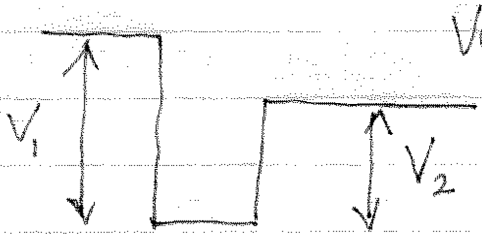
Lecture 12: Solutions to the T.I.S.E.: Piecewise constant potentials in 1D

So far we have considered only two problems: the free particle and the particle in a 1D box of infinite depth. We now extend our repetoir to more general problems. A particular class which is easy to deal with conceptually is piecewise constant potentials

E.g.



Remember, the choice of zero potential energy does not effect any of the physical predictions. To see this in Q.M. consider the T.D.S.E.

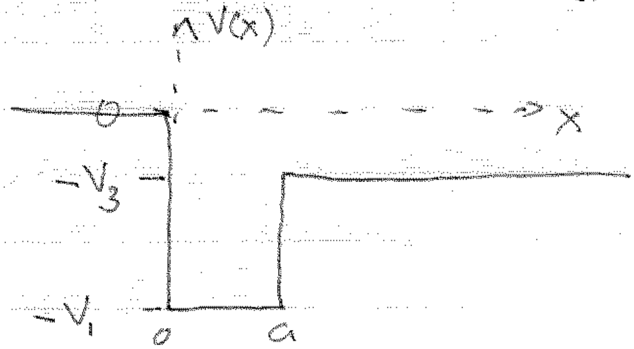
$$\frac{\hbar}{-i}\frac{\partial}{\partial t}\psi = \hat{H}\psi$$

If $\hat{H} \Rightarrow \hat{H}+V_0$ (add a constant everywhere) then the solution $\psi \Rightarrow \psi e^{-iV_0 t}$. But, this overall phase does not effect any probabilities.

Generally, we will take the zero of potential at $x=+\infty$ or $x=-\infty$

Example: $$V(x) = \begin{cases} 0 & -\infty < x < 0 \\ -V_1 & 0 < x < a \\ -V_3 & a < x < +\infty \end{cases}$$

(where $V_3 = V_2 - V_1$



In any region where the potential has a constant value V_c so that the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V_c$,

the T.I.S.E. in that region is

$$\hat{H} u_E = E u_E \Rightarrow \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_c\right) u_E(x) = E\, u_E(x)$$

$$\Rightarrow \frac{d^2 u_E}{dx} + \left(\frac{2m(E - V_c)}{\hbar^2}\right) u_E(x) = 0$$

Classically, the momentum in a region with potential V_c is $p_c = \sqrt{2m(E - V_c)}$. In Q.M. we cannot talk about "momentum in a region of space" since momentum and position are incompatible observables. Nonetheless, we often speak of a "local wave number"

$$k_c = \frac{p_c}{\hbar} = \sqrt{\frac{2m(E - V_c)}{\hbar^2}}$$

The T.I.S.E. in the region with $V(x) = V_c$ is then

$$\frac{d^2 u_E}{dx} + k_c^2 u_E = 0$$

This diff'eqn is of a familiar form.
We must consider two cases:

- $\underline{E > V_c}$ (classically allowed region) $\Rightarrow$ $\underline{k_c \text{ real}}$

$$u_E(x) = A e^{ik_c x} + B e^{-ik_c x}$$

- $\underline{E < V_c}$ (classically forbidden region) $\Rightarrow$ $\underline{k_c \text{ imaginary}}$

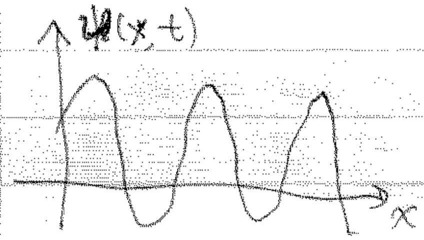
Let $\kappa_c = i k_c \Rightarrow \kappa = \sqrt{\frac{2m}{\hbar^2}(V_c - E)}$

$$u_E(x) = A e^{-\kappa_c x} + B e^{+\kappa_c x}$$

Thus, whereas the region $E < V_c$ is classically forbidden, in Q.M. there is a finite probability to find the particle here.
We see here important general features of the T.I.S.E.

