(1) a) Let us expand the trial wave function φ in terms of the eigenfunctions of the Hamiltonian, ψ_n:

$$\varphi = \sum_{n=0}^{\infty} c_n \psi_n$$

If φ is normalized then

$$1 = \langle\varphi|\varphi\rangle = \left\langle \sum_m c_m \psi_m \middle| \sum_n c_n \psi_n \right\rangle = \sum_m \sum_n c_m^* c_n \underbrace{\langle \psi_m | \psi_n \rangle}_{\delta_{mn}} = \sum_n |c_n|^2$$

For $\langle\varphi|H|\varphi\rangle$ we get

$$\langle\varphi|H|\varphi\rangle = \left\langle \sum_m c_m \psi_m \middle| H \middle| \sum c_n \psi_n \right\rangle = \sum_m \sum_n c_m^* c_n E_n \langle \psi_m | \psi_n \rangle =$$

$$= \sum_n E_n |c_n|^2 \geq \sum_n E_0 |c_n|^2 = E_0 \sum_n |c_n|^2 = E_0$$

b) Let us choose the trial wave function in the following form: $\varphi = C e^{-\alpha|x|}$ $(\alpha > 0)$

From the normalization condition we can determine C:

$$1 = \langle\varphi|\varphi\rangle = |c|^2 \int_{-\infty}^{+\infty} e^{-2\alpha|x|} dx = 2|c|^2 \int_0^{\infty} e^{-2\alpha x} dx = \frac{|c|^2}{\alpha} \Rightarrow C = \sqrt{\alpha}$$

Then

$$E(\alpha) = \langle T \rangle + \langle V \rangle$$

$$\langle T \rangle = \left\langle \varphi \middle| \frac{p^2}{2m} \middle| \varphi \right\rangle = \frac{1}{2m} \langle p\varphi | p\varphi \rangle = \frac{\hbar^2}{2m} \left\langle \frac{d\varphi}{dx} \middle| \frac{d\varphi}{dx} \right\rangle =$$

$$= \frac{\hbar^2 |c|^2}{2m} \int_{-\infty}^{+\infty} \left(\frac{d}{dx} e^{-\alpha|x|} \right)^2 dx = \frac{\hbar^2 \alpha}{m} \int_0^{\infty} \left(-\alpha e^{-\alpha x} \right)^2 dx = \frac{\hbar^2 \alpha^2}{2m}$$

$$\langle V \rangle = \alpha \int_{-\infty}^{+\infty} V(x) e^{-2\alpha|x|} dx$$

When $\alpha \to 0$ (loosely bound state) the latter expession becomes: $\langle V \rangle \approx \alpha \underbrace{\int_{-\infty}^{+\infty} V(x) dx}_{-q,\ q>0} = -\alpha q$

With that the trial energy becomes

$$E(\alpha \to 0) = \frac{\hbar^2}{2m}\alpha^2 - q\alpha$$

It is easy to see how that for small values of α the energy is negative. This proves that there is at least one bound state.

② a) Because L^2 and L_z commute, their simultaneous eigenstates $|lm\rangle$ (spherical harmonics) will also be eigenstates for any linear combination of operators L^2 an L_z. The energy eigenvalues of H_0 are

$$E^{(0)}_{lm} = \alpha \hbar^2 l(l+1) + \beta \hbar m$$

b) The eigenvalues of H_0 are non-degenerate (in general). Therefore we can apply non-degenerate perturbation theory:

$$V = \gamma L_y = \frac{\gamma}{2i}(L_+ - L_-)$$

$$E^{(1)}_{lm} = \langle lm|V|lm\rangle = \frac{\gamma}{2i}\left[\langle lm|L_+|lm\rangle - \langle lm|L_-|lm\rangle\right]$$

Using the property of the ladder operators L_+ and L_-

$$L_\pm |lm\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\,|l, m\pm 1\rangle$$

and the fact that states $|lm\rangle$ are mutually orthogonal it is easy to see that the first order corrections vanish, i.e. $E^{(1)}_{lm} = 0$

In the second order we have:

$$E^{(2)}_{lm} = \sum_{l',m' \neq l,m} \frac{|\langle l'm'|V|lm\rangle|^2}{E^{(0)}_{lm} - E^{(0)}_{l'm'}} = \frac{\gamma^2}{4}\sum_{l',m'\neq l,m} \frac{|\langle l'm'|L_+ - L_-|lm\rangle|^2}{E^{(0)}_{lm} - E^{(0)}_{l'm'}}$$

For any specific value of l only the terms $l' = l$ (but $m' \neq m$) will be different from zero in the latter sum. This is because $L_\pm$ when it act on $|lm\rangle$ does not change the l value. So,

$$E^{(2)}_{lm} = \frac{\gamma^2}{4}\sum_{m'\neq m} \frac{|\langle lm'|L_+|lm\rangle - \langle lm'|L_-|lm\rangle|^2}{\beta\hbar(m - m')} =$$

$$= \frac{\gamma^2}{4}\frac{\hbar}{\beta}\left[\frac{\left|\langle l, m+1|\sqrt{l(l+1)-m(m+1)}\,|l, m+1\rangle\right|^2}{m-(m+1)} + \right.$$

$$\left. + \frac{\left|\langle l, m-1|\sqrt{l(l+1)-m(m-1)}\,|l, m-1\rangle\right|^2}{m-(m-1)}\right] =$$

$$= \frac{\gamma^2\hbar}{4\beta}\left[-\big(l(l+1)-m(m+1)\big) + \big(l(l+1)-m(m-1)\big)\right] = \frac{\gamma^2\hbar}{2\beta}\, m$$

