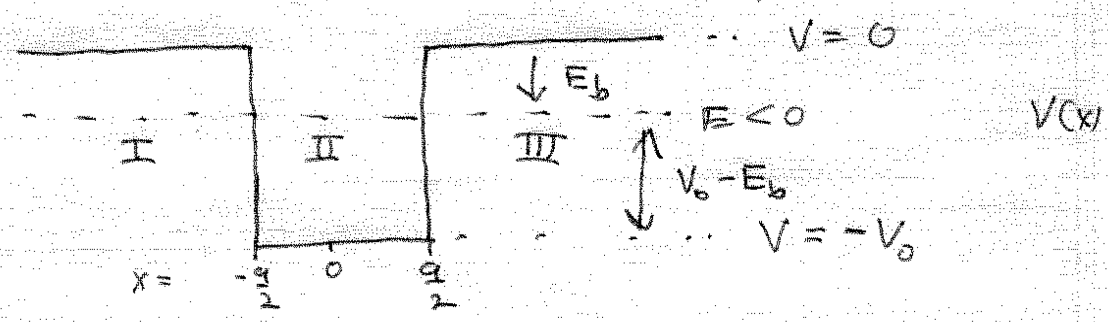
Lecture 13: Bound States for 1D potentials

Symmetric potential Well

Last lecture we considered the potential



With the zero of potential energy as chosen above, the bound states have $E<0$. The "binding energy" is defined $E_b = -E$.

The solutions to the T.I.S.E. come in two forms:

"Even parity": $u_{Even}(-x) = u_{Even}(x)$ reflection symmetric

"Odd parity": $u_{odd}(-x) = -u_{odd}(x)$ reflection anti-sym.

Thus the solutions are

Even: $u^{II}_{even}(x) = A\cos kx$, $u^{I}_{even}(x) = u^{III}_{even}(-x) = Be^{-\kappa x}$

Odd: $u^{II}_{odd}(x) = A\sin kx$, $u^{I}_{odd}(x) = -u^{III}_{odd}(-x) = Be^{-\kappa x}$

where $k = \sqrt{\frac{2m}{\hbar^2}(V_0 - E_b)}$ $\kappa = \sqrt{\frac{2m}{\hbar^2} E_b}$

- We have two independent boundary conditions.

  Continuity of u ~~and~~ at $x = a/2$

  Continuity of $\frac{du}{dx}$ at $x = -a/2$

  and three unknowns A, B, E_b

- The b.c.'s can be used to solve for two of them. We solve for B and E_b. The final constant A is set by normalization $\int_{-\infty}^{\infty} dx\, |u(x)|^2 = 1$

Solving for the energy eigenvalues

Combine the two b.c.'s into the "logarithmic" derivative

$$\frac{1}{u^{II}(\frac{a}{2})} \left.\frac{du^{II}}{dx}\right|_{\frac{a}{2}} = \frac{1}{u^{III}(\frac{a}{2})} \left.\frac{du^{III}}{dx}\right|_{a/2}$$

Even parity: $\left(\frac{1}{A\cos\frac{ka}{2}}\right)\left(-kA\sin\left(\frac{ka}{2}\right)\right) = \frac{1}{Be^{-\kappa a/2}}\left(-\kappa Be^{-\kappa a/2}\right)$

$$\Rightarrow \boxed{\frac{\kappa a}{2} = \frac{ka}{2}\tan\left(\frac{ka}{2}\right)}$$ transcendental eqn for E_b for even parity

