(1) a) Let us first normalize the trial wave function:

$$1 = \langle\psi|\psi\rangle = \int_{-a}^{a} |c|^2 \left(1-\frac{|x|}{a}\right)^2 dx = 2\int_0^a |c|^2 \left(1-\frac{|x|}{a}\right)^2 dx =$$

$$= 2\frac{|c|^2}{a^2}\int_0^a (x^2-2ax+a^2)\,dx = \frac{2|c|^2 a}{3}, \quad \text{so} \quad |C|^2 = \frac{3}{2a}$$

The expectation value of the kinetic energy operator is:

$$\langle T\rangle = |c|^2 \int_{-\infty}^{+\infty} \left(1-\frac{|x|}{a}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(1-\frac{|x|}{a}\right)\right]dx = \frac{|c|^2\hbar^2}{2m}\int_{-\infty}^{+\infty}\left[\frac{d}{dx}\left(1-\frac{|x|}{a}\right)\right]^2 dx =$$

$$= \frac{|c|^2\hbar^2}{2m}\int_{-a}^{a}\left(-\frac{x}{|x|a}\right)^2 dx = \frac{|c|^2\hbar^2}{2ma^2}\cdot 2a = \frac{|c|^2\hbar^2}{ma}$$

The expectation value of the potential energy operator is:

$$\langle V\rangle = |C|^2 \int_{-a}^{a} \beta|x|\left(1-\frac{|x|}{a}\right)^2 = 2|c|^2\beta\int_0^a x\left(1-\frac{x}{a}\right)^2 dx = \frac{2|c|^2\beta}{a^2}\int_0^a (x^3-2ax^2+a^2x)\,dx =$$

$$= \frac{|c|^2\beta a^2}{6}$$

Then the trial energy is

$$E = \langle T\rangle + \langle V\rangle = |C|^2\left(\frac{\hbar^2}{ma}+\frac{\beta a^2}{6}\right) = \frac{3}{2}\frac{\hbar^2}{ma^2} + \frac{1}{4}\beta a$$

For its minimum we compute $\frac{\partial E}{\partial a} = -\frac{3\hbar^2}{ma^3} + \frac{1}{4}\beta = 0$

which yields the optimal value of a: $a_{min} = \left(\frac{12\hbar^2}{m\beta}\right)^{1/3}$

When we substitute a_{min} in E we get

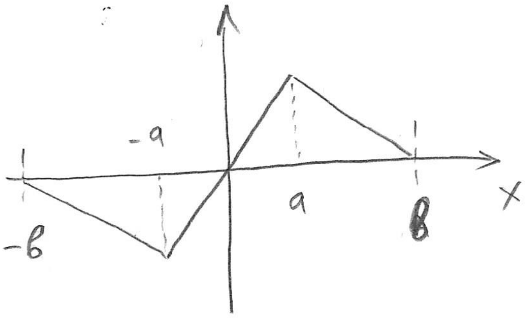
$$E = \frac{3}{2}\frac{\hbar^2}{m}\left(\frac{m\beta}{12\hbar^2}\right)^{2/3} + \frac{1}{4}\beta\left(\frac{12\hbar^2}{m\beta}\right)^{1/3} = \frac{3}{4}\left(\frac{3\hbar^2\beta^2}{2m}\right)^{1/3}$$

b) The potential $V = \beta|x|^2$ does not have any infinite walls. Hence the wave function must be continuous. Function

$$\psi(x) = \begin{cases} C, & -a < x < a \\ 0, & |x| > 0 \end{cases}$$

is not continuous at $x = \pm a$ and thus does not belong to the class of allowed (properly behaved) functions

c) We could use an odd function of this form



$$\psi(x) = \begin{cases} cx \,, & -a < x < a \\ \dfrac{ca}{b-a}(b-x) \,, & a < x < b \\ \dfrac{ca}{b+a}(x-b) \,, & -b < x < -a \\ 0 \,, & |x| > b \end{cases}$$

this function is orthogonal to the ground state so it will give an upper bound to the energy of the first excited state

② Both H_0 and the total Hamiltonian $H = H_0 + V$ have a block-diagonal structure with 1×1, 2×2, and 1×1 blocks. Hence, the energies come as eigenvalues of the corresponding block matrices. Perturbation V can only mix states within a block. The states that correspond to different blocks do not mix. The eigenvalues/eigenstates of H_0 are:

$E_1^{(0)} = a \qquad \psi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

This state does not mix with any other. The energy is not shifted (in any order of the perturbation theory) because $V_{11} = 0$.

