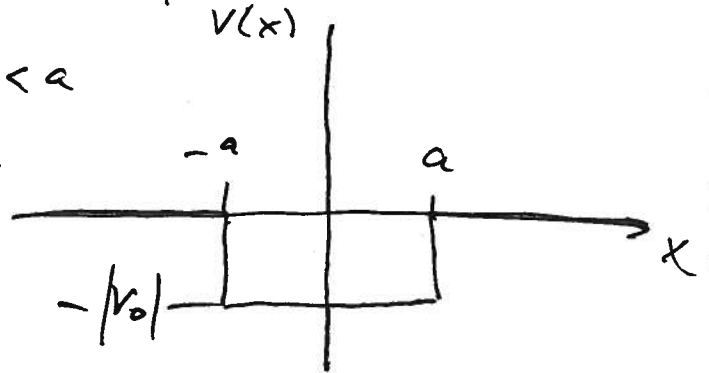


Finite Square Well

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

$$V(x) = \begin{cases} -|V_0| & \text{for } -a < x < a \\ 0 & \text{for } |x| > a \end{cases}$$



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.

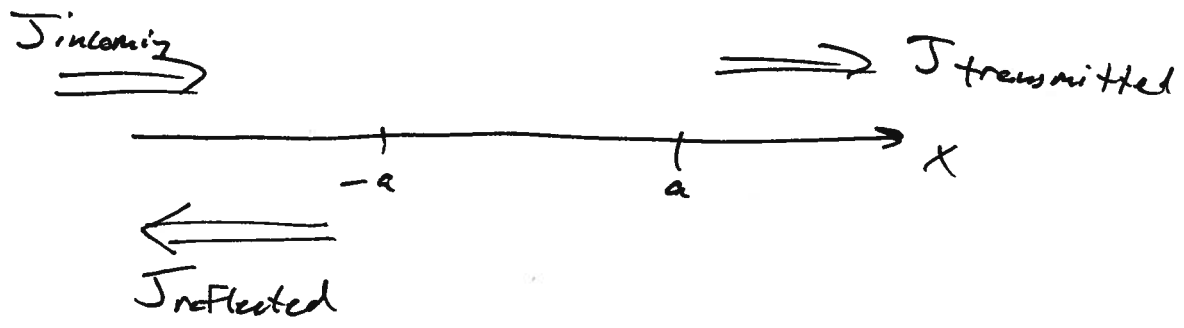
Again we imagine a beam of particles approaching from $x = -\infty$ (moving to the right.)

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 that)
- electrons in a metal scattering on an impurity atom
- a neutron scattering on a proton or other nucleus.

Solution:

incoming beam
reflected beam

↓
↓

$$\psi_I(x) = A e^{ikx} + B e^{-ikx} \text{ as usual, } k^2 = \frac{2m}{\hbar^2} (E)$$

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

$$\psi_{III}(x) = F e^{ikx} + \emptyset$$

↑
↑

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

$$\text{Again, } T \equiv \left| \frac{J_{\text{trans}}}{J_{\text{inc}}} \right| = \left| \frac{E}{A} \right| \quad \& \quad R \equiv \left| \frac{J_{\text{ref}}}{J_{\text{inc}}} \right| = \left| \frac{B}{A} \right| \quad \& \quad T+R=1 \quad (3)$$

Result (from Griffiths)

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

When the \sin^2 term $\rightarrow 0$, then $T=1 \Rightarrow$ Complete transmission