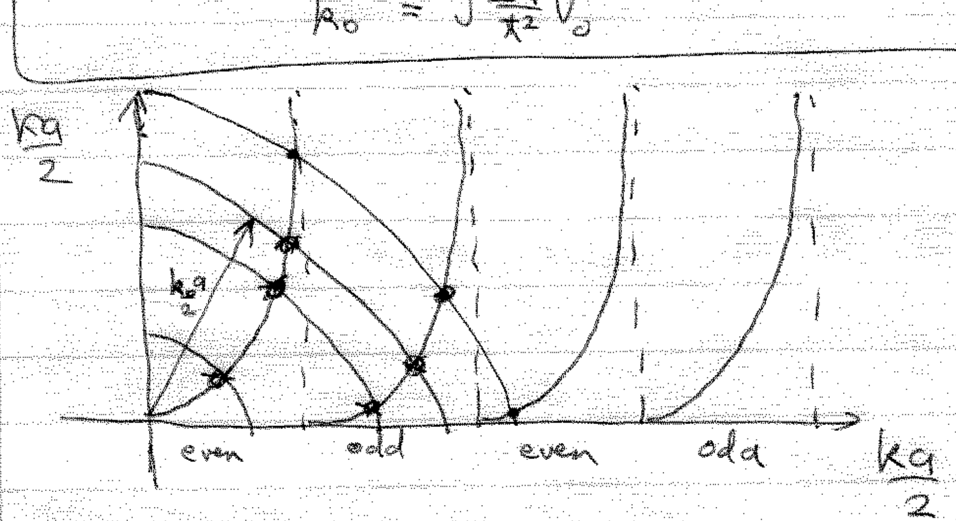
Odd parity: $\frac{1}{(A\sin\frac{ka}{2})}\left(kA\cos\left(\frac{ka}{2}\right)\right) = \frac{1}{Be^{-\kappa a/2}}\left(-\kappa Be^{-\kappa a/2}\right)$

$$\Rightarrow \boxed{\frac{\kappa a}{2} = -\frac{ka}{2}\cot\left(\frac{ka}{2}\right)}$$ eqn. for odd parity

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

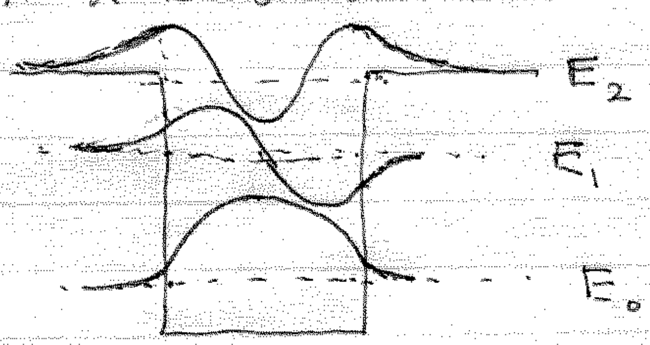
Graphical solution for different V_0

$$k_0 = \sqrt{\frac{2m}{\hbar^2} V_0}$$



The intersection points represent the solution for a given potential depth V_0

A sketch is shown for three a bound-state solutions



Note: I have changed convention here and labeled the states $n = 0, 1, 2, 3$ etc.
ground state, first excited state

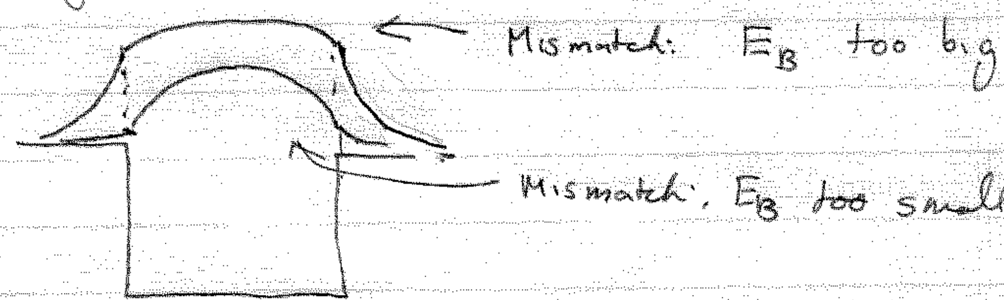
Notes:
- Unlike the ∞-well we cannot find the energy eigenvalues analytically
- The wavefunction is smooth an extends into the classically forbidden region. Penetration into that region is less for larger binding energies
- The ground state has no nodes, and the n^{th} excited state has n nodes

General properties of solutions to the T.I.S.E (1D)

- The restriction of the possible energy eigenvalues is determined by the boundary conditions.

