Some simple QM systems in 1D position space

Schroedinger Eq in position space: $\psi''(x) = -\frac{2m}{\hbar^2}(E-V(x))\psi$

Classically Allowed Region (CAR): $E - V(x) > 0$

$\Rightarrow \psi(x)$ oscillates with spatial ~~wavenumber~~ ~~wavelength~~ wavenumber

Classically Forbidden Region (CFR): $E - V(x) < 0$

$\Rightarrow \psi(x)$ decays

Other conditions for ψ:

1. ψ is continuous
2. ψ' is continuous when $V(x)$ is not infinite
3. ψ should be normalizable. (But we ignore this sometimes when considering "beams of particles")

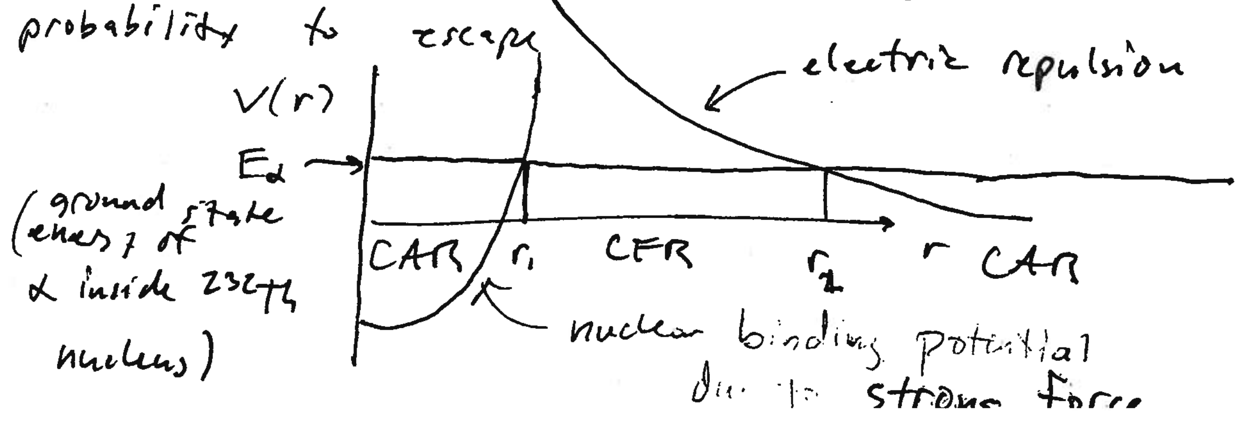
Alpha Decay

Heavy nuclei like U-238 can decay by emitting an alpha-particle (the nucleus of ^4He: p n p n)

Ex: $^{238}U \rightarrow {}^{234}Th + \alpha$ (Half-life ~ 10^9 years)

$N,Z = 238, 92$ $\quad N,Z = 234, 90 \quad N,Z = 4, 2$

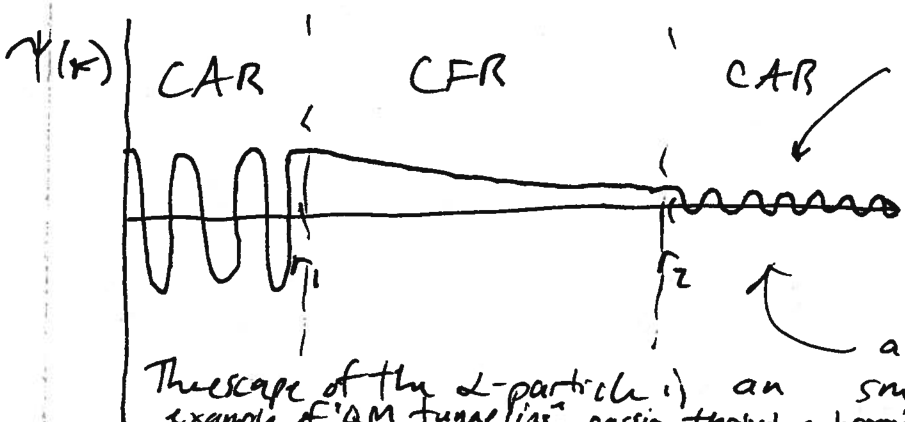
We can think of the alpha particle being bound inside the ^{234}Th nucleus, but having some probability to escape



How does the α-particle escape during α-decay?

Well, an α outside the ^{232}Th nucleus is <u>repelled</u> from the nucleus by the electric force (both are positively charged. So the potential must fall off like $\frac{1}{r}$.

The wavefunction must look like



The amplitude of ψ outside r_2 represents the probability of observing α-decay.

amplitude here is small because of exponential decay in the CF

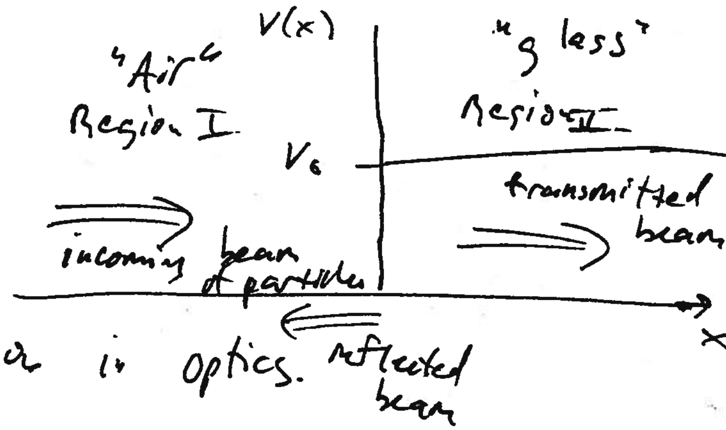
The escape of the α-particle is an example of "QM tunneling" passing through a barrier

α-decay was the first problem in nuclear physics which was explained by QM.