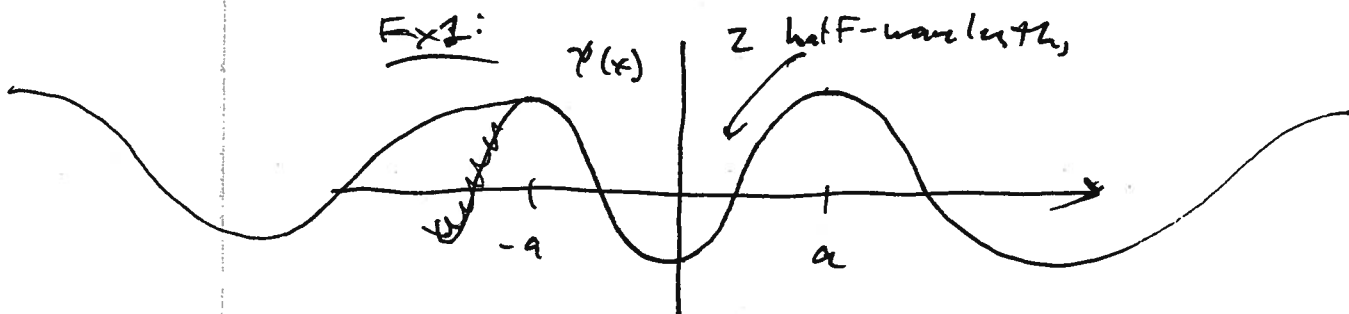
This happens when \leftarrow no reflection.

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

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

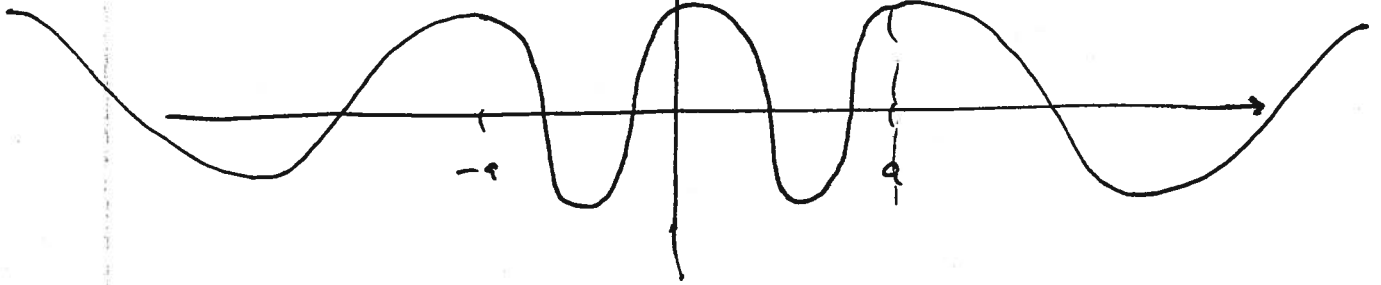
If we measure energy with respect to the bottom of the well ($E' \equiv E+|V_0|$) we see that these ^{special} energies are exactly those of the infinite square well. Why?