– Boundstates: Must go to zero at infinity

$\Rightarrow$ Only discrete possible energies



– Each excited state will have one more node no matter what shape of 1D well

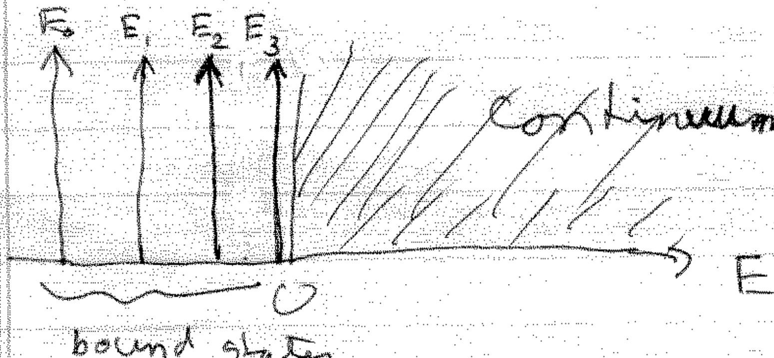
(Only possible way to satisfy b.c.'s)

– Unbound states: stationary state Wave function magnitude

$\Longrightarrow$ Constant as $|x| \to \infty$

$\therefore$ No restriction on E for unbound states

General spectrum

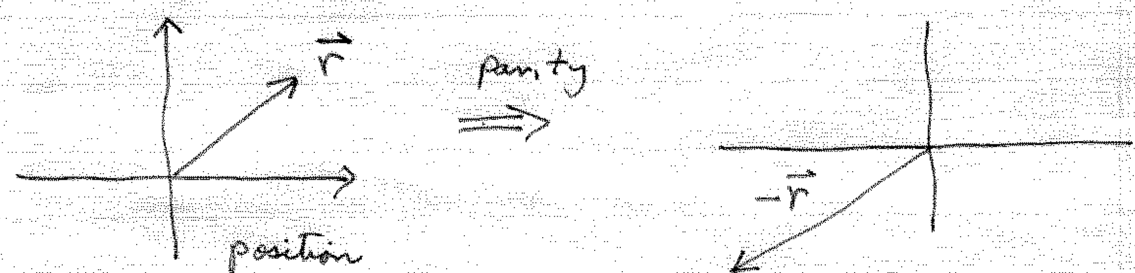


Parity: A discrete symmetry

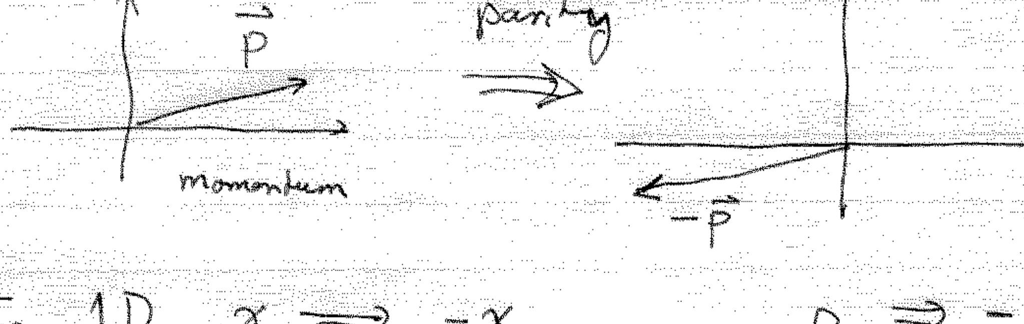
We saw that the energy eigenfunctions for the symmetric finite square well satisfies

$$\underbrace{u(x) = u(-x)}_{\text{reflection symmetric}} \quad \text{or} \quad \underbrace{u(x) = -u(-x)}_{\text{reflection anti-symmetric}}$$

This is an example of the symmetry "parity". Generally, parity refers to inversion of all coordinates through the origin



2D picture



In 1D $\quad x \underset{\text{parity}}{\Longrightarrow} -x \qquad\qquad p \underset{\text{parity}}{\Longrightarrow} -p$

In Quantum mechanics this is implemented by a "symmetry operator" (much more on this next semester)

Parity operator $\equiv \hat{\Pi}$

$$\hat{\Pi} : \hat{x} \Rightarrow -\hat{x}$$

$$\hat{\Pi} : \hat{p} = \hat{\Pi} : \frac{\hbar}{i}\frac{\partial}{\partial x} \Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial(-x)} = -\hat{p}$$

$$\hat{\Pi} : \Psi(x,t) = \Psi(-x,t)$$

Consider then the T.I.S.E in 1D

$$\hat{H}\, u(x) = E\, u(x)$$

$$\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right] u(x) = E\, u(x)$$

Apply Parity operator

$$\hat{\Pi} : \hat{H}\, u(x) = \hat{\Pi} : E\, u(x)$$

$$\Rightarrow \left[\frac{(-\hat{p})^2}{2m} + V(-\hat{x})\right] u(-x) = E\, u(-x)$$