So we can say that

$$E_1^{(1)} = E_1^{(2)} = 0 \quad \text{and} \quad E_1 = a$$

The next state/energy is

$E_4^{(0)} = a \qquad \psi_4^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

The situation with this state is similar to that of $\psi_1^{(0)}$, so

$$E_4^{(1)} = E_4^{(2)} = 0 \quad \text{and} \quad E_4 = a$$

Now let us consider the middle block:

$$a\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} X = E^{(0)} X$$

This 2×2 problem is easy to solve and we find:

$E_2^{(0)} = a \qquad X_2^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \psi_2^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$

$E_3^{(0)} = 3a \qquad X_3^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \psi_3^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$

There is no degeneracy within this middle block so it is safe to use the non-degenerate perturbation theory formulae:

$$E_2^{(1)} = \langle x_2^{(0)} | V | x_2^{(0)} \rangle = \frac{1}{\sqrt{2}} (1 \; -1)\, b \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{b}{2} (1 \; -1) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{b}{2}$$

$$E_3^{(1)} = \langle x_3^{(0)} | V | x_3^{(0)} \rangle = \frac{1}{\sqrt{2}} (1 \; 1)\, b \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{b}{2} (1 \; 1) \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \frac{3b}{2}$$

Now let us proceed to the second order:

$$E_2^{(2)} = \sum_{\substack{m=2 \\ m \neq 2}}^{3} \frac{|\langle x_m^{(0)} | V | x_2^{(0)} \rangle|^2}{E_2^{(0)} - E_m^{(0)}} = \frac{|\langle x_3^{(0)} | V | x_2^{(0)} \rangle|^2}{E_2^{(0)} - E_3^{(0)}}$$

here $\langle x_3^{(0)} | V | x_2^{(0)} \rangle = \frac{1}{\sqrt{2}} (1 \; 1)\, b \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{b}{2} (1 \; 1) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{b}{2}$

so $E_2^{(2)} = \frac{(\frac{b}{2})^2}{(a-3a)} = -\frac{b^2}{8a}$

Similarly,

$$E_3^{(2)} = \frac{|\langle x_2^{(0)} | V | x_3^{(0)} \rangle|^2}{E_3^{(0)} - E_2^{(0)}} = \frac{b^2}{8a}$$

In the end we get

$$E_2 = a - \frac{b}{2} - \frac{b^2}{8a} + O(b^3)$$

$$E_3 = 3a + \frac{3b}{2} + \frac{b^2}{8a} + O(b^3)$$

③ a) $H' = -q\mathcal{E}_0 z \sin\omega t$

b) Recall that s-states are spherically symmetric and for p-states the angular dependence is given by spherical harmonics $Y_1^{+1,0,-1}$, so

$|00\rangle = |1\rangle = f_1(r)$

$|1+1\rangle = |2\rangle = (x+iy) f_2(r)$

$|10\rangle = |3\rangle = z f_3(r)$

$|1-1\rangle = |4\rangle = (x-iy) f_4(r)$

here $f_i(r)$ are some spherically-symmetric functions

Given that $H' \sim z$ most matrix elements H'_{ij} vanish due to the symmetry of the integrand:

$$H' = \begin{array}{c c} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \begin{pmatrix} 0 & 0 & H'_{13} & 0 \\ 0 & 0 & 0 & 0 \\ H'_{31} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

$H'_{13} = -q\mathcal{E}_0 \langle 00|z|10\rangle \sin\omega t$

if we denote

$\Omega = q\mathcal{E}_0 \langle 00|z|10\rangle$

then $H'_{13} = H'_{31} = -\hbar\Omega \sin\omega t$

c) The time-dependent Schrödinger equation in matrix form is

$$i\hbar \frac{dc_n(t)}{dt} = \sum_k{}' H'_{nk} e^{i\omega_{nk}t} c_k(t)$$

where c_n are time-dependend coefficients in the expansion

$$\psi(\vec{r},t) = \sum_n{}' c_n(t) |n\rangle e^{\frac{-iE_n^{(0)}t}{\hbar}}$$

In our case all energies are degenerate, so we can take them to be equal to zero (a common phase factor is not important)