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

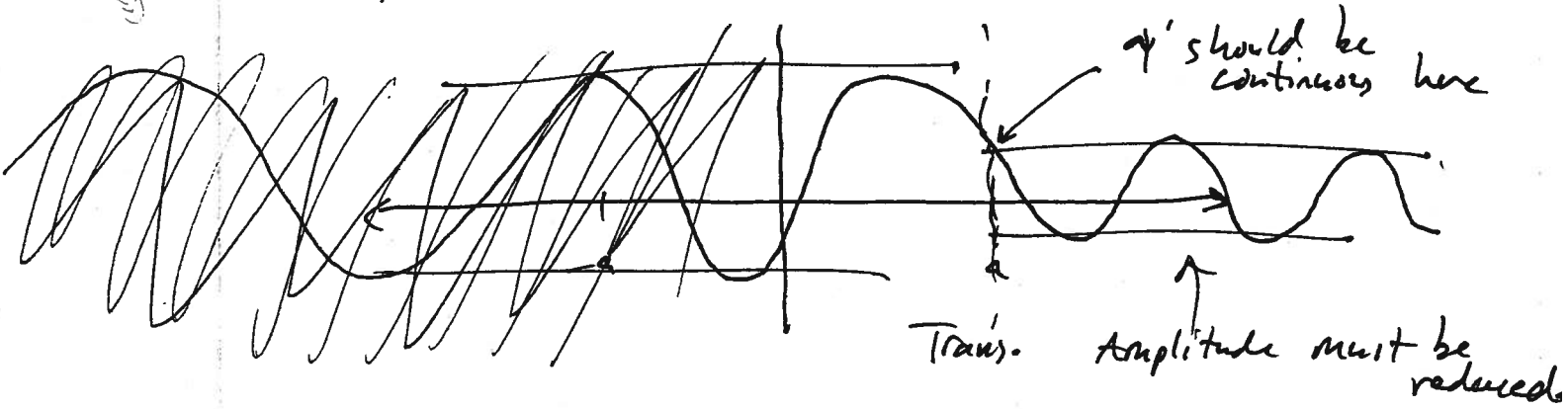


ψ half-wavelengths

$\psi(x)$

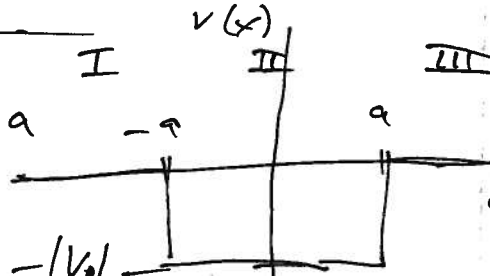


At other energies, the wavefunction ψ crosses the boundary at the "wrong moment".



~~ψ(x)~~

Bound States of the Finite Well

$$V(x) = \begin{cases} -|V_0| & \text{for } -a < x < a \\ 0 & \text{for } |x| > a \end{cases}$$


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

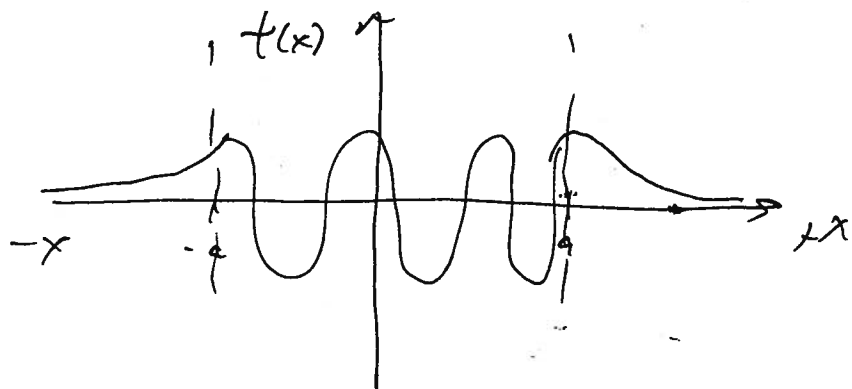
Case 2: $E < 0$ (bound states)
but $E > -|V_0|$

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

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

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

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



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

(Homework #10)

Even Solutions "Solutions with positive Parity"

$\psi(x) = \begin{cases} F e^{-kx} + G e^{kx}, & x > a \\ D \cos(kx), & -a < x < a \\ F e^{kx}, & x < -a \end{cases}$

order

$G = 0$, because this term blows up

Continuity of ψ at $x = a$:

$$F e^{-ka} = D \cos(ka) \quad (1)$$

Continuity of ψ' at $x = a$:

$$-k F e^{-ka} = -D k \sin(ka) \quad (2)$$

Divide (2) by (1):

$$\boxed{k = k \tan(ka)} \leftarrow \text{This equation determines the energy eigenvalues, because } x \text{ \& } k \text{ are both functions of } E$$

