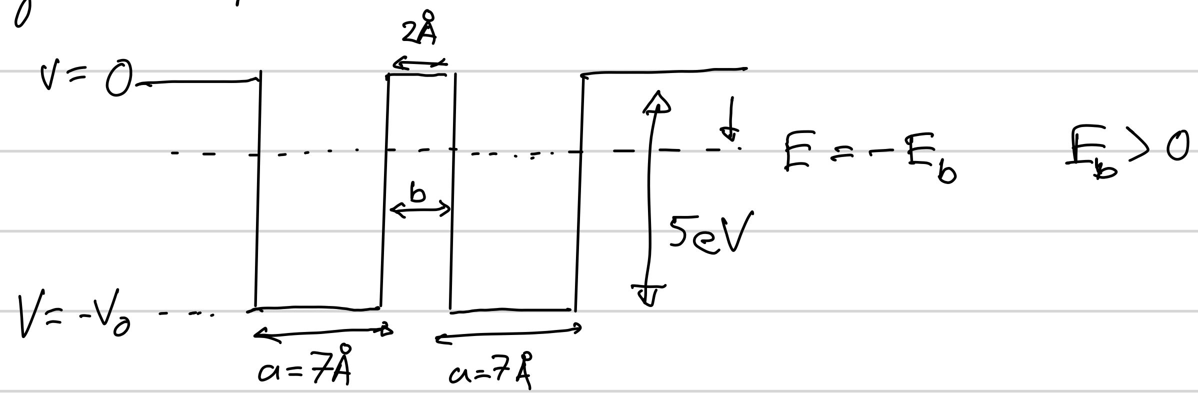
Physics 491: Problem Set # 8 Solutions

Problem 1: Tunnelling in multiple wells

Double-well potential for an electron



the "tunnelling splitting" between states that would be degenerate for an infinite barrier is approximated by $\Delta E_n = E_n e^{-\kappa_n b}$ $\quad \kappa = \sqrt{\frac{2m}{\hbar^2} E_b}$

(a) For an infinitely thick barrier, the bound states are those of a finite square well of depth $V_0 = 5\,\text{eV}$ and width $a = 7\text{Å}$. The key parameter is $\quad k_0 a = \sqrt{\frac{2m V_0 a^2}{\hbar^2}} = \sqrt{V_0/E_c}$

Let us calculate the characteristic energy $\quad E_c = \frac{\hbar^2}{2ma^2} = \frac{(\hbar c)^2}{2(mc^2)\,a^2}$

Useful units: $\hbar c = 1973\ \text{eV Å}$, $\quad mc^2 = 0.511\ \text{MeV}$

$$\Rightarrow E_c = \frac{(1973)^2\ \text{eV}^2\,\text{Å}^2}{2\,(0.511\times 10^6\ \text{eV})\,(7\text{Å})^2} = 0.077\ \text{eV} \quad \Rightarrow k_0 a = \sqrt{\frac{5}{0.077}} \approx 8$$