(3) The Hamiltonian $H = \begin{pmatrix} +E & h(t) \\ h(t) & -E \end{pmatrix}$ can be represented as a sum of H_0 and V:

$$H_0 = \begin{pmatrix} +E & 0 \\ 0 & -E \end{pmatrix} \qquad V = h(t)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \leftarrow \text{perturbation}$$

The eigenvalues and eigenstates of H_0 are

$$E_1 = E \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad E_2 = -E \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

a) According to the time-dependent perturbation theory

$$c_1^{(1)}(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} V_{12}(t')\, e^{i\omega_{12}t'}\, dt' \quad \text{where} \quad \omega_{12} = \frac{E+E}{\hbar} = \frac{2E}{\hbar}$$

$$V_{12}(t) = h(t)$$

So

$$c_1^{(1)}(t=+\infty) = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} h(t)\, e^{i\omega_{12}t}\, dt$$

and

$$P_{2\to 1}(t=+\infty) = |c_1^{(1)}(+\infty)|^2 = \left|\frac{1}{\hbar}\int_{-\infty}^{+\infty} h(t)\, e^{i\omega t}\, dt\right|^2$$

b) The exact solution of the TDSE:

$$i\hbar\frac{dc_n}{dt} = \sum_k V_{nk}\, e^{i\omega_{nk}t}\, c_k(t)$$

or

$$\begin{cases} i\hbar\dfrac{dc_1}{dt} = V_{11}c_1 + V_{12}\, e^{i\omega_{12}t}\, c_2 \\[2mm] i\hbar\dfrac{dc_2}{dt} = V_{21}\, e^{-i\omega_{12}t}\, c_1 + V_{22}c_2 \end{cases}$$

if $E = 0$ the system of equations becomes

$$\begin{cases} i\hbar\dfrac{dc_1}{dt} = h(t)\, c_2 \\[2mm] i\hbar\dfrac{dc_2}{dt} = h(t)\, c_1 \end{cases} \qquad \text{initial conditions:} \quad \begin{matrix} c_1(-\infty) = 0 \\ c_2(-\infty) = 1 \end{matrix}$$

The solution of this system is

$$c_1(t) = \frac{e^{-\frac{i}{\hbar}\int_{-\infty}^{t} h(t')dt'} - e^{\frac{i}{\hbar}\int_{-\infty}^{t} h(t')dt'}}{2}$$

$$c_2(t) = \frac{e^{-\frac{i}{\hbar}\int_{-\infty}^{t} h(t')dt'} + e^{\frac{i}{\hbar}\int_{-\infty}^{t} h(t')dt'}}{2}$$

or simply

$$c_1(t) = -i\sin\alpha(t) \qquad \text{where } \alpha(t) \equiv \frac{1}{\hbar}\int_{-\infty}^{t} h(t')\,dt'$$

$$c_2(t) = \cos\alpha(t)$$

The probability of transition is then

$$P_{2\to 1}(+\infty) = |c_1(+\infty)|^2 = \sin^2\alpha(+\infty)$$

The perturbative result in part a) is valid when α remains small at any t, i.e.

$$\frac{1}{\hbar}\int_{-\infty}^{t} h(t')\,dt' \ll 1$$

4. The incident wave in 1D is e^{ikx}

The Lippman - Schwinger equation is

$$\psi(x) = e^{ikx} + \frac{2m}{\hbar^2}\int_{-\infty}^{+\infty} G(x,x')\, V(x')\, \psi(x')\, dx'$$

In our case we have

$$V(x) = -\alpha\,\delta(x) \qquad \text{and} \qquad G(x,x') = -\frac{i}{2k}\, e^{ik|x-x'|}$$

With that our Lippman-Schwinger equation is

$$\psi(x) = e^{ikx} + \frac{im\alpha}{\hbar^2 k}\int_{-\infty}^{+\infty} e^{ik|x-x'|}\,\delta(x')\,\psi(x')\,dx'$$

or

$$\psi(x) = e^{ikx} + \frac{im\alpha}{\hbar^2 k}\, e^{ik|x|}\,\psi(0)$$

at $x=0$ it becomes

$$\psi(0) = 1 + \frac{im\alpha}{\hbar^2 k}\,\psi(0) \implies \psi(0) = \frac{1}{1-\frac{im\alpha}{\hbar^2 k}} = \frac{1}{1-i\beta} \qquad \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