~~$k(E) = k(E) \tan[k(E)a]$~~

$$k(E) = k(E) \tan[k(E)a]$$

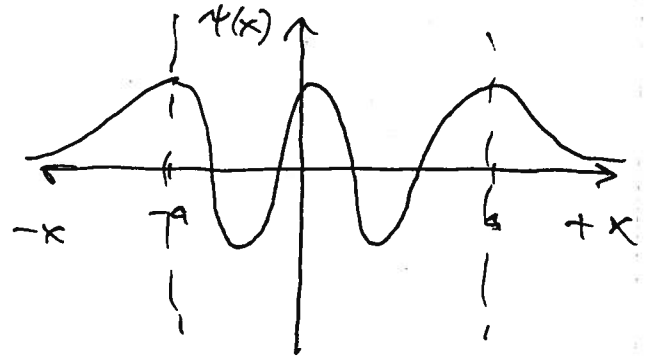
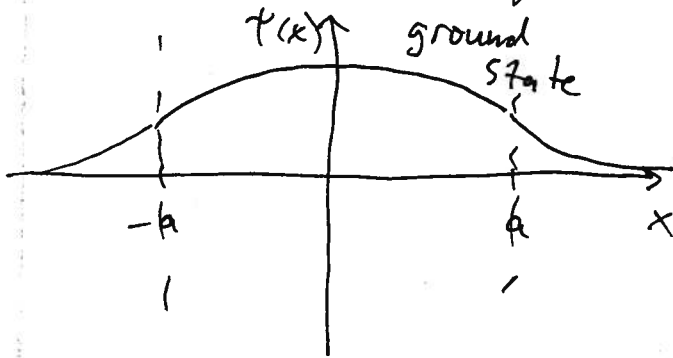
This is a transcendental Eq. for E , it cannot be solved algebraically. Must use a numerical technique

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 high solutions correspond to "fitting more wiggles" in the well. ~~the~~ CAR.



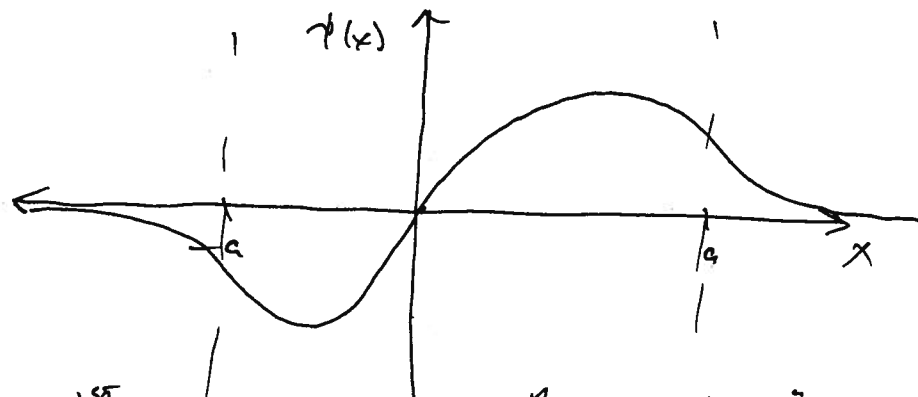
- For any finite a & finite $|V_0|$, there are a finite number of bound states.

Odd Solutions "Solutions with negative parity"

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

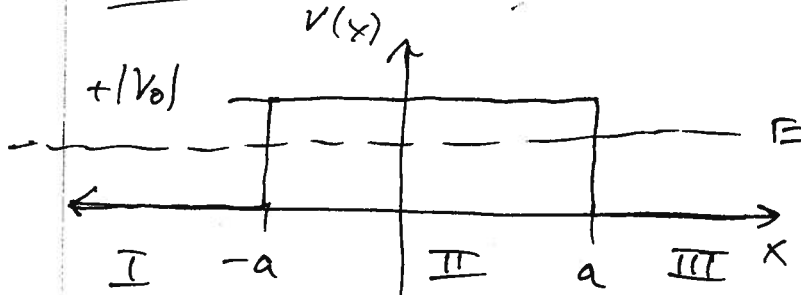
Eigenvalue Eq: $k \cot(ka) = -\kappa$.