<u>Classically allowed</u>: Propagating Waves

$$\mathrm{Re}\left(A e^{ik_c x} e^{-i\omega_c t}\right) = C \cos(k_c x - \omega_c t + \phi)$$

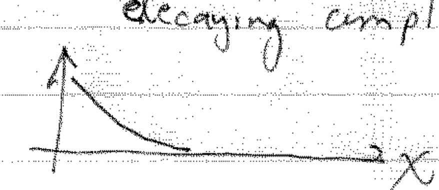


<u>Classically forbidden</u>: Evanescent waves

$$\mathrm{Re}\left(A e^{-\kappa_c x} e^{-i\omega_c t}\right)$$

$$= C e^{-\kappa_c t} \cos(\omega_c t + \phi)$$

decaying amplitude



The solution to the T.I.S.E. is then set by the boundary conditions:

(i) $u_E(x)$ is continuous so its derivative $\frac{du_E}{dx}$ is nonsingular.

(ii) $\frac{du_E}{dx}$ is continuous so $\frac{d^2u_E}{dx^2}$ is nonsingular (unless $V(x)$ blows up somewhere)

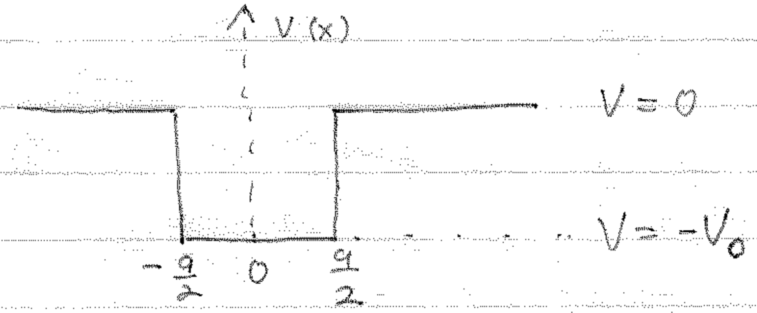
Suppose x_b denotes the boundary between two regions

$$\left.\begin{aligned} \Rightarrow \quad & u_E^{(I)}(x_b) = u_E^{(II)}(x_b) \\ \text{and} \quad & \frac{du_E^{(I)}}{dx}(x_b) = \frac{du_E^{(II)}}{dx}(x_b) \end{aligned}\right\} \Rightarrow \boxed{\frac{1}{u_E^{(I)}(x_b)} \frac{du_E^{(I)}}{dx}(x_b) = \frac{1}{u_E^{(II)}(x_b)} \frac{du_E^{(II)}}{dx}(x_b)}$$

Moreover, $u_E(x)$ cannot "blow up" (i.e. $u_E \to \pm\infty$) as $x \to \pm\infty$. Such states cannot be normalized and thus do not form proper states. These solutions are rejected. Of course, we have already seen that if $|u_E(x)| =$ Constant as $x \to \pm\infty$, these states cannot be normalized either.

However, according to the Fourier theorem, these states form a good basis set and are necessary to include in order to obtain a complete set of stationary states.

Example: The symmetric finite potential well



$$V(x) = \begin{cases} 0 & -\infty < x < -\frac{a}{2} \quad \text{(region I)} \\ -V_0 & -\frac{a}{2} < x < +\frac{a}{2} \quad \text{(region II)} \\ 0 & \frac{a}{2} < x < \infty \quad \text{(region III)} \end{cases}$$

There are two classes of solutions classically

$E > 0 \Rightarrow$ Particle unbound

$E < 0 \Rightarrow$ Particle bound

The same is true quantum mechanically. Let's consider first the <u>bound states</u>

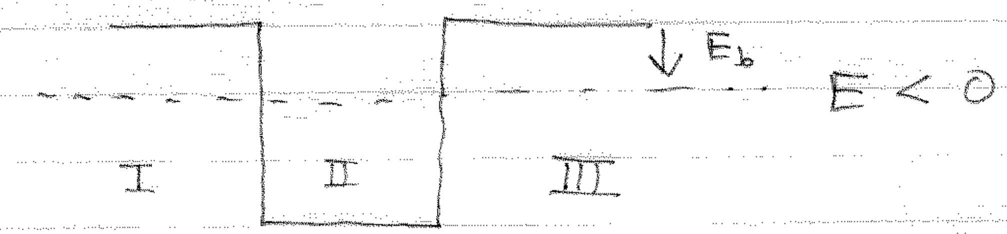
Let $E < 0$. Define $E = -E_b$ where $E_b > 0$ (binding energy)

T.I.S.E. $\Rightarrow \quad \dfrac{-\hbar^2}{2m}\dfrac{d^2u}{dx^2} + V(x)\,u = -E_b\,u$

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}\left(-E_b - V(x)\right)u = 0$$

We consider solutions in each region.