The solution to the Lippmann-Schwinger equation can then be written as

$$\psi(x) = e^{ikx} + i\beta\, e^{ik|x|}\,\frac{1}{1-i\beta} = e^{ikx} + \underbrace{\frac{i\beta}{1-i\beta}}_{\text{scattering amplitude}}\, e^{ik|x|}$$

reflection probability $= |\text{scattering amplitude}|^2$

$$R = \frac{\beta^2}{1+\beta^2}$$

transmission probability:

$$T = 1 - R = \frac{1}{1+\beta^2}$$

(5) a) Between $t=-\infty$ and $t=0^-$ the Hamiltonian is changed continuously from

$$H(-\infty) = \varepsilon \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{to} \quad H(0^-) = \varepsilon \begin{pmatrix} 0 & \sqrt{2} \\ \sqrt{2} & 1 \end{pmatrix}$$

Its eigenvalues and eigenvectors change from

$$E_1(-\infty) = 0 \qquad \psi_1(-\infty) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$E_2(-\infty) = \varepsilon \qquad \psi_2(-\infty) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

to

$$E_1(0^-) = -\varepsilon \qquad \psi_1(0^-) = \begin{pmatrix} -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{1}{3}} \end{pmatrix}$$

$$E_2(0^-) = 2\varepsilon \qquad \psi_2(0^-) = \begin{pmatrix} \sqrt{\frac{1}{3}} \\ \sqrt{\frac{2}{3}} \end{pmatrix}$$

In this time interval ($[-\infty, 0^-]$) the energy spacing $\Delta E = E_2 - E_1$ increses from ε to 3ε, i.e. it is never smaller than ε.

The process remains adiabatic as long as the characteristic time scale for the time evolution of the general wave function

$$\psi = c_1\psi_1 e^{-\frac{iE_1 t}{\hbar}} + c_2\psi_2 e^{-\frac{iE_2 t}{\hbar}} \sim c_1\psi_1 + c_2\psi_2 \underbrace{e^{-\frac{i\Delta E t}{\hbar}}}_{e^{-i\frac{t}{\tau}}}.$$

is shorter then the characteristic time scale T for the change of $H(t)$. In other words, for the adiabadicity we must have

$$\tau \ll T \quad \text{or} \quad \frac{\hbar}{\Delta E} \ll T$$

which yields the condition

$$\frac{\hbar}{\varepsilon} \ll T$$

b) For $t<0$ is adiabatic, so no transition to the excited state occur. At $t=0$, however, there is a sudden change of the Hamiltonian. In this sudden change the wave function of the system remains the same (there is simply no time for it to evolve). The Hamiltonian, however, suddenly has new eigenstates. Hence the probability of transition is

$$P = |\langle \psi^{new}_{excited} | \psi^{old}_{ground} \rangle|^2 = |\langle \psi_2(t=+\infty) | \psi_1(t=0^-) \rangle|^2$$

Note that

$$H(t=0^+) = H(t=-\infty) = H(t=+\infty)$$

So

$$\psi_2(t=0^+) = \psi(t=-\infty) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\psi_1(t=0^-) = \begin{pmatrix} -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{1}{3}} \end{pmatrix}$$

and

$$P = \left| \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{1}{3}} \end{pmatrix} \right|^2 = \frac{1}{3}$$

(6) a) $\gamma_n = i \int_{a_1}^{a_2} \langle \psi_n | \frac{\partial}{\partial a} \psi_n \rangle \, da$ - geometric phase change

where $\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

$$\frac{\partial}{\partial a} \psi_n = -\frac{1}{2} \frac{\sqrt{2}}{a^{3/2}} \sin \frac{n\pi x}{a} - \frac{n\pi x \sqrt{2}}{a^{5/2}} \cos \frac{n\pi x}{a} = -\frac{1}{2a} \psi_n - \frac{n\pi}{a^2} \sqrt{\frac{2}{a}} \, x \cos \frac{n\pi x}{a}$$

With this we have

$$\gamma_n = i \left[-\frac{1}{2} \int_{a_1}^{a_2} \frac{1}{a} \underbrace{\langle \psi_n | \psi_n \rangle}_{1} \, da - 2n\pi \int_{a_1}^{a_2} \frac{1}{a^3} \underbrace{\left(\int_0^a x \sin \frac{n\pi x}{a} \cos \frac{n\pi x}{a} \, dx \right)}_{-\frac{a^2}{4n\pi}} da \right] =$$

$$= -\frac{i}{2} \int_{a_1}^{a_2} \frac{1}{a} \, da + \frac{i}{2} \int_{a_1}^{a_2} \frac{1}{a} \, da = 0$$

b) $\theta_n = -\frac{1}{\hbar} \int_0^t E_n(t') \, dt'$ - dynamic phase change

where $E_n = \frac{\pi^2 \hbar^2 n^2}{2 m a^2}$

$$dt = \frac{da}{da} dt = \frac{da}{C}$$

So

$$\theta_n = -\frac{1}{\hbar} \int_{a_1}^{a_2} \frac{\pi^2 \hbar^2 n^2}{2 m a^2} \frac{da}{C} = -\frac{\pi^2 \hbar n^2}{2 m C} \int_{a_1}^{a_2} \frac{1}{a^2} \, da = \frac{\pi^2 \hbar n^2}{2 m C} \left(\frac{1}{a_2} - \frac{1}{a_1} \right).$$