1st odd state (if it exists)



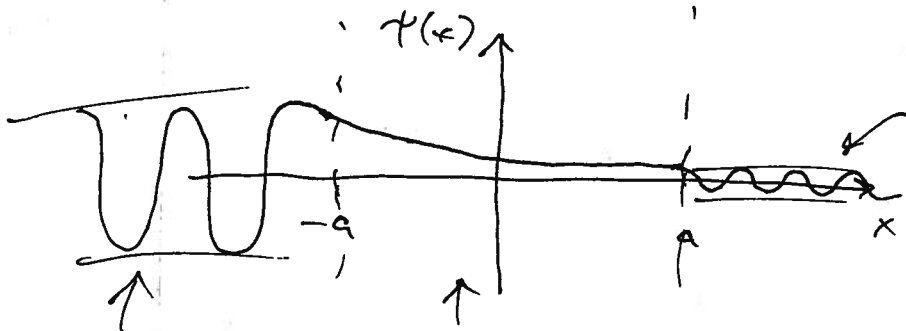
Since the 1st odd state has an "extra wiggle", compared to the ground state it has higher energy. Depending on a & $|V_0|$

Square Barrier



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

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



↑ incoming beam amplitude

↑ exponential decay

amplitude is smaller on output side due to exponential decay in Region II

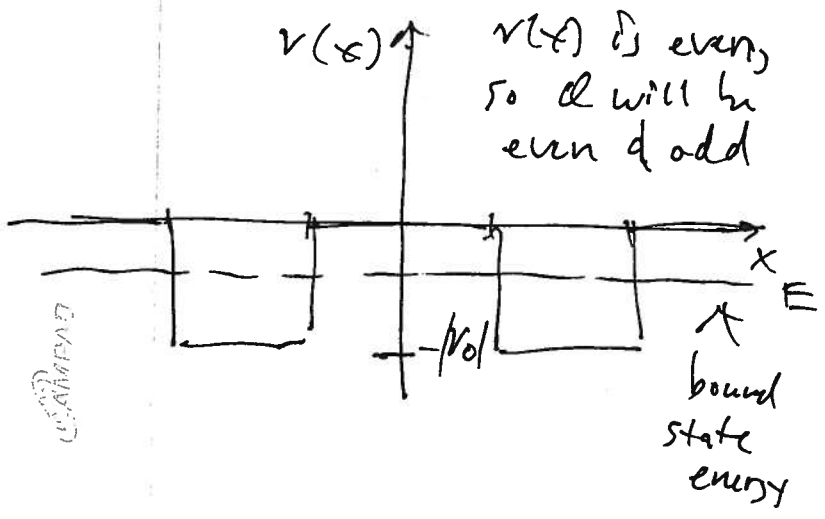
- Classically, no particles should penetrate the barrier. But QM allows some penetration. This is another example of "QM tunneling". (Alpha-decay is similar).
- The exact amplitudes in each region are constrained by require ψ & ψ' to be continuous at $x = a$ & $x = -a$.
- A similar phenomena happens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