Potential Step

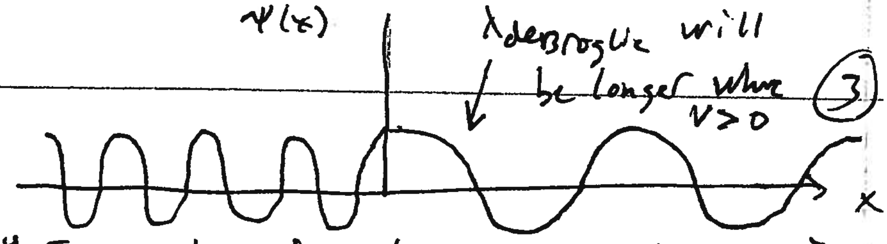
$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x > 0 \end{cases}$$

This is the QM equivalent to ~~a change~~ a change in the index of refraction in optics.



~~Trans~~

We imagine a beam of particles striking the barrier from the left. How much is transmitted, and how much is reflected?



Two Cases

1 $E > V_0$ "Everywhere is classically allowed"

Assume $\psi_{incoming} = Ae^{ikx}$ ← incoming momentum eigenstate, our initial condition

Region I: $\psi_1'' = -k_1^2\psi_1$, $k_1^2 = \frac{2m}{\hbar^2}E$

Region II: $\psi_2'' = -k_2\psi_2$, $k_2^2 = \frac{2m}{\hbar^2}(E-V_0)$

incoming beam

$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ ← reflected beam, travelling to the left. ~~a beam ... incoming~~

$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$

transmitted beam

← this represents a beam travelling to the left in Region II. We assume $D = \emptyset$.

These wavefunctions are momentum eigenstates, which are un-normalizable. So we consider A, B, C, & D to represent the relative intensities of these beams.

Boundary Conditions

(i) $\psi_1(x=0) = \psi_2(x=0) \implies A + B = C$

(ii) $\psi_1'(x=0) = \psi_2'(x=0) \implies k_1(A-B) = k_2C$

Solution: $2k_1A = (k_1+k_2)C$ $\quad(k_1$ (ii) + (i)$)$

$$\boxed{C = \left(\frac{2k_1}{k_1+k_2}\right)A} \quad \& \quad \boxed{B = \left(\frac{k_1-k_2}{k_1+k_2}\right)A}$$

relative incoming amplitude

Suppose there is no potential step: $V_0 = \phi$.
Then $k_1 = k_2$ & $B = \phi \Rightarrow$ no reflected beam
$C = 1 \Rightarrow$ 100% transmission.

/ → Finish here

Probability Current

We can define a "probability current" $\vec{J}$ which is analogous to electric current. Where $J > \phi$, a particle probability is increasing to the right. Where $J < \phi$, particle probability is increasing to the left

We define in 1D $J \equiv \frac{\hbar}{2mi}\left(\psi^* \psi' - \psi \psi^{*\prime}\right)$

(see Homework #10 for the motivation).

For the simple step,

$$J_{incoming} = \frac{\hbar}{2mi}\left(2ik_1|A|^2\right) = \frac{\overset{\hbar k_1}{p_1}}{m}|A|^2$$

$$J_{transmitted} = \frac{\hbar k_2}{m}|C|^2$$

$$J_{reflected} = -\frac{\hbar k_1}{m}|B|^2$$

Define the Transmission Coefficient & Reflection Coefficient:

$$T \equiv \frac{|J_{transmitted}|}{|J_{incoming}|} = \frac{k_2}{k_1}\left|\frac{C}{A}\right|^2 = \frac{4k_1k_2}{(k_1+k_2)^2} = \frac{4(k_2/k_1)}{(1+k_2/k_1)^2}$$

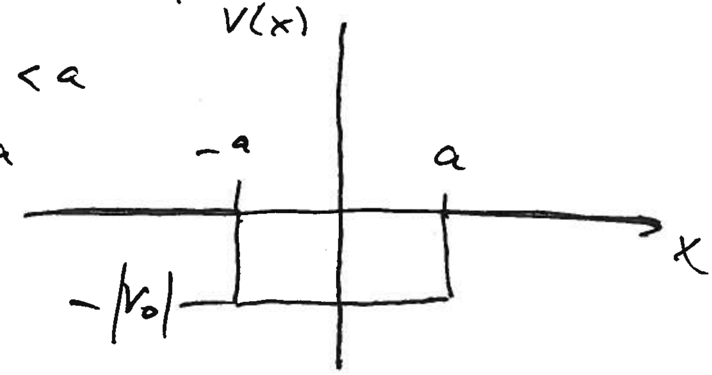
$$R \equiv \frac{|J_{reflected}|}{|J_{incoming}|} = \left|\frac{B}{A}\right|^2 = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{(1-k_2/k_1)^2}{(1+k_2/k_1)^2}$$

Also note that if $E = V_0$, then $k_2 = \phi$, & $T = \phi$, 100% refl

Finite Square Well

If the infinite square well was an artificial potential function, then the finite square well is a step towards a more realistic potential.

$$V(x) = \begin{cases} -|V_0| & \text{for } -a < x < a \\ \emptyset & \text{for } |x| > a \end{cases}$$

