Physics 491

Lecture 14: Unbound States for 1D potentials

Overview: The unbound stationary states are characterized by:

- Continuum of energies
- Unnormalizable states
- Degeneracies

For example: Free particle, eigenstates

$$u_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\hat{H} u_k(x) = \frac{(\hbar k)^2}{2m} u_k(x), \qquad E_k = \frac{(\hbar k)^2}{2m}$$

all k's allowed

"Delta function normalization"

$$\langle u_k | u_{k'} \rangle = \int_{-\infty}^{\infty} dx \; u_k^*(x) \, u_{k'}(x) = \int_{-\infty}^{\infty} dx \frac{e^{i(k'-k)x}}{2\pi}$$

$$\Rightarrow \langle u_k | u_{k'} \rangle = \delta(k-k') = \begin{cases} 0 & k \neq k' \\ \infty & k = k \end{cases} \quad !$$

Contrast with discrete bound spectrum

$$\hat{H} u_n = E_n u_n \qquad E_n \text{ discrete}$$

$$\langle u_n | u_m \rangle = \underset{\substack{\uparrow \\ \text{Kronecker delta}}}{\delta_{nm}} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

<u>Degeneracy</u>: $u_k(x) = \dfrac{e^{ikx}}{\sqrt{2\pi}}$ and $u_{-k}(x) = \dfrac{e^{-ikx}}{\sqrt{2\pi}}$

have the same energy $\dfrac{(\hbar k)^2}{2m}$

> So, if all possible energies are allowed, what are we solving for?

$\Rightarrow$ <u>Scattering</u>:

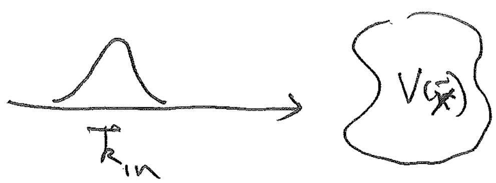
We seek the probability for the potential to scatter an incomming ~~free~~ unbound particle from one state into another.

Really wave packet:

$$\psi(\vec{x}, t) = \int d^3k \; \tilde{\psi}(\vec{k}) \; u_{\vec{k}}(\vec{x}) \; e^{-iE_{\vec{k}}t/\hbar}$$

$\tilde{\psi}(\vec{k})$: expansion coefficients

$u_{\vec{k}}(\vec{x})$: Unbound eigenfunctions



Thus, if we know the unbound eigenfunctions we know how particles scatter.

Probability Current:

Recall from lecture 5, we defined

$$\rho(\vec{x},t) \equiv |\psi(\vec{x},t)|^2 = \text{Probability density} = \frac{\text{prob}}{\text{Volum}}$$

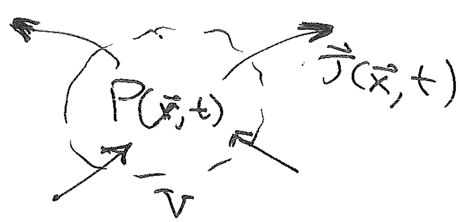
$$\vec{J}(\vec{x},t) \equiv \frac{1}{2}\left(\psi^* \frac{\hat{\vec{p}}}{m}\psi + \left(\frac{\hat{\vec{p}}}{m}\psi\right)^* \psi\right)$$

$$= \text{Im}\left(\psi^* \frac{\hbar}{m}\vec{\nabla}\psi\right) = \text{Probability current density}$$

$$= \frac{\text{prob}/\text{time}}{\text{Area}}$$

Continuity Equation: $\dfrac{\partial \rho}{\partial t} = -\vec{\nabla}\cdot\vec{J}$

or: $$\frac{d}{dt}\int_V \rho \, d^3x = \oint_S \vec{J}\cdot d\vec{a}$$



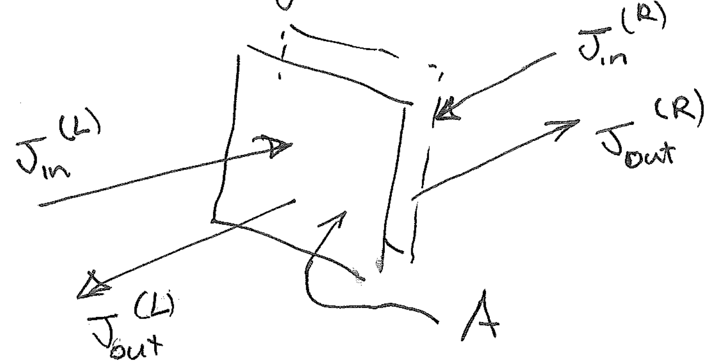
Probability to find particle in volume changes due to flow into/out of V