Summary of "Rules" for 1D wave mechanics

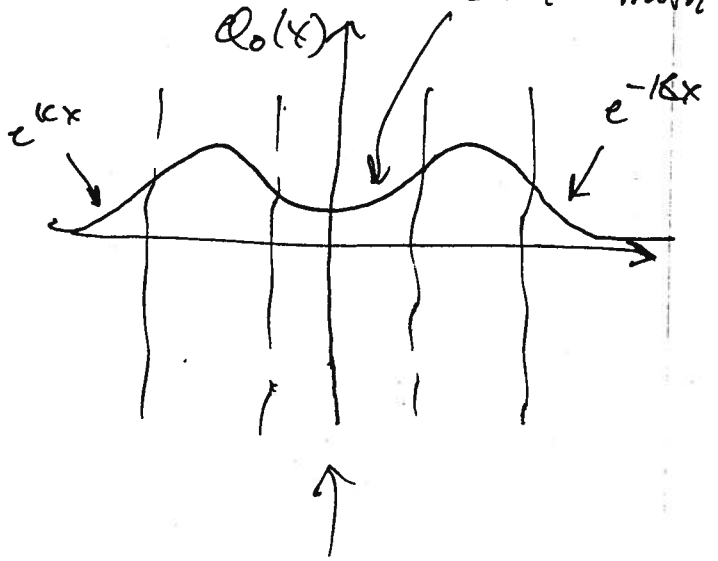
- Where $E > V(x)$ (KE is positive), ψ oscillates
- Where $E < V(x)$ (KE is negative), ψ decays
- Where KE is large, wavelength is short
- " " " small, " " long.
- ψ & ψ' are continuous where $V(x)$ is finite.
- ψ'' will be discontinuous where $V(x)$ changes suddenly
- The amplitudes of ψ in various regions are constrained by the requirement of continuity of ψ & ψ' .
- For bound states we look for normalizable wavefunctions.
- For free-particle states we "accept" ^{often} 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 .