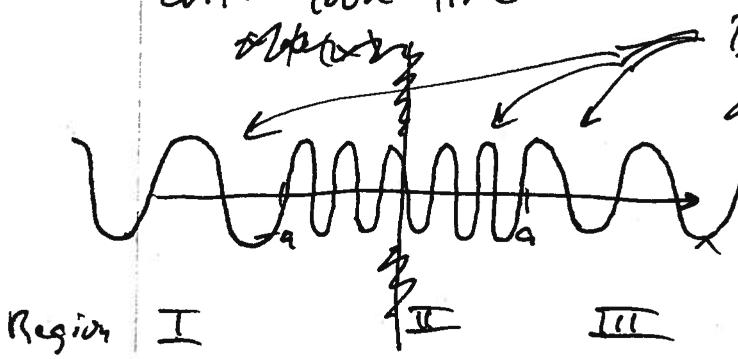


Case 1 $E > 0 \Rightarrow$ Everywhere is classically allowed.

We call these solutions $(E>0)$ "scattering states", since for $E>0$, no bound state will exist.

Again we imagine a beam of particles approaching from ~~-∞~~ $x = -\infty$ (moving to the right.)

In terms of DeBroglie wavelength, the solution will look like:

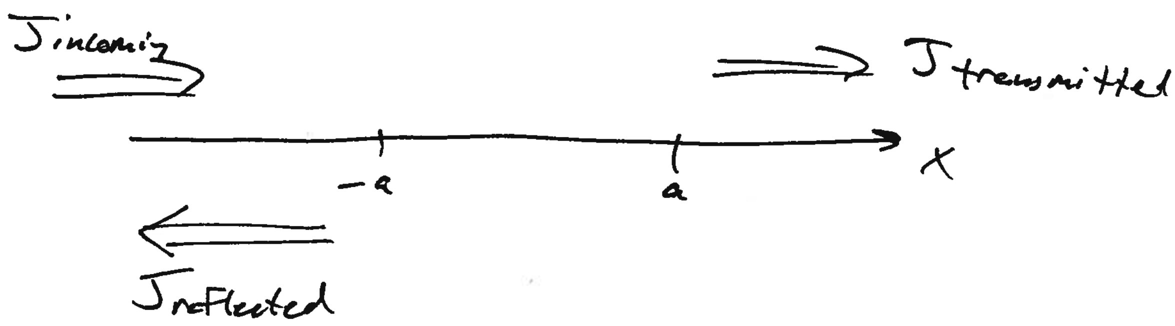


But the relative amplitudes are determined by the TDSE & the boundary conditions:

① ψ is continuous

② ψ' is continuous

In terms of Probability Currents we have



The Finite Square Well is a good 1st model to use for

- electrons scattering on atoms (at least the 1-D version of this)
- electrons in a metal scattering on an impurity atom
- a neutron scattering on a proton or other nucleus.

Solution:

incoming beam / reflected beam

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad \text{as usual}, \quad k^2 = \frac{2m}{\hbar^2}(E)$$

$$\psi_{II}(x) = Ce^{igx} + De^{-igx}, \quad g^2 \equiv \frac{2m}{\hbar^2}(E + |V_0|)$$

$$\psi_{III}(x) = Fe^{ikx} + \phi$$

transmitted beam; no left-moving beam in Region III

Boundary Conditions:

$$\psi_I(x=-a) = \psi_{II}(x=-a)$$

$$\psi_{II}(x=a) = \psi_{III}(x=a)$$

$$\psi_I'(x=-a) = \psi_{II}'(x=-a)$$

$$\psi_{II}'(x=a) = \psi_{III}'(x=a)$$

Applying these 4 boundary conditions, we can find $B, C, D, \& F$ in terms of A

Again, $T \equiv \left|\frac{J_{trans}}{J_{inc}}\right| = \left|\frac{F}{A}\right|$ & $R \equiv \left|\frac{J_{ref}}{J_{inc}}\right| = \left|\frac{B}{A}\right|$ & $T + R = 1$.

Result (from Griffiths)

$$T = \frac{1}{1 + \frac{|V_0|^2}{4E(E+|V_0|)} \sin^2\left[\frac{2a}{\hbar}\sqrt{2m(E+|V_0|)}\right]}$$

When the $\sin^2$ term $\to \phi$, the $T = 1 \Rightarrow$ complete transmission

This happens when no reflection.

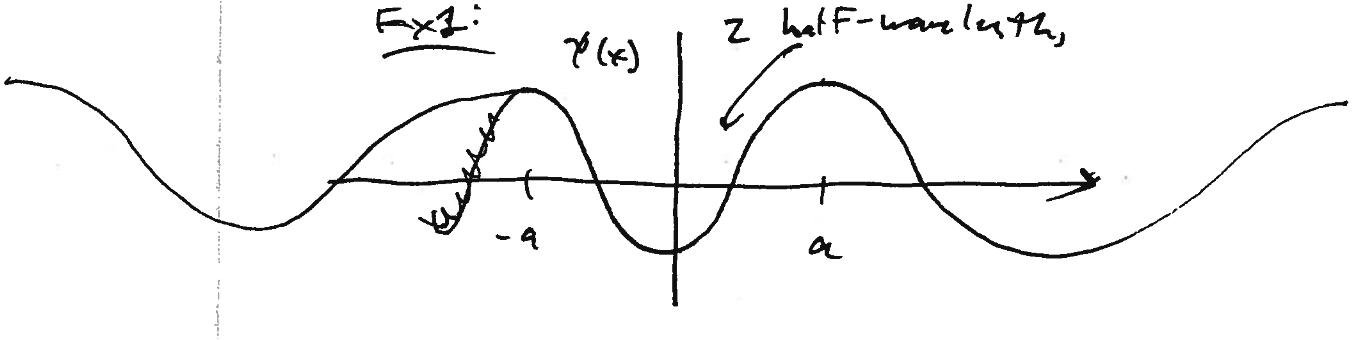
$$\frac{2a}{\hbar}\sqrt{2m(E+|V_0|)} = n\pi$$

