PHY 712 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 7:
Continue reading Chapter #5 in Shankar; Quantum mechanical systems in 1-dim

1. **Particle in the presence of a potential step**
2. **Probability density and current density**

PHY 741 Quantum Mechanics

MWF 12 PM - 12:50 PM	OPL 103	http://www.wfu.edu/~natalie/f17phy741/

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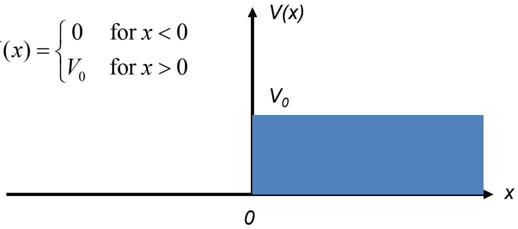
Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

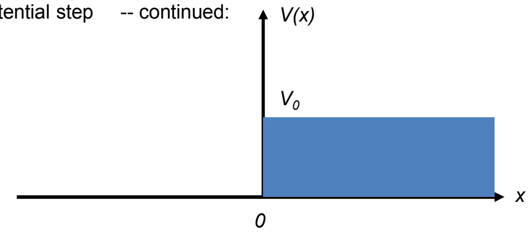
	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2	Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3	Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4	Mon, 9/04/2017	Chap. 4	Principles of Quantum Mechanics	#4	9/8/2017
5	Wed, 9/06/2017	Chap. 5	Examples in 1 dimension		
6	Fri, 9/08/2017	Chap. 5	Schrödinger equation in one-dimension	#5	9/13/2017
7	Mon, 9/11/2017	Chap. 5	Schrödinger equation in one-dimension		
8	Wed, 9/13/2017	Chap. 5	Schrödinger equation in one-dimension	#6	9/15/2017
9	Fri, 9/15/2017				
10	Mon, 9/18/2017				

Consider a particle of mass *m* in the presence of an infinite potential step:

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



Consider a particle of mass *m* in the presence of an infinite potential step -- continued:

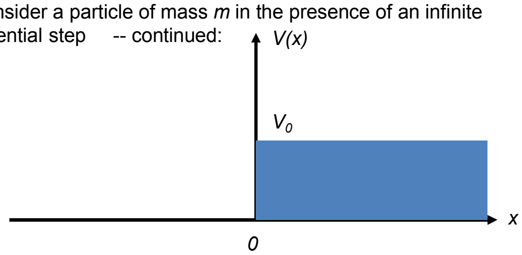


Eigenfunctions of the Schroedinger equation:

$x < 0$ $\qquad$ $x > 0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \qquad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \left(E - V_0\right)\psi(x)$$

Consider a particle of mass *m* in the presence of an infinite potential step -- continued:



Energy eigenfunction:

$x < 0$ $\qquad$ $x > 0$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\left(e^{i\left(\sqrt{2mE}/\hbar\right)x} + Re^{-i\left(\sqrt{2mE}/\hbar\right)x}\right) \qquad \psi(x) = \frac{1}{\sqrt{2\pi}}Te^{i\left(\sqrt{2m(E-V_0)}/\hbar\right)x}$$

coefficients

Consider a particle of mass *m* in the presence of an infinite potential step -- continued:

Note that when we find the solution, its complex conjugate and a linear combination of the two will also be a solution.

Digression on the notion of current density and the continuity equation. Recall the time dependent Schroedinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi$$

$$-i\hbar\frac{\partial\psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi^*$$

Note that: $i\hbar\psi^*\frac{\partial\psi}{\partial t} = \psi^*\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi$

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi \qquad -i\hbar\frac{\partial\psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi^*$$

$$i\hbar\psi^*\frac{\partial\psi}{\partial t} = \psi^*\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi$$

Define probability density: $\rho(\mathbf{r},t) \equiv P(\mathbf{r},t) = \psi^*(\mathbf{r},t)\psi(\mathbf{r},t)$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

where $\mathbf{j} \equiv \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$

Example: $\psi(\mathbf{r},t) = \psi(x,t) = \frac{1}{\sqrt{2\pi}}e^{ikx} \quad \Rightarrow \quad \mathbf{j} = \frac{\hbar k}{m}\hat{\mathbf{x}}$