(Next Page)



Regions I and III (Classically forbidden)

Region II (Classically allowed)

Solution region I

$$\frac{d^2u^{(I)}}{dx^2} - \frac{2mE_b}{\hbar^2}u^{(I)} = 0 \qquad \text{Let } \kappa = \sqrt{\frac{2mE_b}{\hbar^2}}$$

$$\Rightarrow u^{(I)}(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

Solution region II

$$\frac{d^2u^{(II)}}{dx^2} + \left[\frac{2m(V_0 - E_b)}{\hbar^2}\right]u^{(II)} = 0 \qquad \text{let } k = \sqrt{\frac{2m(V_0 - E_b)}{\hbar^2}}$$

$$\Rightarrow u^{(II)}(x) = Ce^{ikx} + De^{-ikx}$$

Solution region III

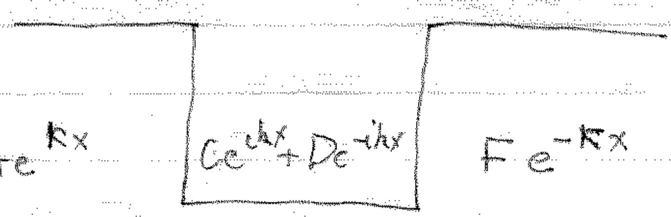
$$u^{(III)}(x) = Fe^{-\kappa x} + Ge^{+\kappa x}$$

We thus have to use the boundary conditions at $x = \pm \frac{a}{2}$ and $x = \pm\infty$ to determine the unknown constants.

Using b.c. at $x = -\infty \Rightarrow B = 0$

$x = +\infty \Rightarrow G = 0$

Otherwise the solution blows up at $\pm\infty$



B.C. Continuity of u at $\pm \frac{a}{2}$

(1) $x = \frac{a}{2}$: $\quad Ce^{ika/2} + De^{-ika/2} = Fe^{-\kappa a/2}$

(2) $x = -\frac{a}{2}$: $\quad Ce^{-ika/2} + De^{ika/2} = Ae^{-\kappa a/2}$

B.C. Continuity of $\frac{du}{dx}$ at $\pm a$

(3) $x = \frac{a}{2}$: $\quad ik\left(Ce^{ika/2} - De^{-ika/2}\right) = -\kappa F e^{-\kappa a/2}$

(4) $x = -\frac{a}{2}$: $\quad ik\left(Ce^{-ika/2} - De^{-ika/2}\right) = +\kappa A e^{-\kappa a/2}$

Multiply (1) by κ and then add to (3)

$$(ik + \kappa)Ce^{ika/2} + (-ik + \kappa)De^{-i\frac{ka}{2}} = 0$$

$$\Rightarrow \frac{C}{D} = -\left(\frac{\kappa - ik}{\kappa + ik}\right)e^{-ika}$$

Similary, Multiply (2) by κ and add to 4

$$\Rightarrow \frac{C}{D} = -\left(\frac{\kappa + ik}{\kappa - ik}\right)e^{+ika}$$

Putting these together

$\Rightarrow \quad \frac{C^2}{D^2} = 1 \quad \Longrightarrow \quad \boxed{C = \pm D}$

Two classes of solutions:

Region II

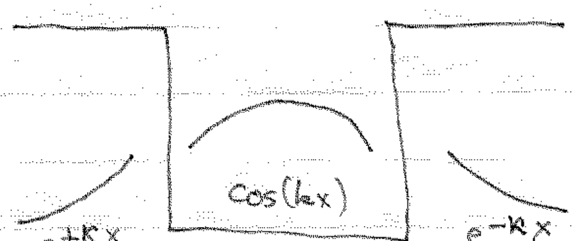
(+) "Even parity": $2C\cos(kx)$

(−) "Odd parity": $2iC\sin(kx)$

<u>For even parity</u>

- Continuity of u at $x = \pm a/2$

$$\left.\begin{array}{ll} (5)\ x = \frac{a}{2} & 2C\cos\left(\frac{ka}{2}\right) = F e^{-Ka/2} \\ (6)\ x = -\frac{a}{2} & 2C\cos\left(\frac{ka}{2}\right) = A e^{-Ka/2} \end{array}\right\} \Rightarrow A = F$$



← Sketch

In order to match all b.c.'s restriction on possible k and K $\Longrightarrow$ <u>Quantize energy</u>

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

$x = \frac{a}{2} \qquad -2Ck\sin\left(k\frac{a}{2}\right) = -KAe^{-Ka/2}$ (7)