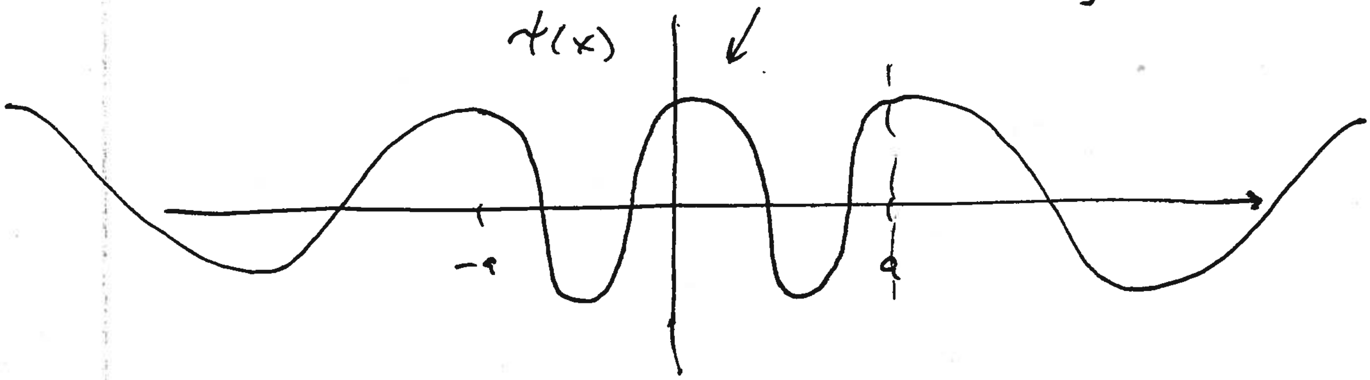
or when $E + |V_0| = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$ $\leftarrow$ condition for full transmission

If we measure energy with respect to the bottom of the well ($E' \equiv E + |V_0|$) we see that these special energies are exactly those of the infinite square well. Why?

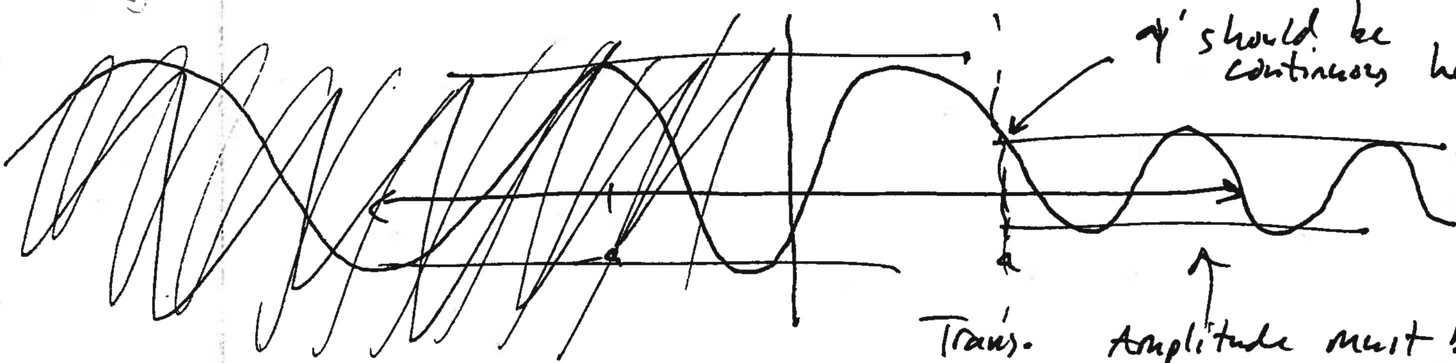
$\Rightarrow$ ~~At~~ Answer: at these energies, an integral # of half-wavelengths fit inside the well:

Ex 1:



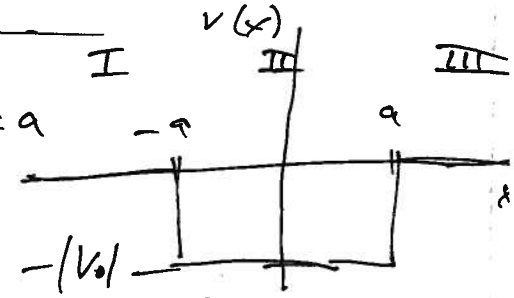


At other energies, the wavefunction crosses the boundary at the "wrong moment".



Bound States of the Finite Well

$$V(x) = \begin{cases} -|V_0| & \text{for } -a < x < a \\ \emptyset & \text{for } |x| > a \end{cases}$$



We've looked at the scattering states (we found the Transmission Coefficient, for example). Now lets look for Bound states.