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Consider a particle of mass *m* in the presence of an infinite potential step -- continued:

Energy eigenfunction:

$x<0$ $\qquad$ $x>0$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\left(e^{i\left(\sqrt{2mE}/\hbar\right)x} + Re^{-i\left(\sqrt{2mE}/\hbar\right)x}\right) \qquad \psi(x) = \frac{1}{\sqrt{2\pi}}Te^{i\left(\sqrt{2m(E-V_0)}/\hbar\right)x}$$

$$\rho(x) = \frac{1}{2\pi}\left(1+|R|^2 + 2\Re\left(R^*e^{2i\left(\sqrt{2mE}/\hbar\right)x}\right)\right) \qquad \rho(x) = \frac{1}{2\pi}|T|^2$$

$$j(x) = \frac{\sqrt{2mE}}{2\pi m}\left(1-|R|^2\right) \qquad j(x) = \begin{cases} \frac{\sqrt{2m(E-V_0)}}{2\pi m}|T|^2 & \text{For } E > V_0 \\ 0 & \text{For } E < V_0 \end{cases}$$

(corrected 9/18/2017 thanks to Sajant)

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Consider a particle of mass *m* in the presence of an infinite potential step -- continued:

Energy eigenfunction:

$x<0$ $\qquad$ $x>0$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\left(e^{i\left(\sqrt{2mE}/\hbar\right)x} + Re^{-i\left(\sqrt{2mE}/\hbar\right)x}\right) \qquad \psi(x) = \frac{1}{\sqrt{2\pi}}Te^{i\left(\sqrt{2m(E-V_0)}/\hbar\right)x}$$

Continuity of wavefunction at $x=0$:

$1 + R = T$

Continuity of derivative of wavefunction at $x=0$:

$$\frac{\sqrt{2mE}}{\hbar}(1-R) = \frac{\sqrt{2m(E-V_0)}}{\hbar}T$$

$$T = \frac{2}{1+\sqrt{\frac{E-V_0}{E}}} \qquad R = T-1$$

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Consider a particle of mass *m* in the presence of an infinite potential step -- continued:

Energy eigenfunction:

$x < 0$ $\qquad\qquad$ $x > 0$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\left(e^{i\left(\sqrt{2mE}/\hbar\right)x} + Re^{-i\left(\sqrt{2mE}/\hbar\right)x}\right) \qquad \psi(x) = \frac{1}{\sqrt{2\pi}}Te^{i\left(\sqrt{2m(E-V_0)}/\hbar\right)x}$$

$$T = \frac{2}{1+\sqrt{\frac{E-V_0}{E}}} \qquad R = T - 1$$

For $E > V_0$ $\qquad j = \frac{\sqrt{2m(E-V_0)}}{2\pi m}\frac{4}{\left(1+\sqrt{\frac{E-V_0}{E}}\right)^2}$

For $V_0 > E$ $\qquad j = 0$

Reflectance and transmittance of matter wave

Energy eigenfunction:

$x < 0$ $\qquad\qquad$ $x > 0$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\left(e^{i\left(\sqrt{2mE}/\hbar\right)x} + Re^{-i\left(\sqrt{2mE}/\hbar\right)x}\right) \qquad \psi(x) = \frac{1}{\sqrt{2\pi}}Te^{i\left(\sqrt{2m(E-V_0)}/\hbar\right)x}$$

incident wave $\qquad$ reflected wave $\qquad$ transmitted wave

where: $T = \frac{2}{1+\sqrt{\frac{E-V_0}{E}}} \qquad R = T - 1$

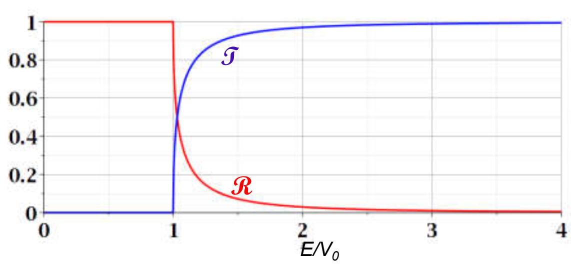
$$\mathcal{R} = \left|\frac{j_{refl}}{j_{inc}}\right| = |R|^2$$

$$j_{inc} = \frac{\sqrt{2mE}}{2\pi m} \qquad j_{refl} = -\frac{\sqrt{2mE}}{2\pi m}|R|^2$$

$$\mathcal{T} = \left|\frac{j_{trans}}{j_{inc}}\right| = \sqrt{\frac{E-V_0}{E}}|T|^2$$