EXERCISE

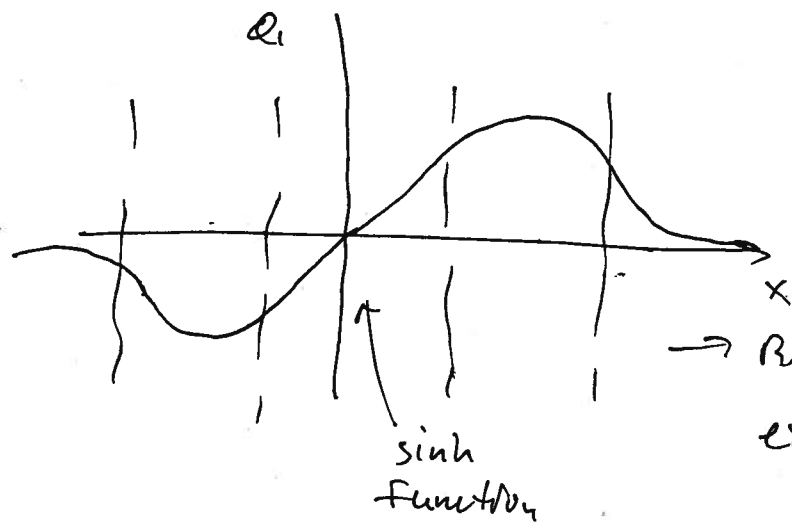
Double square well



Ground: even function
Cosh function



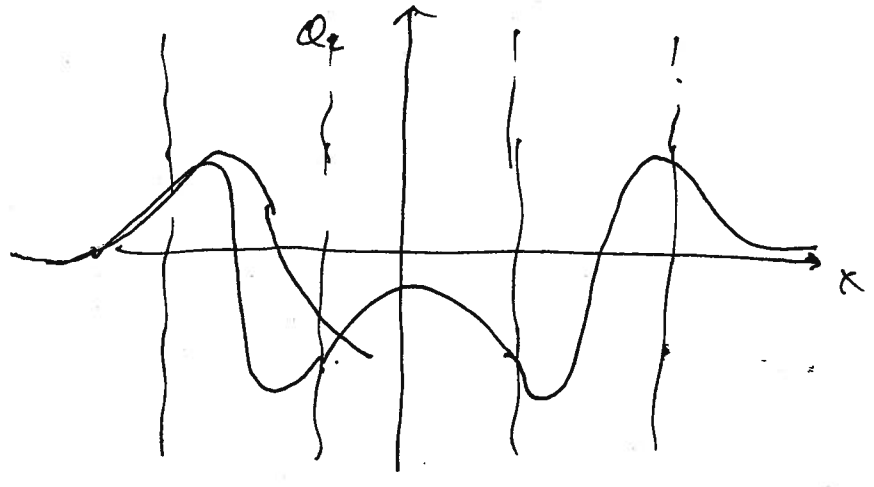
1st excited: odd function



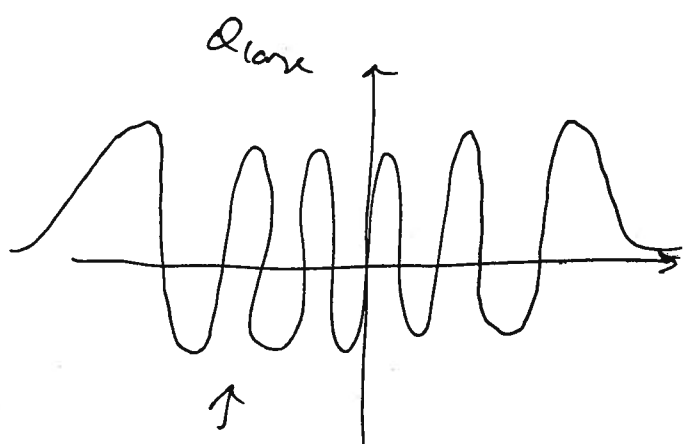
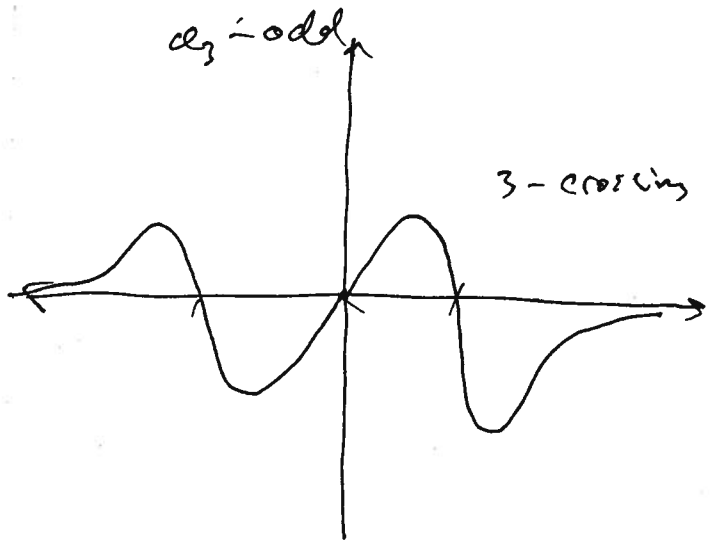
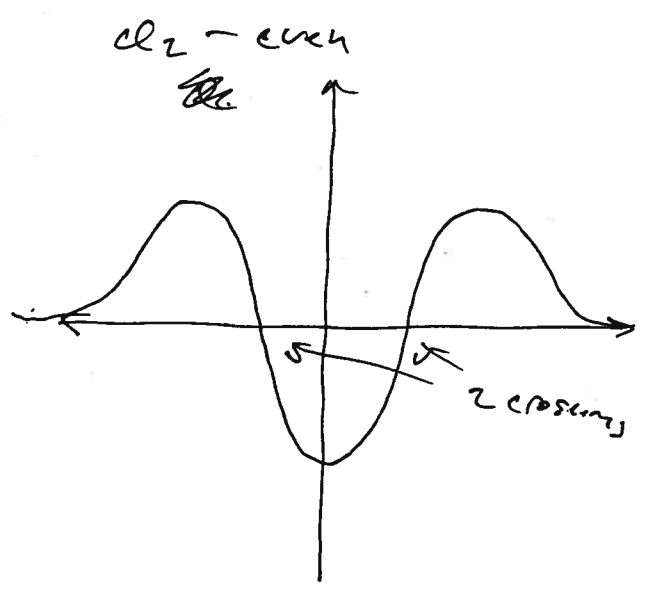