$E_n^{(0)} = 0 \qquad \omega_{nk} = 0$

Then we have

$$i\begin{pmatrix}\dot{c}_1\\ \dot{c}_2\\ \dot{c}_3\\ \dot{c}_4\end{pmatrix} = \begin{pmatrix}0 & 0 & -\Omega\sin\omega t & 0\\ 0 & 0 & 0 & 0\\ -\Omega\sin\omega t & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}c_1\\ c_2\\ c_3\\ c_4\end{pmatrix}$$

We can see that equations for c_2 and c_4 are decoupled:

$$i\frac{dc_2}{dt} = 0 \qquad i\frac{dc_4}{dt} = 0$$

since given the initial condition ($c_2(t=0)=0$, $c_4(t=0)=0$ since the system was prepared in state $|1\rangle$) we conclude

$$c_2(t) = 0 \qquad P_2(t) = |c_2(t)|^2 = 0$$

$$c_4(t) = 0 \qquad P_4(t) = |c_4(t)|^2 = 0$$

The system of equations for c_1 and c_3 is:

$$i\frac{dc_1}{dt} = -\Omega\sin\omega t\, c_3$$

$$i\frac{dc_3}{dt} = -\Omega\sin\omega t\, c_1$$

or

$$i\begin{pmatrix}\dot{c}_1\\ \dot{c}_3\end{pmatrix} = -\Omega\sin\omega t\underbrace{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}}_{M}\begin{pmatrix}c_1\\ c_2\end{pmatrix}$$

To decouple equations for c_1 and c_3 we can make a linear transformation that diagonalizes matrix M

$$\begin{vmatrix}\lambda & 1\\ 1 & \lambda\end{vmatrix} = 0 \qquad \lambda = \pm 1$$

$$x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix}$$

$$a = \frac{c_1 + c_3}{\sqrt{2}} \qquad c_1 = \frac{a+b}{\sqrt{2}}$$

$$b = \frac{c_1 - c_3}{\sqrt{2}} \qquad c_3 = \frac{a-b}{\sqrt{2}}$$

Then

$$i\begin{pmatrix}\dot{a}\\ \dot{b}\end{pmatrix} = -\Omega\sin\omega t\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}$$

The solution is

$$\ddot{a} = \alpha e^{-\frac{i\Omega}{\omega}\cos\omega t} \qquad b = \beta e^{\frac{i\Omega}{\omega}\cos\omega t}$$

where α, β are constants

Given the initial conditions

$$C_1(0) = 1 \qquad C_3(0) = 0 \quad \Longrightarrow \quad a(0) = \frac{1}{\sqrt{2}} \qquad b(0) = \frac{1}{\sqrt{2}}$$

we find α and β:

$$a = \frac{1}{\sqrt{2}} e^{\frac{i\Omega}{\omega}(1-\cos\omega t)} \qquad b = \frac{1}{\sqrt{2}} e^{-\frac{i\Omega}{\omega}(1-\cos\omega t)}$$

Going back to C_1 and C_3 we obtain

$$C_1 = \frac{a+b}{\sqrt{2}} = \cos\left[\frac{\Omega}{\omega}(1-\cos\omega t)\right]$$

$$C_3 = \frac{a-b}{\sqrt{2}} = i\sin\left[\frac{\Omega}{\omega}(1-\cos\omega t)\right]$$

Lastly,

$$P_1(t) = |C_1|^2 = \cos^2\left[\frac{\Omega}{\omega}(1-\cos\omega t)\right]$$

$$P_3(t) = |C_3|^2 = \sin^2\left[\frac{\Omega}{\omega}(1-\cos\omega t)\right]$$

(4) Here we can use the Bohr-Sommerfeld quantization rules for potentials with no vertical walls

$$\int_{-b}^{b} \sqrt{2m\left[E - V(x)\right]}\, dx = \left(n - \frac{1}{2}\right)\pi\hbar$$

where $\pm b$ are classical turning points

$$E = \frac{1}{2} m\omega^2 (b-a)^2 \leftarrow \text{condition for finding } b$$

The above integral becomes

$$2\int_0^a \sqrt{2mE}\, dx + 2\int_a^b \sqrt{2m\left[E - \frac{m\omega^2 (x-a)^2}{2}\right]}\, dx = \left(n-\frac{1}{2}\right)\pi\hbar$$

or

$$2a\sqrt{2mE} + 2m\omega \int_a^b \sqrt{\frac{2E}{m\omega^2} - (x-a)^2}\, dx = \left(n - \frac{1}{2}\right)\pi\hbar$$