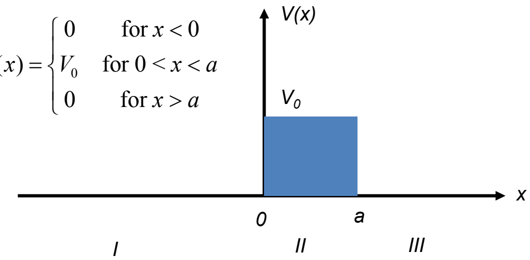
$$j_{trans} = j = \frac{\sqrt{2m(E-V_0)}}{2\pi m}|T|^2$$

for $E > V_0$ only



Consider a particle of mass *m* in the presence of a finite potential step:

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



Consider a particle of mass *m* in the presence of a finite potential step -- continued

Energy eigenstates of the Hamiltonian

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

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

Define $k=\sqrt{2mE}/\hbar \quad \text{for } E>0$

$$k_1=\sqrt{2m(E-V_0)}/\hbar \quad \text{for } E>V_0$$

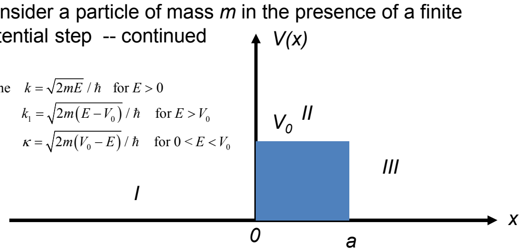
$$\kappa=\sqrt{2m(V_0-E)}/\hbar \quad \text{for } 0<E<V_0$$

Consider a particle of mass *m* in the presence of a finite potential step -- continued

Define $k=\sqrt{2mE}/\hbar \quad \text{for } E>0$

$$k_1=\sqrt{2m(E-V_0)}/\hbar \quad \text{for } E>V_0$$

$$\kappa=\sqrt{2m(V_0-E)}/\hbar \quad \text{for } 0<E<V_0$$



$$\psi_I(x)=\frac{1}{\sqrt{2\pi}}\left(e^{ikx}+Re^{-ikx}\right) \qquad \psi_{III}(x)=\frac{1}{\sqrt{2\pi}}Te^{ikx}$$

$$\psi_{II}(x)=\frac{1}{\sqrt{2\pi}}\begin{cases}\left(Ae^{ik_1x}+Be^{-ik_1x}\right) & \text{for } E>V_0\\ \left(Ae^{\kappa x}+Be^{-\kappa x}\right) & \text{for } 0<E<V_0\end{cases}$$

Consider a particle of mass *m* in the presence of a finite potential step -- continued

Define $k = \sqrt{2mE}/\hbar$ for $E > 0$

$k_1 = \sqrt{2m(E - V_0)}/\hbar$ for $E > V_0$

$\kappa = \sqrt{2m(V_0 - E)}/\hbar$ for $0 < E < V_0$

note that $\kappa = ik_1$

Satisfying boundary conditions:

$$1 + R = A + B \qquad 1 - R = \frac{k_1}{k}(A - B)$$

$$Ae^{ik_1 a} + Be^{-ik_1 a} = Te^{ik_1 a} \qquad Ae^{ik_1 a} - Be^{-ik_1 a} = \frac{k}{k_1}Te^{ik_1 a}$$

$$\mathcal{T} = \begin{cases} \dfrac{4k^2k_1^2}{\left(k^2 - k_1^2\right)^2 \sin^2(k_1 a) + 4k^2k_1^2} & \text{for } E > V_0 \\ \dfrac{4k^2\kappa^2}{\left(k^2 + \kappa^2\right)^2 \sinh^2(\kappa a) + 4k^2\kappa^2} & \text{for } 0 < E < V_0 \end{cases}$$