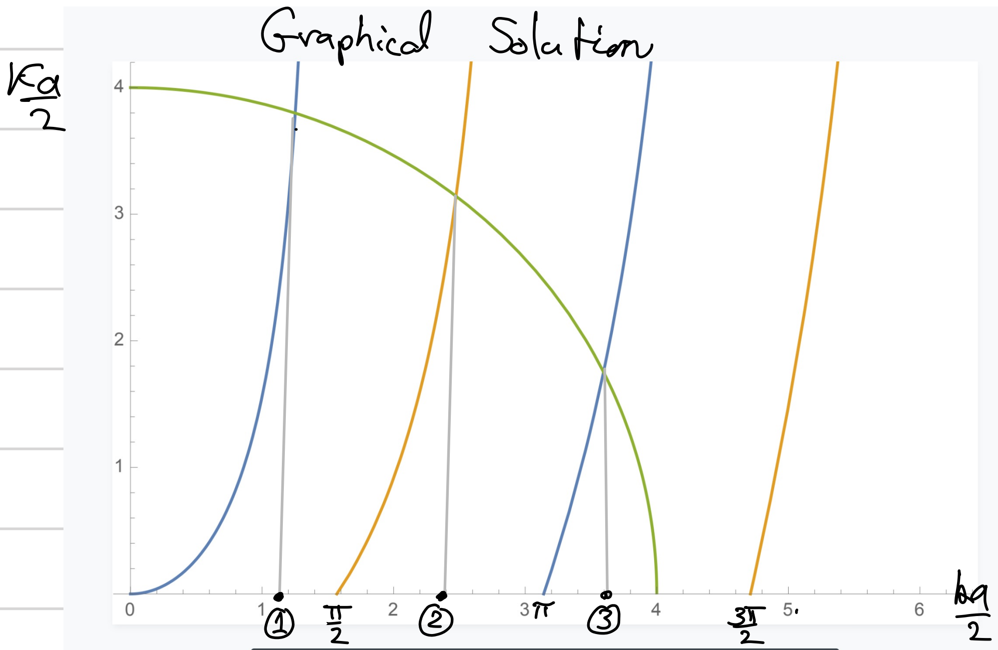
Single finite well

$$ka = \sqrt{\frac{2ma^2}{\hbar^2}(E-V)} = \sqrt{\frac{V_0 - E_b}{E_c}} \Rightarrow E_b = V_0 - (ka)^2 E_c$$

Binding energy

$$\begin{cases} \frac{ka}{2}\tan\left(\frac{ka}{2}\right) = \frac{\kappa a}{2}, & \text{even parity} \\ -\frac{ka}{2}\cot\left(\frac{ka}{2}\right) = \frac{\kappa a}{2}, & \text{odd parity} \end{cases};$$

$$\left(\frac{ka}{2}\right)^2 + \left(\frac{\kappa a}{2}\right)^2 = \left(\frac{k_0 a}{2}\right)^2$$



① $\frac{k_1 a}{2} \approx 1.2 \Rightarrow E_b^1 \approx 4.55$ eV

② $\frac{k_2 a}{2} \approx 2.4 \Rightarrow E_b^2 \approx 3.22$ eV

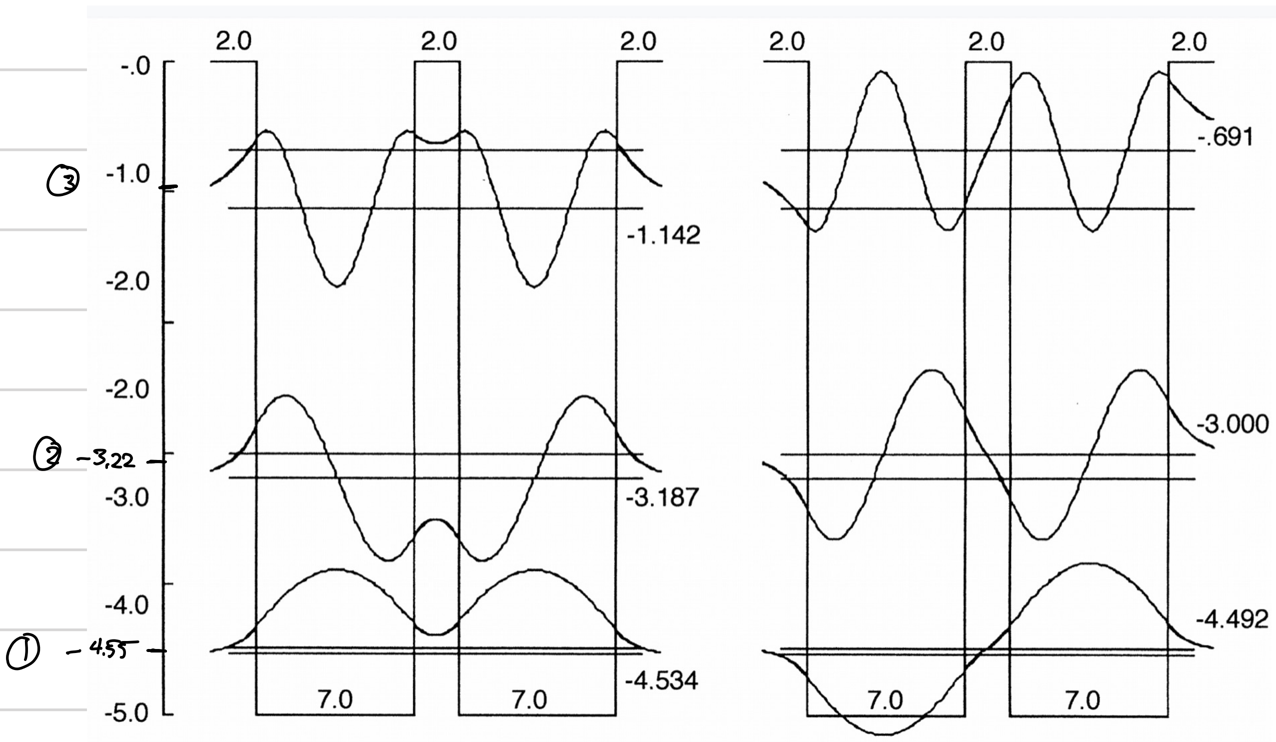
③ $\frac{k_3 a}{2} \approx 3.6 \Rightarrow E_b^3 \approx 1$ eV