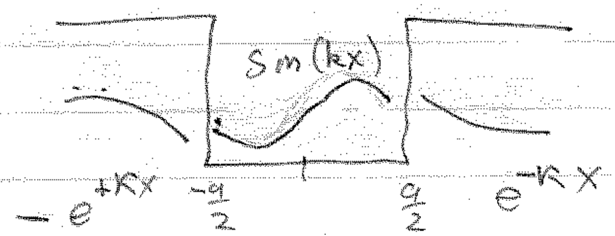
$x = -\frac{a}{2} \qquad$ (no new information)

Dividing (7) by (6)

even parity

$$\Rightarrow -k \tan \frac{ka}{2} = -\kappa \Rightarrow \boxed{\left(\frac{ka}{2}\right) \tan\left(\frac{ka}{2}\right) = \frac{\kappa a}{2}}$$

<u>For odd parity</u>



Continuity of u

$$\Rightarrow F = -A$$

Logarithmic derivative: $\frac{1}{u^{II}(\frac{a}{2})} \frac{du^{(II)}}{dx}\Big|_{\frac{a}{2}} = \frac{1}{u^{(III)}} \frac{du^{(III)}}{dx}\Big|_{\frac{a}{2}}$

$$\Rightarrow \frac{2ikC\cos\left(\frac{ka}{2}\right)}{2iC\sin\left(\frac{ka}{2}\right)} = \frac{-A\kappa e^{-\frac{\kappa a}{2}}}{A e^{-\kappa a/2}}$$

odd parity

$$\Rightarrow k \cot\left(\frac{ka}{2}\right) = \kappa \Rightarrow \boxed{\frac{ka}{2}\cot\left(\frac{ka}{2}\right) = \frac{\kappa a}{2}}$$

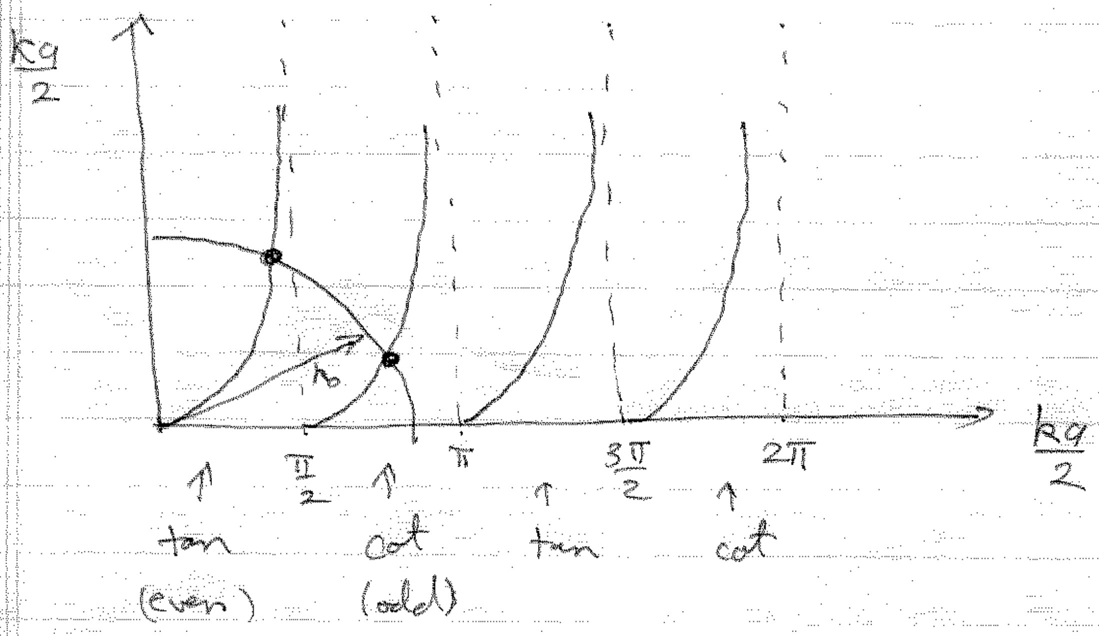
Finally we have the constraint $\kappa^2 = \frac{2mE_b}{\hbar^2}$

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

$$\Rightarrow k^2 = \frac{2m}{\hbar^2}V_0 - \kappa^2 \Rightarrow \boxed{\left(\frac{ka}{2}\right)^2 + \left(\frac{\kappa a}{2}\right)^2 = \left(\frac{k_0 a}{2}\right)^2}$$

Where $k_0 \equiv \sqrt{\frac{2mV_0}{\hbar^2}}$

These transidental equation cannot be solved analytically. We resort to numerical solution



For a given choice of k_0 (i.e. V_0) there are possible solutions shown as dots.