$$\left[\frac{\hat{p}^2}{2m} + V(-\hat{x})\right] u(-x) = E\, u(-x)$$

For the special case $V(\hat{x}) = V(-\hat{x})$
(i.e. $V(\hat{x})$ is reflection symmetric)

$$\Rightarrow \quad \hat{H}\, u(-x) = E\, u(-x)$$

$\Rightarrow$ $u(x)$ and $u(-x) = \hat{\Pi}\, u(x)$ are eigenfunctions of $\hat{H}$ with the <u>same eigenvalue</u>

If there are <u>no degeneracies</u> then

$$u(-x) = \lambda\, u(x) \quad \text{(they must be proportional)}$$

$$\Rightarrow \quad \hat{\Pi}\, u(x) = \lambda\, u(x)$$

$\Rightarrow$ The stationary state must be an eigenstate of parity

<u>Eigenstates of parity:</u>

Note $\hat{\Pi}^2 u(x) = \hat{\Pi}\, u(-x) = u(x)$

$\Rightarrow$ $\hat{\Pi}^2$ has eigenvalue $+1$

$\Rightarrow$ $\hat{\Pi}$ has eigenvalues $+1$ and -1

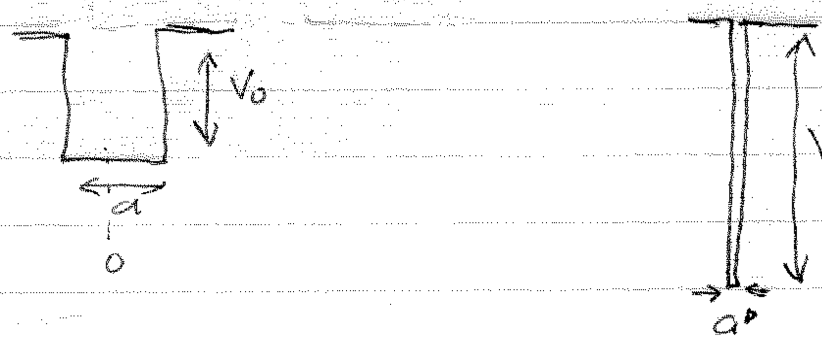
$$\hat{\Pi}\, u_{even}(x) = u_{even}(x) \qquad \hat{\Pi}\, u_{odd}(x) = -u_{odd}(x)$$

To Summarize:

$\boxed{\begin{array}{l}\text{If the } \underline{\text{Hamiltonian is invariant under parity}} \\ \quad \text{(true when the potential is parity invariant)} \\ \text{and there are no degeneracies} \\ \quad \Rightarrow \underline{\text{Stationary states are eigenstates of Parity}}\end{array}}$

The Delta-function potential

Let us consider a potential well which becomes very deep and narrow, approaching a delta-function



Let us take the limit such that $V_0 a \equiv \mathcal{V}_0$ is constant

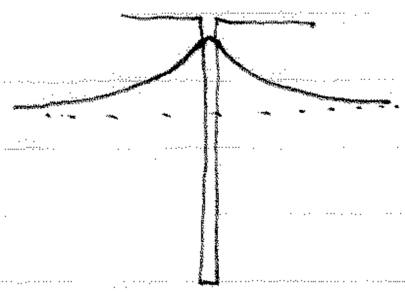
i.e. $a' V_0' = a V_0 = \mathcal{V}_0$

Then in the limit $a \to 0$ $V_0 \to \infty$ but

$$a V_0 \to \mathcal{V}_0$$

$$\boxed{V(x) = -\mathcal{V}_0\, \delta(x)} \text{ delta function potential}$$

If there is at least one bound state, it is the limit of the ground state of the finite well



Now to solve ~~this~~ the T.I.S.E with $V(x) = V_0 \delta(x)$ we need to think carefully about the boundary condition at $x = 0$. Because $V(x) \to \infty$ at $x = 0$ the derivative of $u(x)$ will be discontinuous.