Each of the three bound states is split in a "tunnelling doublet" with energy splitting $\Delta E_n \simeq E_n e^{-\kappa_n b}$, where $\kappa_n = \sqrt{\frac{2m E_b^n}{\hbar}}$ Binding energy nth level

$$\Rightarrow \kappa_n b = \sqrt{\frac{E_b^n}{E_c}}\,\frac{b}{a} = \sqrt{\frac{E_b^n}{E_c}}\,\frac{2}{7} \Rightarrow \kappa_1 b \approx 2.2, \quad \kappa_2 b \approx 1.84, \quad \kappa_3 b \approx 1$$

$$\Rightarrow \Delta E_1 = (V_0 - E_b^1)\, e^{-\kappa_1 b} = 0.05 \text{ eV}, \quad \Delta E_2 = (V_0 - E_b^2)\, e^{-\kappa_2 b} \approx 0.28 \text{ eV}, \quad \Delta E_3 \approx 1.47 \text{ eV}$$

The energy level diagram and wave functions are shown. For comparison to the approximate tunnelling splitting, shown are the exact eigenvalues found numerically.



$\Delta E_2 = 0.451$

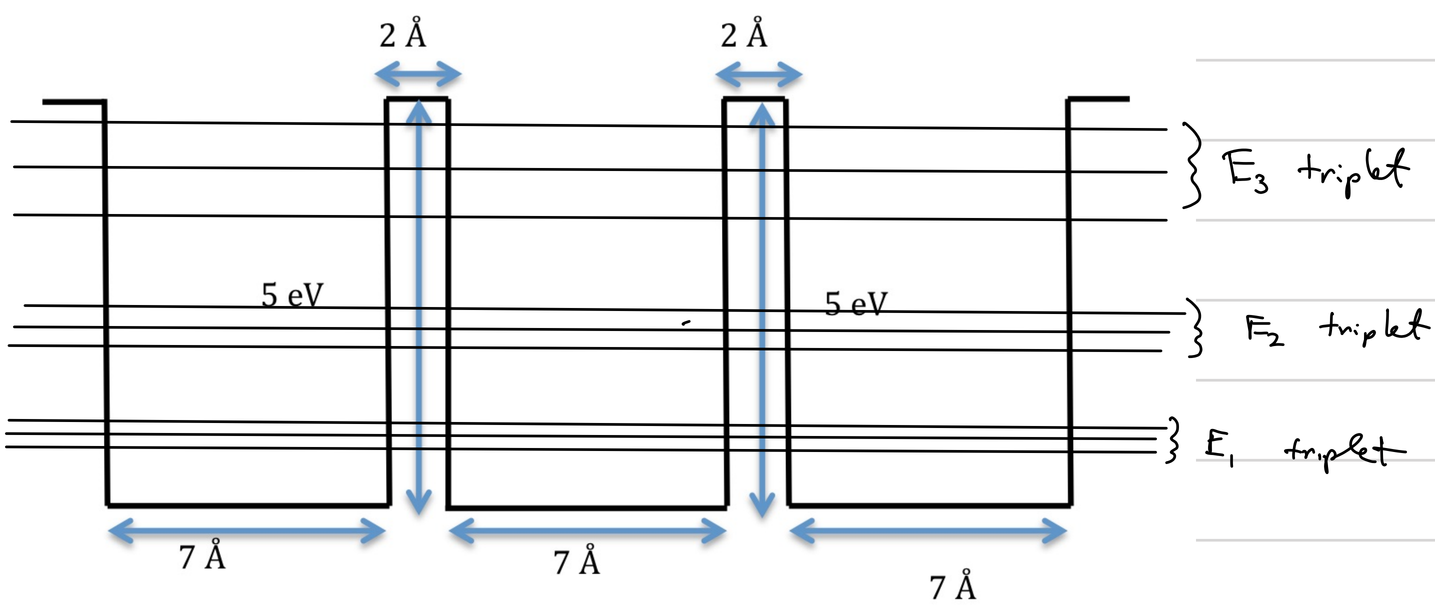
$\Delta E_2 = 0.187$

$\Delta E_1 = 0.042$

(c) We now consider a triple well

If the barrier were infinite, we woud have triply degenerate bound states. The energy levels would be, $E_1 = -4.55\,eV$, $E_2 = -3.22\,eV$, $E_3 = -1\,eV$ each triply degenerate - a total of 9 bound states. With finite tunnelling, each of these levels will split into three, nondegenerate levels. The tunnelling splitting will be smallest for the most tightly bound states