Case 2: $E < 0$ but $E > -|V_0|$ (bound states)

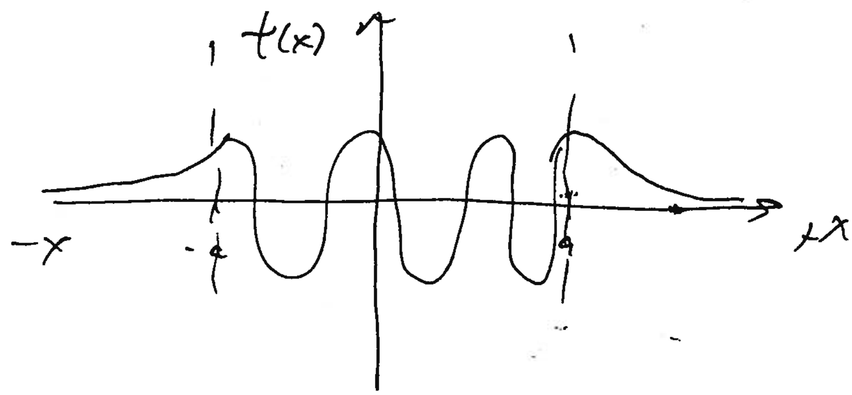
Region I: (Classically Forbidden) $\psi'' = \kappa^2 \psi$, $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$ ($E<0$, so κ is real)

"kappa"

Region II: (Classically Allowed) $\psi'' = -k^2\psi$, $k = \frac{\sqrt{2m(E+|V_0|)}}{\hbar}$

Region III: Classically Forbidden $\psi'' = \kappa^2 \psi$ again

Roughly speaking, $\psi(x)$ will be something like



<u>Theorem</u>: If $V(x)$ is an even function, then the energy eigenstates will be <u>even</u> and/or <u>odd</u> functions. (Homework #10)

<u>Even Solutions</u> "Solutions with positive Parity"

$$\varphi(x) = \begin{cases} Fe^{-\kappa x} + Ge^{\kappa x}, & x > a \\ D\cos(kx), & -a < x < a \\ Fe^{\kappa x}, & x < -a \end{cases}$$

$G = 0$, because this term blows up

re-order

Continuity of φ at $x = a$:

$$Fe^{-\kappa a} = D\cos(ka) \qquad ①$$

Continuity of φ' at $x = a$:

$$-\kappa Fe^{-\kappa x} = -Dk\,\cancel{\cos}\,\sin(ka) \qquad ②$$

Divide ② by ①:

$$\boxed{\kappa = k\tan(ka)}$$

← This equation determines the energy eigenvalues, because κ & k are both functions of E:

$$\cancel{\frac{\sqrt{-2mE}}{\hbar} = \frac{\sqrt{2m(E+V_0)}}{\hbar}\tan}$$

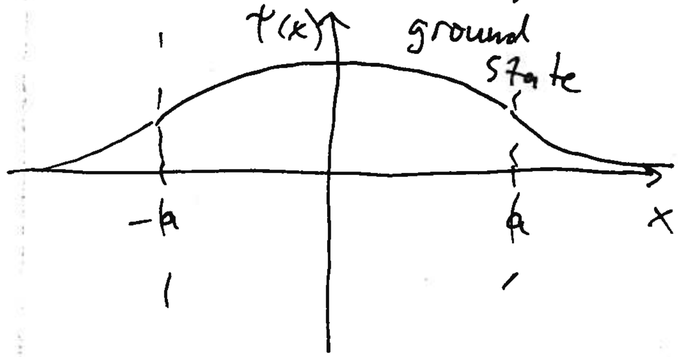
$$\kappa(E) = k(E)\tan\left[k(E)a\right]$$

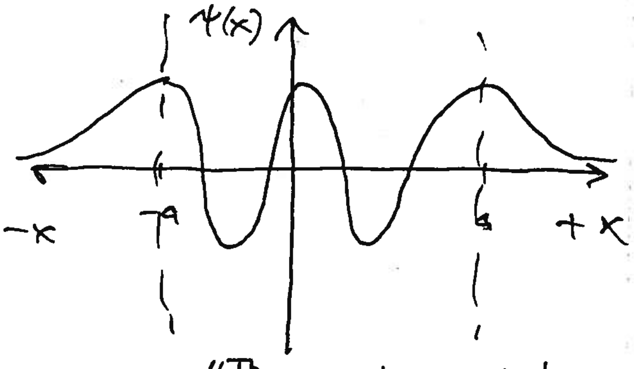
This is a trancendental Eq. for E, it cannot be solved algebraically. Must use a numerical technique

Some properties:

- There is always at least one solution
  $\Rightarrow$ there is always at least one bound state with even parity

- If the well is deep and/or wide (a large and or $|V_0|$ large), there will be many solutions. The higher solutions correspond to "fitting more wiggles" in the the ~~[illegible]~~ CAR:





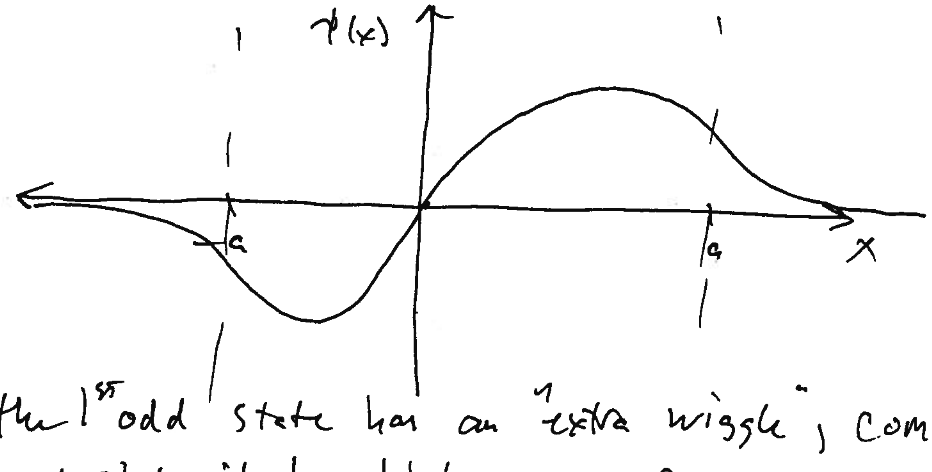
- For any finite a & finite $|V_0|$, there are a finite number of bound states.

