Lecture 10

Free particle: summary

The free particle: V(x) = 0 everywhere.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

We introduce $k \equiv \frac{\sqrt{2mE}}{\hbar}$: $\boxed{\frac{d^2\psi}{dx^2} = -k^2\psi}$

The "stationary states" of the free particle are propagating waves with wavelength

$$\lambda = \frac{2\pi}{|k|}, \quad p = \frac{2\pi\hbar}{\lambda} \quad \Rightarrow p = \hbar k.$$

$$\Psi_k(x,t) = A\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}$$

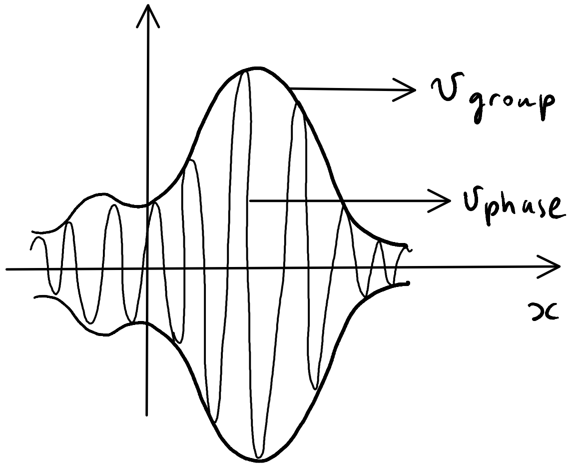
$k \equiv \pm \frac{\sqrt{2mE}}{\hbar}$, with $\begin{cases} k > 0 & \text{traveling to the right} \\ k < 0 & \text{traveling to the left} \end{cases}$

<u>**General solution (wave packet):**</u>

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk}$$

If the initial wave function $\Psi(x,0)$ at time t=0 is known, the function $\phi(k)$ may be found using:

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ikx}\, dx}.$$



A wave packet

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk$$

$$\omega = \frac{\hbar k^2}{2m}$$

Group velocity

$$v_{group} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = v_{classical}$$

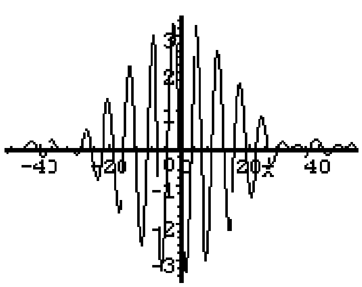
Phase velocity

$$v_{phase} = \frac{\omega}{k} = \frac{\hbar k}{2m}$$

A. John Mallinckrodt
http://www.csupomona.edu/~ajm/materials/animations/packets.html
The following movies show wave packets with various combinations of phase and group velocity. Each waveform is the sum of five sinusoids with the general format

$$\begin{aligned} f(x,t) = \; & A^2 \sin\left[\left(\omega_o + 2\Delta\omega\right)t - \left(k_o + 2\Delta k\right)x\right] \\ & + A \sin\left[\left(\omega_o + \Delta\omega\right)t - \left(k_o + \Delta k\right)x\right] \\ & + \sin\left[\omega_o t - k_o x\right] \\ & + A \sin\left[\left(\omega_o - \Delta\omega\right)t - \left(k_o - \Delta k\right)x\right] \\ & + A^2 \sin\left[\left(\omega_o - 2\Delta\omega\right)t - \left(k_o - 2\Delta k\right)x\right] \end{aligned}$$

which yields



Movie 1:
Phase Velocity = Group Velocity [179K]
A=0.7, $w_o = k_o = 1$, Dw = Dk = 0.05
The entire waveform—the component waves *and* their envelope—moves as one. Kind'a boring.

Movie 2:
Group Velocity = 0 [18K]
A=0.7, $w_o = k_o = 1$, Dw = 0, Dk = 0.05
The envelope is stationary while the component waves move underneath.

Movie 3:
Phase Velocity = 0 [178K]
A=0.7, $w_o = 0$, $k_o = 1$, Dw = Dk = 0.05
Now *only* the envelope moves over stationary component waves.