To see how the dervative changes across the delta-function. let us integrate the T.I.S.E. from $x = -\epsilon$ to $x = \epsilon$

$$\int_{-\epsilon}^{\epsilon} dx \left(\hat{H} u(x) \right) = \int_{-\epsilon}^{\epsilon} E u(x) \, dx$$

$$\Rightarrow \int_{-\epsilon}^{\epsilon} dx \left(\frac{-\hbar^2}{2m} \frac{d^2 u}{dx^2} - V_0 \delta(x) u(x) \right) = E \int_{-\epsilon}^{\epsilon} u(x) \, dx$$

$$\Rightarrow \underbrace{-\frac{\hbar^2}{2m} \int_{-\epsilon}^{+\epsilon} dx \frac{d^2 u}{dx^2}}_{-\frac{\hbar^2}{2m}\left(\left.\frac{du}{dx}\right|_{+\epsilon} - \left.\frac{du}{dx}\right|_{-\epsilon} \right)} - V_0 u(0) = E \int_{-\epsilon}^{\epsilon} u(x) \, dx$$

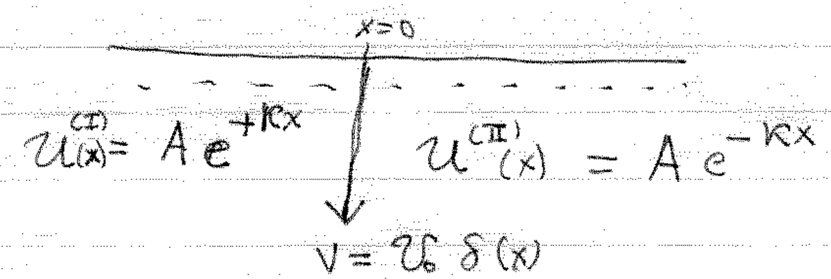
Now take the limit as $\epsilon \to 0$

If $u(x)$ does not blow up $\int_{-\epsilon}^{\epsilon} u(x) \, dx \to 0$

$\therefore$ The change in derivative across the singularity is

$$\boxed{\lim_{\epsilon \to 0} \left. \frac{du}{dx} \right|_{-\epsilon} - \left. \frac{du}{dx} \right|_{+\epsilon} = \frac{2m\mathcal{V}_0}{\hbar^2} u(0)}$$

We can now solve for the eigenfunctions and eigenvalues of the Hamiltonian



even parity

where $\kappa = \sqrt{\frac{2mE_b}{\hbar^2}}$

$$\Rightarrow \lim_{\epsilon \to 0} \left(\kappa A e^{\kappa \epsilon} - \left(-\kappa A e^{-\kappa\epsilon} \right) \right) = 2\kappa A = \frac{2m\mathcal{V}_0}{\hbar^2} A$$

$$\therefore \quad \boxed{\kappa = \frac{m\mathcal{V}_0}{\hbar^2}}$$

Binding energy: $\quad \frac{m\mathcal{V}_0}{\hbar^2} = \sqrt{\frac{2mE_b}{\hbar^2}}$

$$\Rightarrow \quad \boxed{E_b = \frac{m\mathcal{V}_0^2}{2\hbar^2}}$$

<u>Note:</u> Only <u>one</u> bound state. Odd parity is impossible single $u(x)$ would be discontinuous. Only one even parity solution.

Solution: One bound state

$$u(x) = A\, e^{-\kappa |x|}, \quad \boxed{\kappa = \frac{m V_0}{\hbar^2}}$$

$$\boxed{E = -E_b = -\frac{m V_0^2}{2\hbar^2} = -\frac{(\hbar\kappa)^2}{2m}}$$

to find this coefficient, use normalization condition.

$$\underline{1} = \int_{-\infty}^{\infty} |u(x)|^2\, dx = |A|^2 \int_{-\infty}^{\infty} dx\, e^{-\kappa|x|} = 2|A|^2 \int_0^{\infty} dx\, e^{-\kappa x}$$

$$= 2|A|^2 \left(\frac{e^{-\kappa x}}{-\kappa} \right)_0^{\infty} = \frac{2|A|^2}{\kappa} = 1$$

$$\Longrightarrow |A| = \sqrt{\frac{\kappa}{2}} = \sqrt{\frac{m V_0}{2\hbar^2}}$$

$$\Longrightarrow \boxed{u(x) = \sqrt{\frac{\kappa}{2}}\, e^{-\kappa|x|}}$$