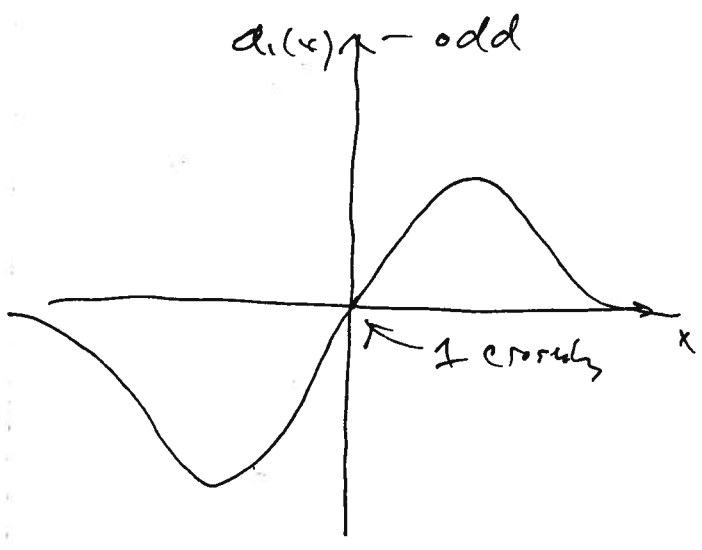
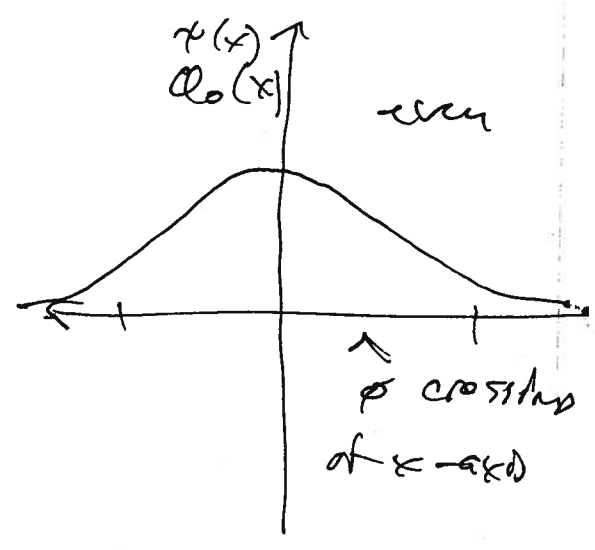
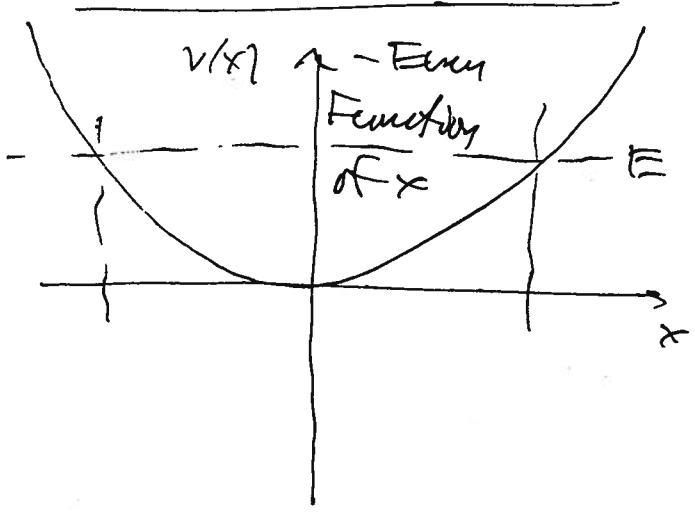
Should decay here, but ψ should be even
Use a cosh(x) function:
$$\cosh(x) = \frac{1}{2}(e^{-kx} + e^{kx})$$

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)

SANTIAO