A sketch of the energy levels in shown here



(d) The eigenvectors of the Hamiltonian for the triple well must be eigenfunctions of parity. As the number of nodes increases with each excited state, the lowest energy level is even parity, and the excited state alternate: odd-even. Thus we can write each triplet in energy order (lowest to highest)

$$|u_n^{(+,1)}\rangle = \frac{1}{\sqrt{3}}\left(|u_{n,left}\rangle + |u_{n,middle}\rangle + |u_{n,right}\rangle\right)$$

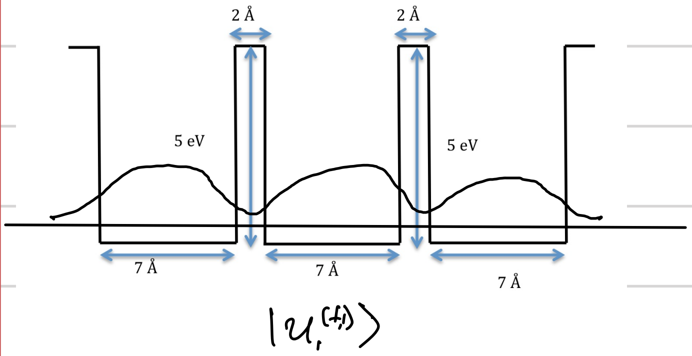
$$|u_n^{(-)}\rangle = \frac{1}{\sqrt{2}}\left(|u_{n,left}\rangle - |u_{n,right}\rangle\right)$$

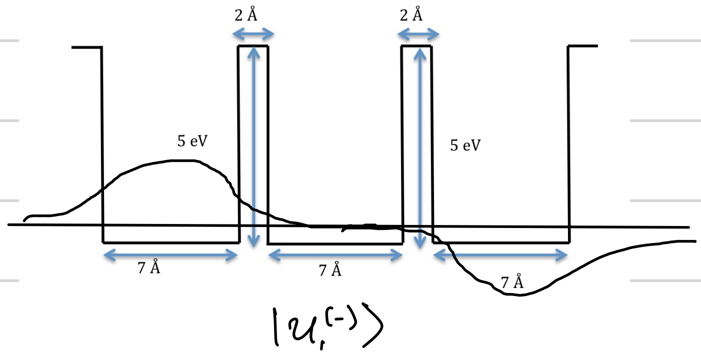
$$|u_n^{(+,2)}\rangle = \frac{1}{\sqrt{6}}\left(|u_{n,left}\rangle - 2|u_{n,middle}\rangle + |u_{right}\rangle\right)$$

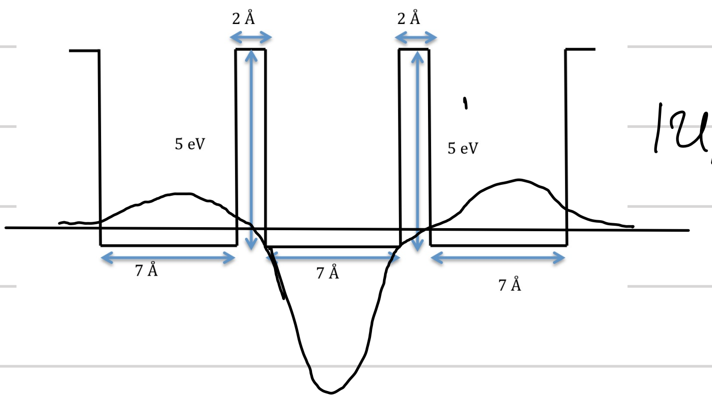
The state $|u_{n,left}\rangle$, $|u_{n,right}\rangle$, $|u_{n,middle}\rangle$ are the n^{th} energy eigenstates of the finite well, centered in the left, right, and middle. These are parity eigenstates because the action of the parity operator is

$$\hat{\Pi}|u_{n,left}\rangle = |u_{n,right}\rangle, \quad \hat{\Pi}|u_{n,middle}\rangle = |u_{n,middle}\rangle, \quad \hat{\Pi}|u_{n,right}\rangle = |u_{n,left}\rangle$$