Odd Solution "Solutions with negative Parity"

Result:
$$\psi(x) = \begin{cases} -Fe^{\kappa x}, & x<-a \\ D\sin(kx), & -a<x<a \\ Fe^{-\kappa x} & x>a \end{cases}$$

Eigenvalue Eq: $k\cot(ka) = -\kappa$.

1st odd state (if it exists)



Since the 1st odd state has an "extra wiggle", compared to the ground state it has higher energy. Depending on a & $|V_0|$

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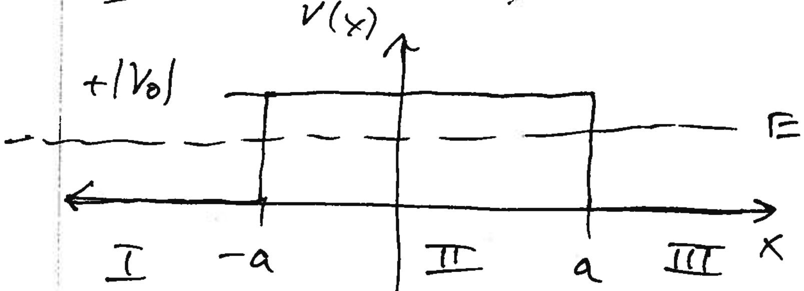
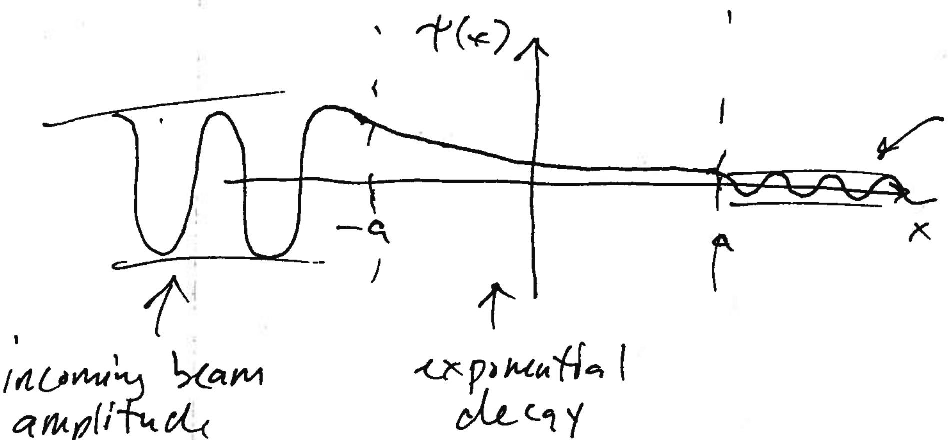
Square Barrier



Suppose ~~E~~ $0 < E < |V_0|$. Then Region I & III are Classically Allowed, But R II is Classically Forbidden

Scattering states: ~~E~~ particle is not bound. Solutions will look like (for a beam travelling to the right:



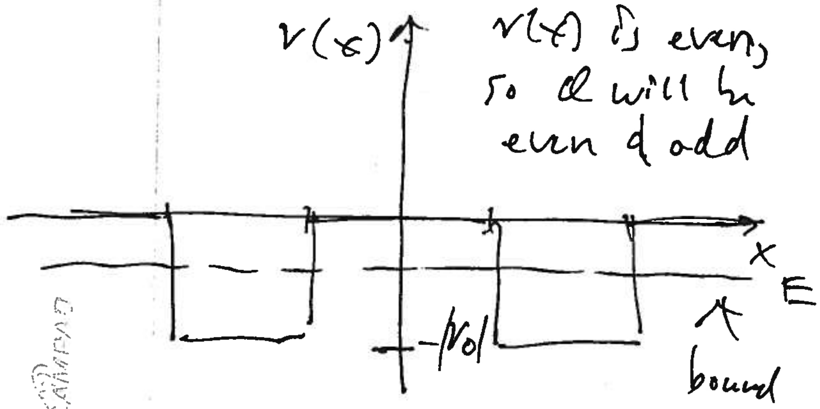
- Classically, no particles should penetrate the barrier. But QM allows some penetration. This is another example of "QM tunneling". (Alpha-decay is similar).
- The exact amplitudes in each region are constrained by require ψ & ψ' to be continuous at $x = a$ & $x = -a$.
- A similar phenomena happens in optics. When light reflects off a barrier where there should be 100% reflection, such as ~~[illegible]~~ when total internal reflection should occur, If the barrier thickness is small,