Stationary state $\dfrac{\partial \rho(\vec{x},t)}{\partial t} = 0$

$$\Rightarrow \quad \vec{\nabla}\cdot\vec{J} = 0$$

$$\Rightarrow \quad \oint_S \vec{J}\cdot d\vec{a} = 0$$

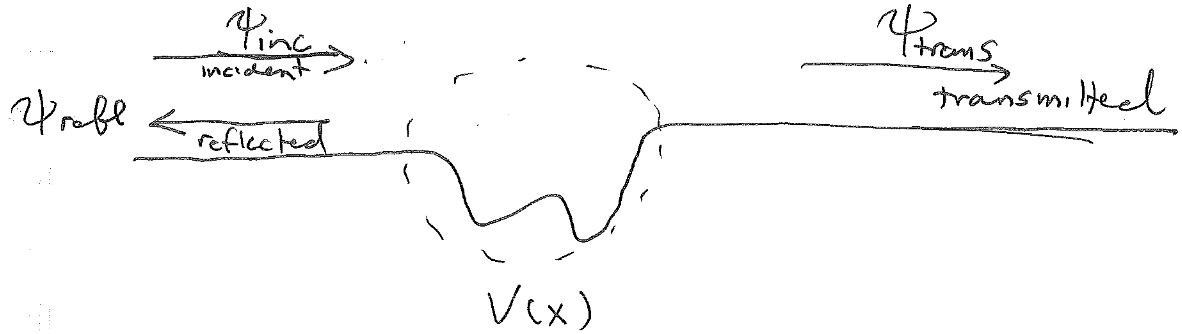
1D scattering: $J = \frac{\hbar}{m} \mathrm{Im}\left(\psi^* \frac{d\psi}{dx}\right)$



$$\oint \vec{J} \cdot da = A\left(J_{in}^{(L)} + J_{in}^{(R)} - J_{out}^{(L)} - J_{out}^{(R)}\right) \underset{\text{stationary}}{=} 0$$

$$\Rightarrow \quad J_{in}^{(L)} + J_{in}^{(R)} = J_{out}^{(L)} + J_{out}^{(R)}$$

Typically, we consider input from one direction (e.g. $J_{in}^{(R)} = 0$). Also take $V \to$ Constant at $x = \pm\infty$



Assumptotically, the incident, transmitted, and reflected waves look like plane waves

$$\psi = A e^{ikx}$$

$$J = \underbrace{\left(\frac{\hbar k}{m}\right)}_{v_{group}} |A|^2 = (v_{group})\left(\frac{\text{prob}}{\text{Volume}}\right) = \rho v$$

<u>Define:</u>

Reflection coeff: $R \equiv \dfrac{J_{ref}(\infty)}{J_{inc}(\infty)}$

Transmission coeff: $T \equiv \dfrac{J_{trans}(\infty)}{J_{inc}(\infty)}$

Continuity Eq: $J_{inc} = J_{trans} + J_{ref}$

$\Rightarrow T + R = 1$ (conservation of particles)

Assumptotic plane waves

$\psi_{inc} = A e^{ik_1 x} \longrightarrow$ $\quad V(x) \quad$ $\longrightarrow \psi_{trans} = C e^{ik_2 x}$

$\psi_{refl} = B e^{-ik_1 x} \longleftarrow$

region 1 $\qquad\qquad$ region 2

$$\Rightarrow \quad R = \frac{|B|^2 \frac{\hbar k_1}{m}}{|A|^2 \frac{\hbar k_1}{m}} = \left|\frac{B}{A}\right|^2$$

$$T = \frac{|C|^2 \frac{\hbar k_2}{m}}{|A|^2 \frac{\hbar k_1}{m}} = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1}$$