Thus, for example, for the E_1 triplet, we sketch:

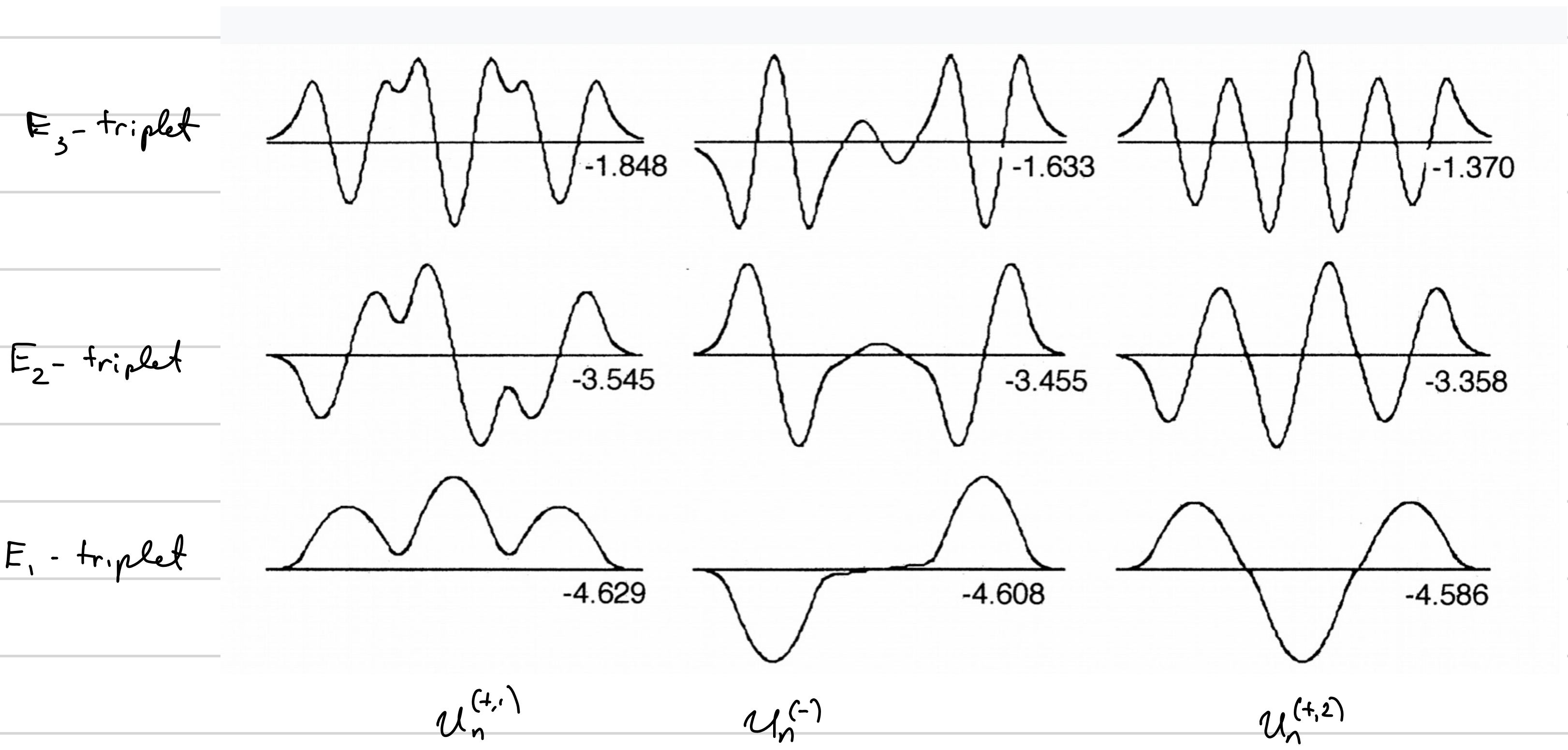






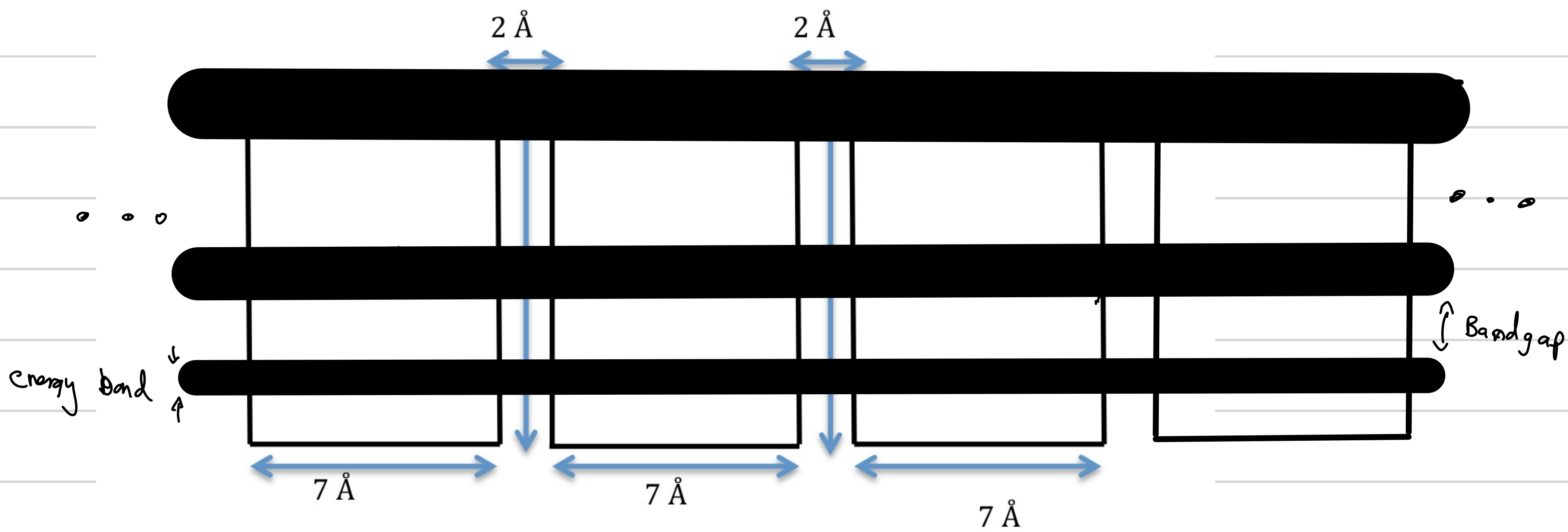
$|u_1^{(+,2)}\rangle$

A more precise sketch of all wavefunctions is shown below



Notice: The number of nodes in the wave function determine the number of the excited state: 2 nodes = second excited state, etc.

(e) Extra credit. As the number of wells increases, we get increasing splitting – 4 wells = quadruplet, 5 well = cinquet, etc.
For an infinite number of wells, the splitting becomes increasingly fine, ultimately resulting in a continuous band of energies for each E_n, with a "forbidden gap of energies" between them

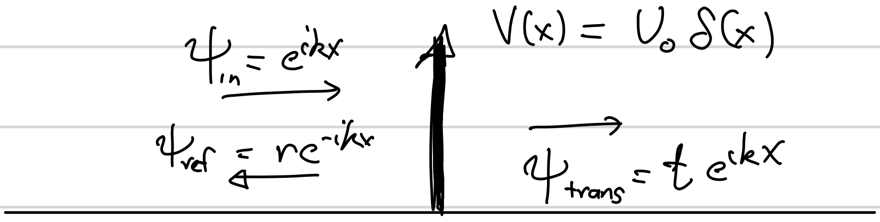


"Band structure" defines the energy spectrum of the energy eigenstates in a periodic potential. It is the fundamental feature of the "solid state" where atoms are arranged in a periodic crystal, and valence electrons experience the periodic attraction of the ions. the nature of the band structure and band gaps determines whether a material is "conducting" "insulating" or "semi conducting"

Problem 2

(a) Consider a repulsive delta function potential

$$V(x) = U_0\,\delta(x)$$



$$k \equiv \sqrt{\frac{2m}{\hbar^2}E}$$
$$\kappa \equiv \frac{mU_0}{\hbar^2}$$

We show here a "scattering eigenstate" (with energy E) corresponding to an incoming wave from $x=-\infty$, reflected with probability amplitude r, and transmitted with probability amplitude t. We can find these amplitudes using the boundary conditions:

$$\psi(0_+) = \psi(0_-)\,, \qquad \left.\frac{d\psi}{dx}\right|_{0_-} - \left.\frac{d\psi}{dx}\right|_{0_+} = -\frac{2mU_0}{\hbar^2}\psi(0)$$