Summary of "Rules" for 1-D wave mechanics

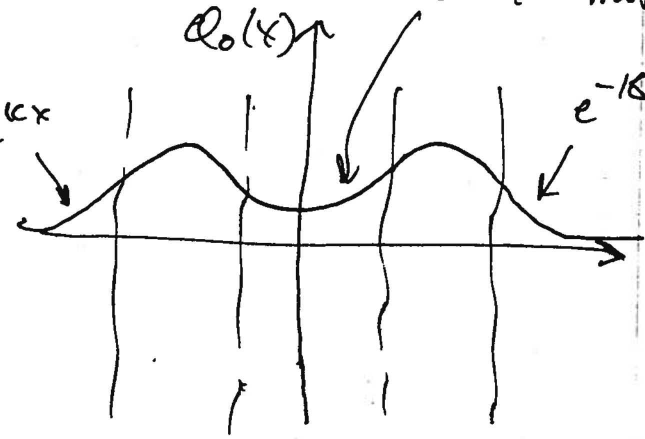
- Where $E > V(x)$ (KE is positive), ψ ~~oscillates~~ ~~oscillates~~ oscillate.
- Where $E < V(x)$ (KE is negative), ψ decays
- Where KE is large, wavelength is short
- " small, " long.
- ψ & ψ' are continuous where $V(x)$ is finite.
- ψ'' will be discontinuous where $V(x)$ changes suddenly
- The amplitudes of ψ in various regions are constrained by the requirement of continuity of ψ & ψ'.
- For bound states we look for normalizable wavefunctions.
- For free-particle states we often "accept" un-normalizable wavefunctions. Usually we calculate beam currents using the J vector.
- For bound states, the ground state has the minimum number of wiggles. Excited states have more wiggles.
- If $V(x)$ is an even function of x, we look for $\psi_n(x)$ to be even & odd functions of x.

Double square well

V(x) is even, so ψ will be even & odd



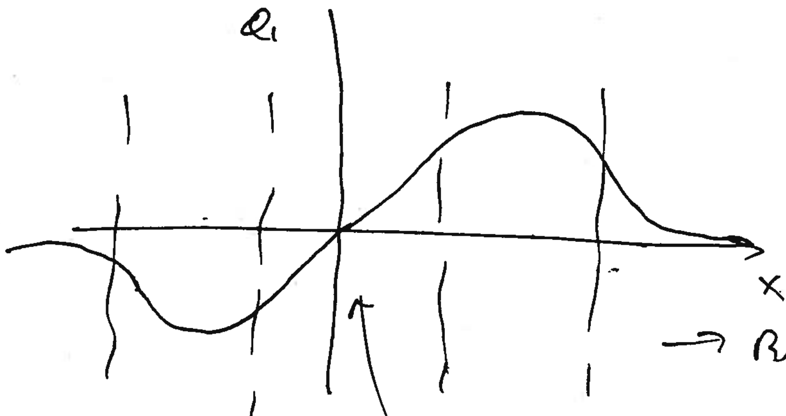
Ground: even function



Should decay here, but ψ should be even like a cosh(x) function:

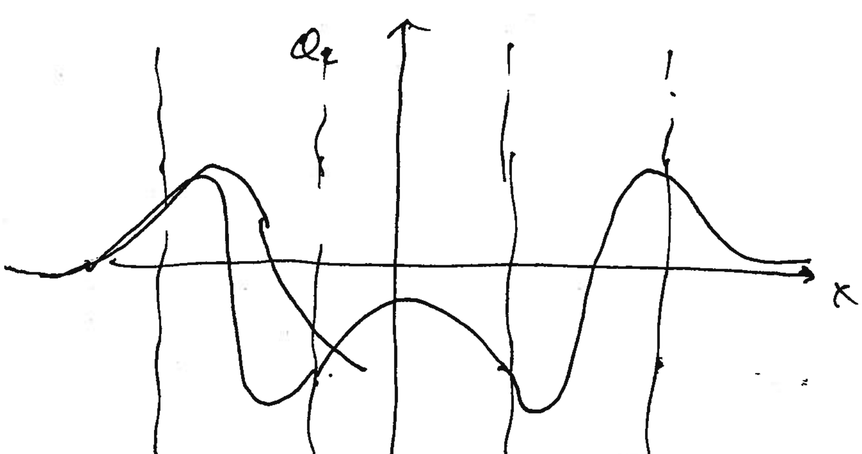
$\cosh(x) = \frac{1}{2}\left(e^{-\kappa x} + e^{\kappa x}\right)$

1st excited: odd function

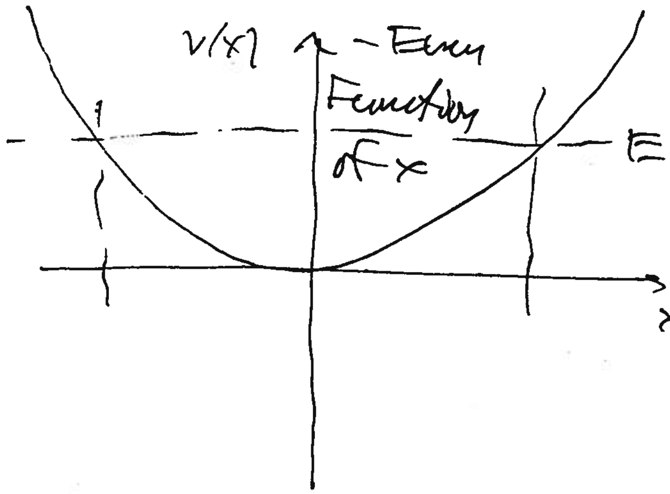


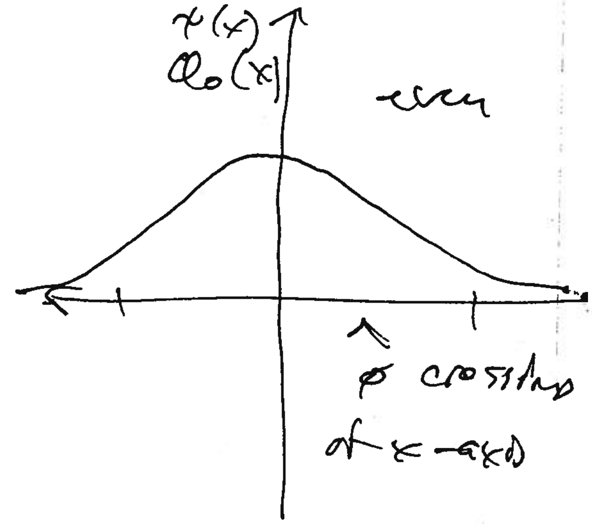
→ Remember, ψ_1 might not exist at all if $|V_0|$ is small or if the wells are very narrow.