<u>Note:</u> Often $k_1 = k_2 \equiv k$. In that case

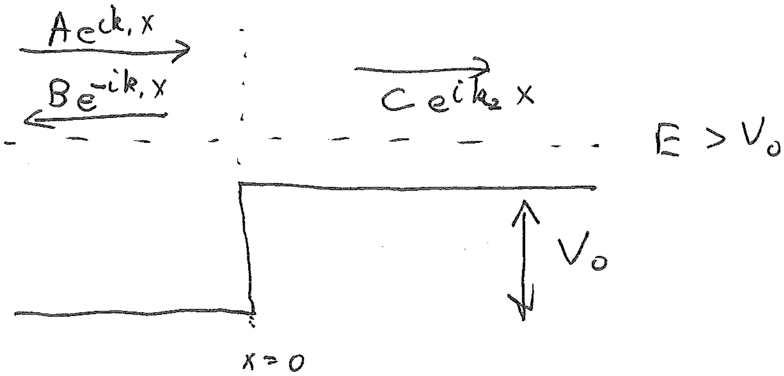
$$R = \left|\frac{B}{A}\right|^2 \quad \& \quad T = \left|\frac{C}{A}\right|^2$$

We define $\dfrac{B}{A} = r$ = <u>reflection amplitude</u>

$\dfrac{C}{A} \equiv t$ = <u>transmission amplitude</u>

Example: Step potential

Case (i): $E > V_0$



$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

Boundary conditions:

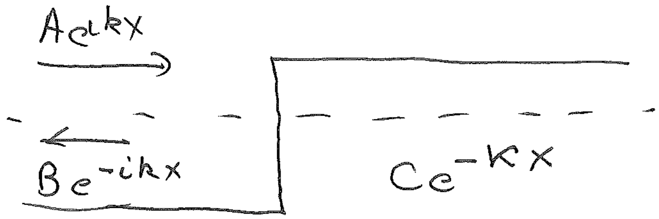
$$u^{(1)}(0) = u^{(2)}(0) \Rightarrow A + B = C$$

$$\frac{du^{(1)}}{dx}(0) = \frac{du^{(2)}}{dx}(0) \Rightarrow ik_1(A-B) = ik_2 C$$

$$\Rightarrow ik_2 = ik_1\left(\frac{A+B}{A-B}\right) \Longrightarrow \begin{cases} B = \left(\dfrac{k_1 - k_2}{k_2 + k_1}\right) A \\[2ex] C = \dfrac{2k_1}{k_1 + k_2} A \end{cases}$$

$$\boxed{\begin{aligned} R &= \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 = \left(\frac{1 - \frac{k_1}{k_2}}{1 + \frac{k_2}{k_1}}\right)^2 \\ T &= \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1} = \frac{4\frac{k_2}{k_1}}{\left(1 + \frac{k_2}{k_1}\right)^2}, \quad \text{Note: } T + R = 1 \end{aligned}}$$

Case (ii) $E < V_0$



$k_1 \to k = \sqrt{\frac{2mE}{\hbar^2}}$

$k_2 \to i\kappa = i\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

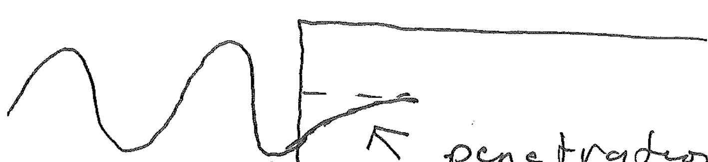
$$\therefore \quad \frac{B}{A} = \frac{1 - i\frac{\kappa}{k}}{1 + i\frac{\kappa}{k}}, \qquad \frac{C}{A} = \frac{2}{1 + \frac{i\kappa}{k}}$$

$$\therefore \quad R = \left|\frac{B}{A}\right|^2 = \frac{\left|1 - i\frac{\kappa}{k}\right|^2}{\left|1 + i\frac{\kappa}{k}\right|^2} = \frac{1 + \frac{\kappa^2}{k^2}}{1 + \frac{\kappa^2}{k^2}} = 1$$

$T = ?$ Note: $J_{trans} \propto \mathrm{Im}\left(e^{-\kappa x} \frac{d}{dx} e^{-\kappa x}\right) = 0$

$\therefore \quad T = 0$

$\Rightarrow$ 100% reflection.



penetration into classically forbidden region, but no propagation

Sketch of stationary state