$$\int_a^b \sqrt{\frac{2E}{m\omega^2} - (x-a)^2}\, dx = \int_0^{b-a} \sqrt{\frac{2E}{m\omega^2} - x^2}\, dx = \frac{1}{2}\left(x\sqrt{\frac{2E}{m\omega^2} - x^2} + \right.$$

$$\left. + \frac{2E}{m\omega^2} \arctan\left[\frac{x}{\sqrt{\frac{2E}{m\omega^2} - x^2}}\right]\right)\Bigg|_0^{\sqrt{\frac{2E}{m\omega^2}}} = \frac{E}{m\omega^2}\frac{\pi}{2}$$

So we have

$$2a\sqrt{2mE} + \pi\frac{E}{\omega} = \left(n - \frac{1}{2}\right)\pi\hbar$$

This is a quadratic equation with respect to $\sqrt{E} \equiv q$

$$q^2 + \frac{2\sqrt{2m}\, a\omega}{\pi} q - \hbar\omega\left(n - \frac{1}{2}\right) = 0$$

The solution is (keeping in mind that $E > 0$)

$$q = -\frac{\sqrt{2m}\, a\omega}{\pi} + \sqrt{\frac{2ma^2\omega^2}{\pi^2} + \hbar\omega\left(n - \frac{1}{2}\right)}$$

and

$$E = \frac{2ma^2\omega^2}{\pi^2}\left(-1 + \sqrt{1 + \frac{\pi^2\hbar}{2\omega m a^2}\left(n - \frac{1}{2}\right)}\right)^2$$

We can check what happens when $a \to 0$

$$E \approx \frac{2ma^2\omega^2}{\pi^2} \cdot \frac{\pi^2 \hbar}{2\omega m a^2}\left(n-\frac{1}{2}\right) \approx \hbar\omega\left(n-\frac{1}{2}\right) \approx \hbar\omega n$$

For large n (semiclassicall appoach is valid in this regime) we reproduce the energies of quantum harmonic oscillator.

If $a \to \infty$ we get

$$\sqrt{1+\frac{\pi^2\hbar}{2\omega m a^2}\left(n+\frac{1}{2}\right)} \approx 1 + \frac{\pi^2\hbar}{4\omega m a^2}\left(n+\frac{1}{2}\right) + \dots$$

and

$$E \approx \frac{2ma^2\omega^2}{\pi^2}\left(\frac{\pi^2\hbar}{4\omega m a^2}\left(n+\frac{1}{2}\right)\right)^2 \approx \frac{\pi^2\hbar^2 n^2}{8ma^2}$$

this reproduces the energies of the infinite potential well of length $2a$

(5) The interaction is described by the following potential:

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

The scattering amplitude in the Born approximation is

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int V(\vec{r}\,')\, e^{i\vec{q}\cdot\vec{r}\,'}\, d\vec{r}\,' \quad \text{where} \quad \vec{q} = \vec{k}\,' - \vec{k} \quad q = 2k\sin\frac{\theta}{2}$$

Using the known formula for the Fourier transform of $\frac{1}{|\vec{r}|}$: $\int \frac{1}{|\vec{r}|} e^{i\vec{q}\vec{r}}\, d\vec{r} = \frac{4\pi}{q^2}$

we obtain

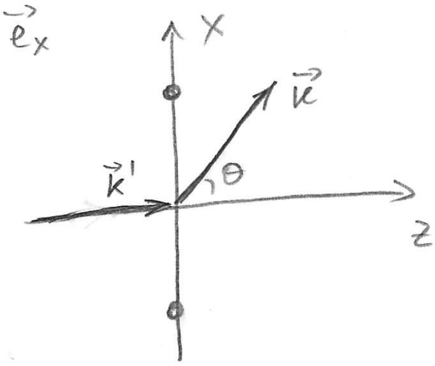
$$f(\theta,\phi) = -\frac{me^2}{8\pi^2\hbar^2\varepsilon_0}\left[\int \frac{e^{i\vec{q}\cdot\vec{r}\,'}}{|\vec{r}\,'-\vec{a}|}\, d\vec{r}\,' - \int \frac{e^{i\vec{q}\cdot\vec{r}\,'}}{|\vec{r}\,'+\vec{a}|}\, d\vec{r}\,'\right] =$$

$$= -\frac{me^2}{2\pi\hbar^2\varepsilon_0}\left[\frac{e^{i\vec{q}\cdot\vec{a}}}{q^2} - \frac{e^{-i\vec{q}\cdot\vec{a}}}{q^2}\right] = -\frac{ime^2}{\pi\hbar^2\varepsilon_0}\frac{\sin\vec{q}\cdot\vec{a}}{q^2}$$

