Phi_3^{(0)} | H' | \Phi_1^{(0)} \rangle = \frac{\alpha\epsilon}{\sqrt{2}}\left(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{\sqrt{2}}\right)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = 0$$

$$\langle \Phi_2^{(0)} | H' | \Phi_3^{(0)} \rangle = \langle \Phi_3^{(0)} | H' | \Phi_2^{(0)} \rangle = \frac{\alpha\epsilon}{\sqrt{2}}\left(\frac{1}{2}\ \frac{1}{2}\ -\frac{1}{\sqrt{2}}\right)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = 0$$

Therefore,

$$\Phi_1^{(1)} = \Phi_2^{(1)} = \Phi_3^{(1)} = 0$$

P.S. Because all $H'_{ij} = 0$ we can also say immediately that $E_1^{(2)} = E_2^{(2)} = E_3^{(2)} = 0$

(3) According to the time-dependent perturbation theory, the first order transition amplitude from state i to state f is given by

$$c_f^{(1)}(t) = \frac{1}{i\hbar}\int_{t_0}^{t} \langle \psi_f | V(x,t') | \psi_i \rangle\, e^{i\omega_{fi}t'}\, dt' \qquad \text{where } \omega_{fi} = \frac{E_f - E_i}{\hbar}$$

In our case $\omega_{fi} = \omega_{41} = \dfrac{(4^2-1^2)\pi^2\hbar^2}{2ma^2} = \dfrac{15\pi^2\hbar^2}{2ma^2} \equiv \omega$,

$t_0 = 0$, $t = +\infty$ (after long time). So we have

$$c_4^{(1)} = \frac{\beta}{i\hbar}\underbrace{\langle \psi_4(x) | x | \psi_1(x) \rangle}_{-\frac{32a}{15^2\pi^2}} \underbrace{\int_0^{\infty} t' e^{-\frac{t'}{\tau}} e^{i\omega t'}\, dt'}_{\frac{1}{\left(\frac{1}{\tau} - i\omega\right)^2}} = -\frac{\beta}{i\hbar}\frac{(4\sqrt{2})^2 a}{15^2\pi^2}\frac{\tau^2}{(1-i\omega\tau)^2}$$

The corresponding probability is

$$P_4^{(1)} = |c_4^{(1)}|^2 = \frac{\beta^2 a^2}{\hbar^2}\left(\frac{4\sqrt{2}}{15\pi}\right)^4 \frac{\tau^4}{(1+\omega^2\tau^2)^2}$$

This probability must remain small, otherwise the perturbative treatment is not valid. Hence, we must require that

$$\frac{\beta^2 a^2 \tau^4}{\hbar^2} \ll 1 \qquad \text{or} \qquad \beta \ll \frac{\hbar}{a\tau^2}$$

(4) Bohr-Sommerfeld quantization rule for a potential with no vertical walls:

$$\int_a^b p(x)\,dx = (n-\tfrac{1}{2})\pi\hbar \qquad n = 1,2,3,\ldots \qquad p(x) = \sqrt{2m(E-V(x))}$$

Classical turning points are found by solving $\alpha|x| = E$

$$a = -\frac{E}{\alpha} \qquad b = +\frac{E}{\alpha}$$

With that we have

$$\int_{-E/\alpha}^{+E/\alpha} \sqrt{2m(E-\alpha|x|)}\,dx = (n-\tfrac{1}{2})\pi\hbar$$

$$\int_{-E/\alpha}^{0} \sqrt{\frac{E}{\alpha}+x}\,dx + \int_{0}^{E/\alpha} \sqrt{\frac{E}{\alpha}-x}\,dx = \frac{1}{\sqrt{2m\alpha}}(n-\tfrac{1}{2})\pi\hbar$$

$$\frac{2}{3}\left(\frac{E}{\alpha}+x\right)^{3/2}\Bigg|_{-E/\alpha}^{0} - \frac{2}{3}\left(\frac{E}{\alpha}-x\right)^{3/2}\Bigg|_{0}^{E/\alpha} = \frac{1}{\sqrt{2m\alpha}}(n-\tfrac{1}{2})\pi\hbar$$