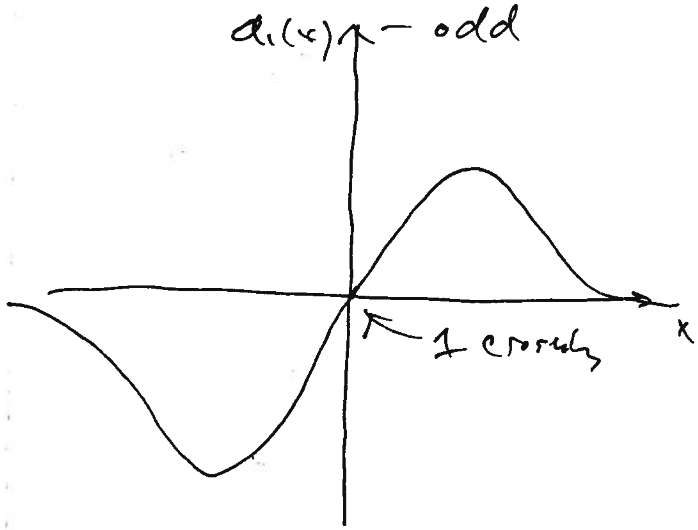
2nd excited: even function

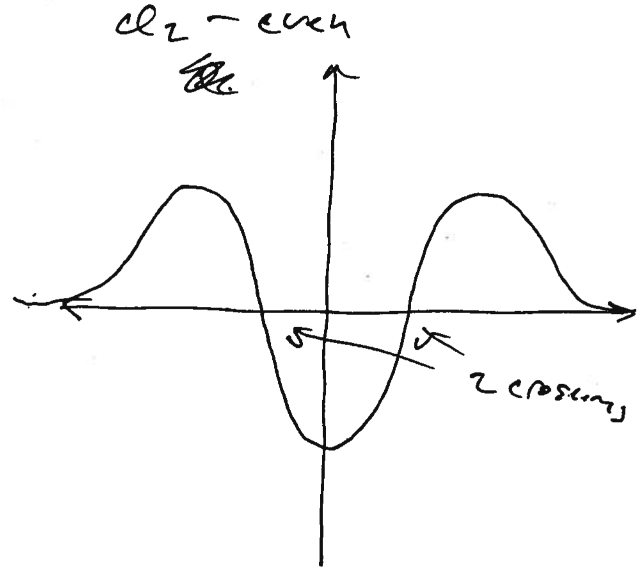


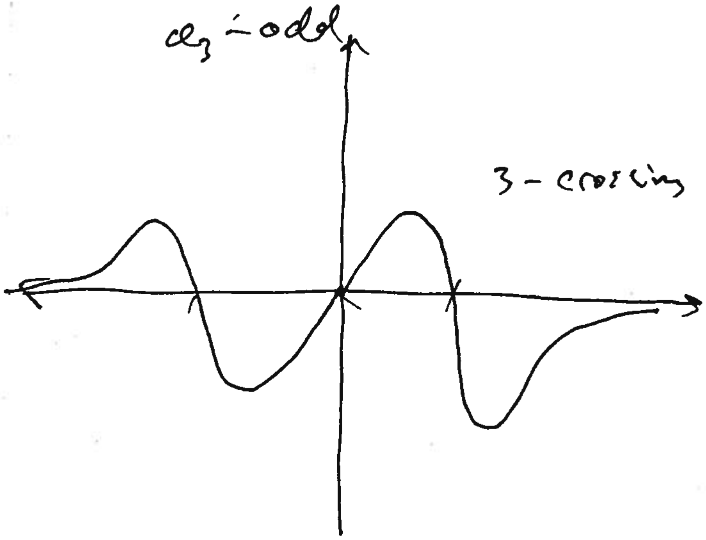
Harmonic Oscillator

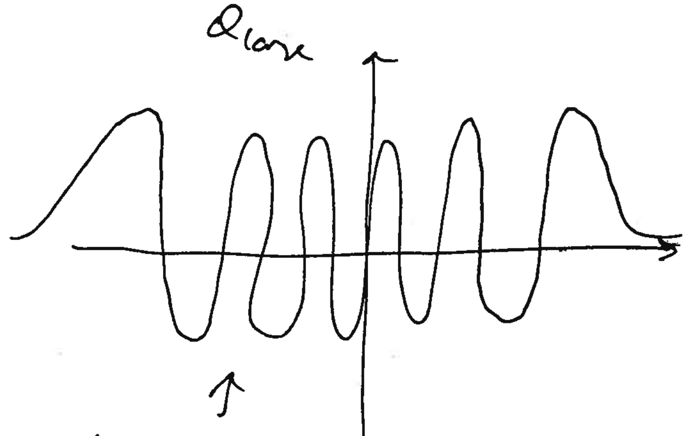












λ continuously changes because $V(x)$ continuously changes (E - KE continuously