Now if we consider scattering specifically in xz-plane then:

$$\vec{q}\cdot\vec{a} = (\vec{k}\,' - \vec{k})\cdot\vec{a} = \left(k\vec{e}_z - [k\sin\theta\,\vec{e}_x + k\cos\theta\,\vec{e}_z]\right)\cdot a\vec{e}_x$$

$$= -ka\sin\theta$$



$$q^2 = 4k^2\sin^2\frac{\theta}{2} = 2k^2(1-\cos\theta)$$

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{m^2e^4}{4\pi^2\hbar^4\varepsilon_0^2k^4}\frac{\sin^2(ka\sin\theta)}{(1-\cos\theta)^2}$$

Maxima are reached when $ka\sin\theta = \pi(n+\frac{1}{2})$ $\quad n = 0, \pm1, \ldots$

$$\theta_{max} = \arcsin\left[\frac{\pi(n+1/2)}{ka}\right] = \arcsin\left[\frac{\lambda(n+1/2)}{2a}\right]$$

where $\lambda = \frac{2\pi}{k}$

6) a) The energy can be found by plugging $\psi(x)$ into the Schrödinger equation. At any point $x \neq 0$ we have that $E = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}$ $\quad \psi = \left(\frac{m\alpha}{\hbar^2}\right)^{1/2} e^{-\frac{m\alpha}{\hbar^2}|x|}$

for $x > 0$ $\quad \psi' = -\left(\frac{m\alpha}{\hbar^2}\right)^{3/2} e^{-\frac{m\alpha}{\hbar^2}x}$ $\quad \psi'' = \left(\frac{m\alpha}{\hbar^2}\right)^{5/2} e^{-\frac{m\alpha}{\hbar^2}x}$

So $$E = -\frac{\hbar^2}{2m\left(\frac{m\alpha}{\hbar^2}\right)^{1/2}}\left(\frac{m\alpha}{\hbar^2}\right)^{5/2} = -\frac{m\alpha^2}{2\hbar^2}$$

b) $$\gamma(t) = i\int_{\alpha_i}^{\alpha_f} \langle \psi | \frac{\partial}{\partial\alpha}\psi \rangle \, d\alpha$$

$$\frac{\partial\psi}{\partial\alpha} = \left[\frac{1}{2}\frac{1}{\alpha} - \frac{m}{\hbar^2}|x|\right] e^{-\frac{m\alpha}{\hbar^2}|x|} \left(\frac{m\alpha}{\hbar^2}\right)^{1/2}$$

$$\langle \psi | \frac{\partial\psi}{\partial\alpha} \rangle = \int_{-\infty}^{+\infty} \left(\frac{m\alpha}{\hbar^2}\right)\left[\frac{1}{2}\frac{1}{\alpha} - \frac{m}{\hbar^2}|x|\right] e^{-\frac{2m\alpha}{\hbar^2}|x|} dx =$$

$$= \frac{m\alpha}{\hbar^2} 2\int_0^{\infty} \left[\frac{1}{2}\frac{1}{\alpha} - \frac{m}{\hbar^2}x\right] e^{-\frac{2m\alpha}{\hbar^2}x} dx = \frac{2m\alpha}{\hbar^2}\left[\frac{1}{2}\frac{1}{\alpha}\frac{\hbar^2}{2m\alpha} - \frac{m}{\hbar^2}\frac{\hbar^4}{4m^2\alpha^2}\right] = 0$$

So $\gamma(t) = 0$

c) $$\theta(t) = -\frac{1}{\hbar}\int_0^t E(t')\,dt = \frac{1}{\hbar}\int_0^t \frac{m\alpha^2(t')}{2\hbar^2} dt' = \frac{m}{2\hbar^3}\int \alpha^2 \frac{dt'}{d\alpha} d\alpha$$

$$= \frac{m}{2\hbar^3}\int_{\alpha_i}^{\alpha_f} \alpha^2\left(\frac{1}{\beta}\right) d\alpha = \frac{m}{6\hbar^3\beta}\left(\alpha_f^3 - \alpha_i^3\right)$$