$$\frac{2}{3}\left(\frac{E}{\alpha}\right)^{3/2} + \frac{2}{3}\left(\frac{E}{\alpha}\right)^{3/2} = \frac{1}{\sqrt{2m\alpha}}(n-\tfrac{1}{2})\pi\hbar \qquad \text{or} \qquad \left(\frac{E}{\alpha}\right)^{3/2} = \frac{3}{4}\frac{(n-\tfrac{1}{2})\pi\hbar}{(2m\alpha)^{1/2}}$$

$$E_n = \frac{\left[\frac{3}{4}(n-\tfrac{1}{2})\pi\hbar\alpha\right]^{2/3}}{[2m]^{1/3}}$$

At large n $\quad E_n \sim n^{\frac{2}{3}}$ which makes sense because for the particle in a box ($V \sim x^{\infty}$) we have $E_n \sim n^2$ and for the harmonic oscillator ($V \sim x^2$) we have $E_n \sim n^1$

(5) The interaction of the positron with the nucleus is given by $V_n(r) = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$. If we represent the electron as a cloud centered at the nucleus, the corresponding charge distribution is given by the square of the ground state wave function of the hydrogen atom:

$$\rho(r) = -e|\psi(r)|^2 = -e\left|\frac{1}{\pi^{1/2}a^{3/2}}e^{-\frac{r}{a}}\right|^2 = -\frac{e}{\pi a^3}e^{-\frac{2r}{a}}$$

a is the Bohr radius

It is spherically symmetric. Hence the interaction of this charge distribution with the positron, $V_e(r)$, is determined by the total charge inside the sphere of radius r (r is the distance of the positron from the nucleus):

$$Q(r) = \int_{\text{sphere}} \rho(r')\,d\vec{r}' = 4\pi\int_0^r \rho(r')r'^2dr = -\frac{4e}{a^3}\int_0^r e^{-\frac{2r'}{a}}r'^2dr'$$

Note that $\int_0^r x^2e^{-\gamma x}dx = \frac{2}{\gamma^3}\left(1-e^{-\gamma r}\left[1+\gamma r+\frac{\gamma^2r^2}{2}\right]\right)$

So

$$Q(r) = -\frac{8e}{a^3}\frac{1}{\left(\frac{2}{a}\right)^3}\left(1-e^{-\frac{2r}{a}}\left[1+2\frac{r}{a}+2\frac{r^2}{a^2}\right]\right) = -e\left(1-e^{-\frac{2r}{a}}\left[1+2\frac{r}{a}+2\frac{r^2}{a^2}\right]\right)$$

Then

$$V_e(r) = \frac{e}{4\pi\varepsilon_0}\frac{Q(r)}{r} = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r}-\frac{1}{r}\left(1-e^{-\frac{2r}{a}}\left[1+2\frac{r}{a}+2\frac{r^2}{a^2}\right]\right)\right)$$

The total interaction is:

$$V(r) = V_n(r)+V_e(r) = \frac{e^2}{4\pi\varepsilon_0}e^{-\frac{2r}{a}}\left(1+2\frac{r}{a}+2\frac{r^2}{a^2}\right)$$

Since the positron is fast we can adopt the Born approximation, in which the scattering amplitude is given by

$$f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty V(r)\,r\sin qr\,dr \qquad q = 2k\sin\frac{\theta}{2} \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

The integral can be evaluated by noting that $\sin qr = \frac{e^{iqr}-e^{-iqr}}{2i}$

The result is:

$$\int_0^\infty e^{-\frac{2r}{a}}\left(1+2\frac{r}{a}+2\frac{r^2}{a^2}\right) r \sin qr \, dr = 32a^2 \frac{aq(20-a^2q^2)}{(4+a^2q^2)^4}$$

and

$$f(\theta) = -\frac{16 e^2 m a^3}{\pi \hbar^2 \varepsilon_0} \frac{(20-a^2q^2)}{(4+a^2q^2)^4}$$

The differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{256 e^4 m^2 a^6}{\pi^2 \hbar^4 \varepsilon_0^2} \frac{(20-a^2q^2)^2}{(4+a^2q^2)^8}$$

(6) a) In this process the Hamiltonian changes suddenly from that of the hydrogen-like atom with $Z=2$ to the one corresponding to $Z=1$. Thus, the probability of finding the atom in the new ground state is determined by the square of the expansion coefficient of the old wave function in terms of the new basis of hydrogenic states:

$$P = \left| \langle \psi^{new}_{ground} | \psi^{old}_{ground} \rangle \right|^2 = \left| \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} r^2 dr \; \psi^{new}_{100}(r)\, \psi^{old}_{100}(r) \right|^2$$

$$= \left| 4\pi \int_0^{\infty} r^2 \frac{1}{\pi^{1/2} a_{new}^{3/2}} e^{-\frac{r}{a_{new}}} \frac{1}{\pi^{1/2} a_{old}^{3/2}} e^{-\frac{r}{a_{old}}} dr \right|^2 = \left| \frac{4}{a_{new}^{3/2} a_{old}^{3/2}} \int_0^{\infty} e^{-\beta r} r^2 dr \right|$$

where $\beta = \frac{1}{a_{new}} + \frac{1}{a_{old}} = \frac{a_{new} + a_{old}}{a_{new} a_{old}}$ and $a_{old,new}$ are Bohr radii for $Z=2$ and $Z=1$.

$$P = \left| \frac{4}{a_{new}^{3/2} a_{old}^{3/2}} \frac{2}{\beta^3} \right|^2 = \left| 8 \frac{a_{new}^{3/2} a_{old}^{3/2}}{(a_{new} + a_{old})^3} \right|^2 = 64 \left[\frac{\sqrt{a_{new} a_{old}}}{a_{new} + a_{old}} \right]^6 =$$

Now we know that $a_{new} = 2 a_{old}$ (recall $a \equiv \frac{4\pi\varepsilon_0 \hbar^2}{Z m e^2}$)

With that we get:

$$P = 64 \left[\frac{\sqrt{2 a_{old} \cdot a_{old}}}{2 a_{old} + a_{old}} \right]^6 = 64 \left[\frac{\sqrt{2}}{3} \right]^6 = \frac{512}{729} \approx 0.702$$

b) In this case we can use the adiabatic theorem, which states that the system will stay in the ground state if it started in the ground state. The final ground state is obviously a linear combination (with equal coefficients) of the configurations that involve nucleus 1 (h_1), nucleus 2 (h_2), and electron (e):

1) $(n_1 + e)_{ground} + (n_2)$

2) $(n_1) + (n_2 + e)_{ground}$

This is because we cannot expect the electron to discriminate between the two identical nuclei (it can stick to any). Therefore the probability to get an atom (nucleus + electron) if we randomly pick only one subsystem is

$$P = \frac{1}{2}$$

Now in order for the adiabatic theorem to hold the process must be slow. Specifically the characteristic time scale of the change of the Hamiltonian (T) must be much larger than the characteristic time scale of the (time-dependent) wave function, τ, which is determined by the energy gap between the ground and first excited state

$$\tau \sim \frac{1}{\omega} = \frac{\hbar}{\Delta E} \approx \frac{\hbar}{|E_{n=1}|} \approx \frac{\hbar}{\frac{\hbar^2}{ma^2}} = \frac{ma^2}{\hbar}$$

m - electron mass
a - Bohr radius

as τ we can take the time it will take for the two nuclei to move apart by distance a ($\approx$ atom size)

$$T \approx \frac{a}{v}$$ (v is relative velocity of nuclei)

$$2\frac{Mv^2}{2} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{R} \quad \text{or} \quad Mv^2 = \frac{\hbar^2}{ma}\frac{1}{R} \Rightarrow v = \sqrt{\frac{\hbar^2}{mMaR}} = \frac{\hbar}{\sqrt{mMaR}}$$

So

$$a\sqrt{\frac{mMaR}{\hbar}} \gg \frac{ma^2}{\hbar} \quad \text{or} \quad R \gg \frac{m}{M}a$$