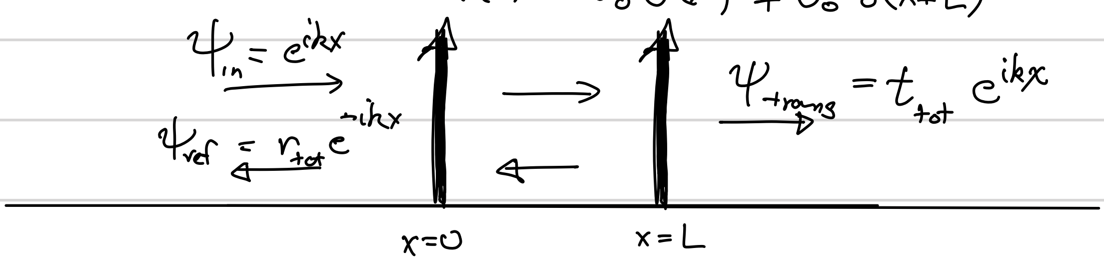
$$\Rightarrow 1+r = t \qquad ik(1-r) - ikt = -\frac{2mU_0}{\hbar^2}t = -2\kappa t$$

$$\Rightarrow ik(1-r) - ik(1+r) = -2\kappa(1+r) \Rightarrow ikr = \kappa(1+r) \Rightarrow r(ik-\kappa) = \kappa$$

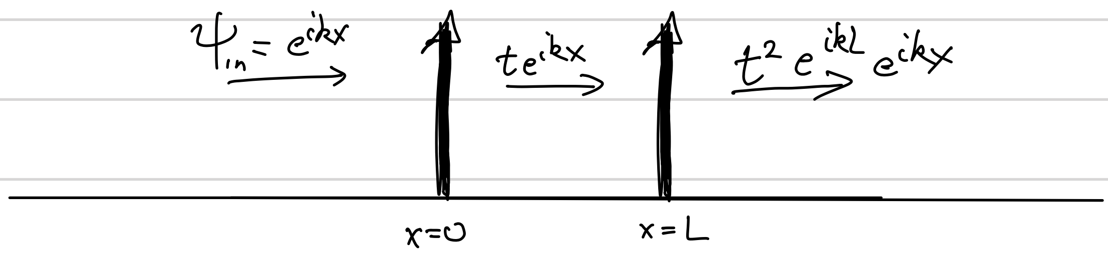
$$\Rightarrow \boxed{\begin{aligned} r &= \frac{\kappa}{ik-\kappa} = \sqrt{R}\,e^{i\phi_r} \quad \text{where } R = |r|^2 = \frac{\kappa^2}{k^2+\kappa^2}\,, \quad \phi_r = -\mathrm{Arctan}\left(\frac{k}{-\kappa}\right) \\ t &= 1+r = \frac{ik}{ik-\kappa} = i\sqrt{T}\,e^{i\phi_r}\,, \quad T = |t|^2 = \frac{k^2}{k^2+\kappa^2} \end{aligned}}$$

(b) Now we consider two delta-function barriers. This is like a "Fabry-Perot cavity" in optics, with each delta function barrier acting like a partially reflecting mirror

$$V(x) = U_0\,\delta(x) + U_0\,\delta(x+L)$$



Between the two barriers, the eigenstate consists of a superposition to forward and backward propagating plane waves. Instead of directly matching all the boundary conditions, which is horribly tedious, we can instead consider the interference of indistinguishable histories



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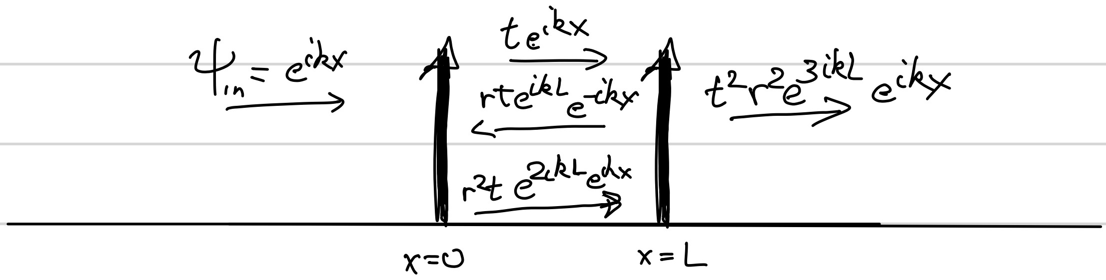

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- In the first "history" the particle transmits through each barrier.
- In the second "history" the particle transmits through the first barrier, propagate to the second barrier where it is reflect, probagate back to the first and reflected back to the second where it is transmitted.

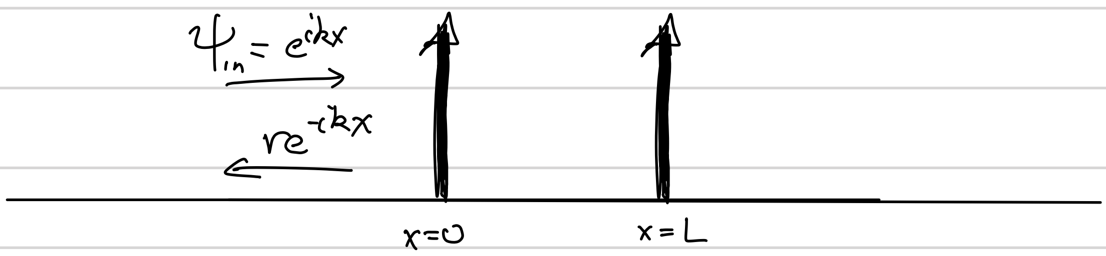
Generalizing:

$$t_{total} = \underset{\text{no reflects}}{t^2 e^{ikL}} + \underset{\text{two reflections}}{t^2 r^2 e^{3ikL}} + \underset{\text{four reflections}}{t^2 r^4 e^{5ikL}} + \dots + \underset{\text{n-reflections}}{t^2 r^{2n} e^{i(2n+1)kL}} + \dots$$

$$= t^2 e^{ikL} \sum_{n=0}^{\infty} (r^2 e^{i2kL})^n$$

$$\boxed{t_{total} = t^2 \frac{e^{ikL}}{1 - r^2 e^{2ikL}}}$$

We now repeat for reflection



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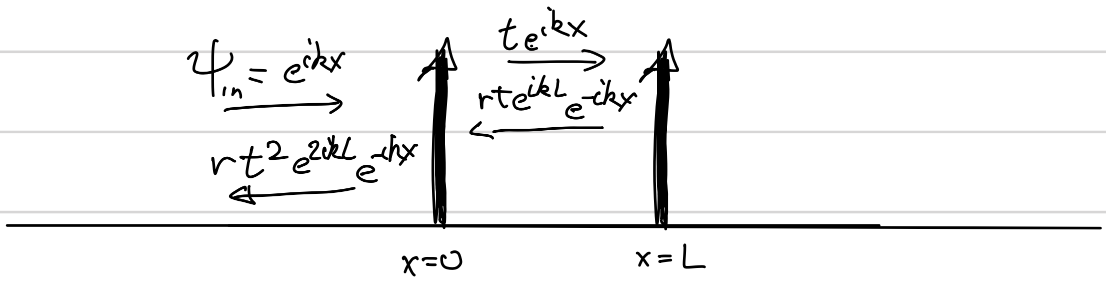

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$$r_{total} = r + r t^2 e^{2ikL} + r^3 t^2 e^{4ikL} + \dots + t^2 r^{(2n+1)} e^{i2nkL} + \dots$$
$$= r\left(1 + t^2 e^{2ikL} \sum_{n=0}^{\infty} \left(r^2 e^{2ikL}\right)^n\right)$$

$$\Rightarrow \boxed{r_{total} = r\left(1 + t^2 \frac{e^{2ikL}}{1 - r^2 e^{2ikL}}\right)}$$

(c) First note: $t_{total} = t^2 \dfrac{e^{ikL}}{1 - r^2 e^{2ikL}} = -T \dfrac{e^{2i\phi_r} e^{ikL}}{1 - R e^{2i(kL+\phi_r)}}$

Having used $R = \sqrt{R}\, e^{i\phi_r}$, $T = i\sqrt{T}\, e^{i\phi_r}$ from part (a)

- If $kL + \phi_r = n\pi \Rightarrow t_{total} = \dfrac{-T}{1-R} = -1 \Rightarrow |T_{total}| = 1$

Similarly, $r_{total} = r\left(1 - T \dfrac{e^{2i(kL+\phi_r)}}{1 - R e^{i(2kL+\phi_r)}}\right) = 0$ if $kL + \phi_r = \pi$

If general $|r_{total}|^2 + |t_{total}|^2 = 1$