Movie 4:
Phase Velocity = -Group Velocity [179K]
A=0.7, $w_o = k_o = 1$, Dw = -0.05, Dk = 0.05

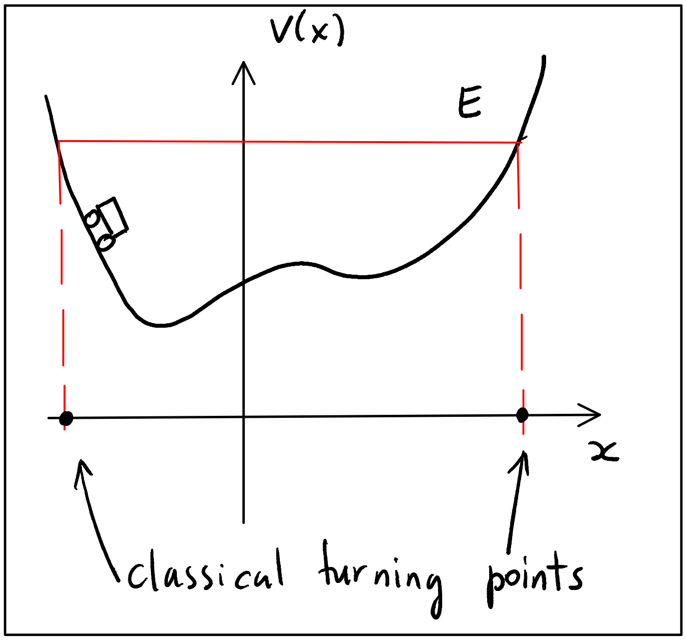
Bound and scattering states

We have now two types of solutions to Schrödinger equation:

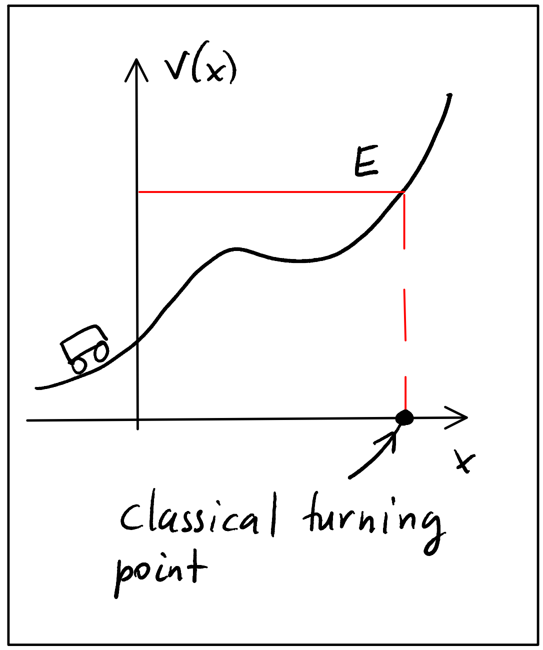
(1) normalizable and labeled by discrete index n (infinite well, harmonic oscillator)

(2) non-normalizable and labeled by continuous index k (free particle).

Classical mechanics



Bound state

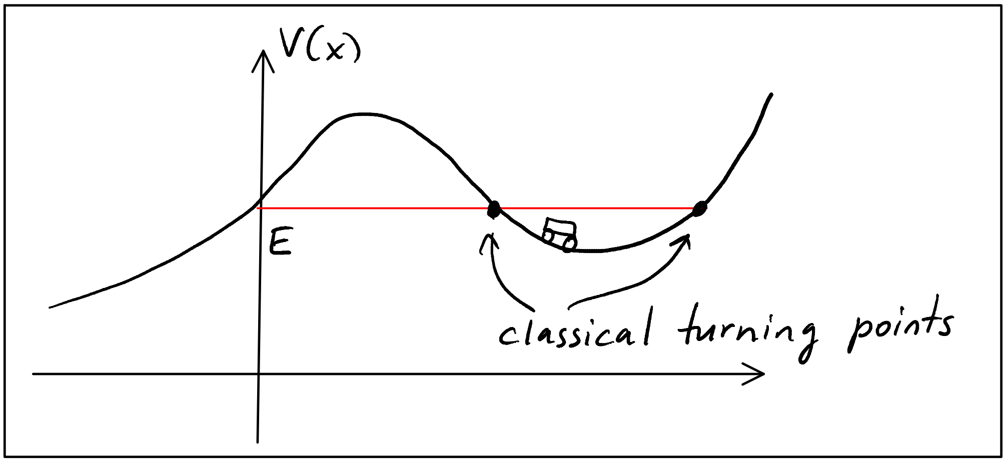


Scattering state

Simulations:

Classical: Energy Skate Park
http://phet.colorado.edu/new/simulations/sims.php?sim=Energy_Skate_Park

Quantum: Quantum Tunneling and Wave Packets
http://phet.colorado.edu/new/simulations/sims.php?sim=Quantum_Tunneling_and_Wave_Packets

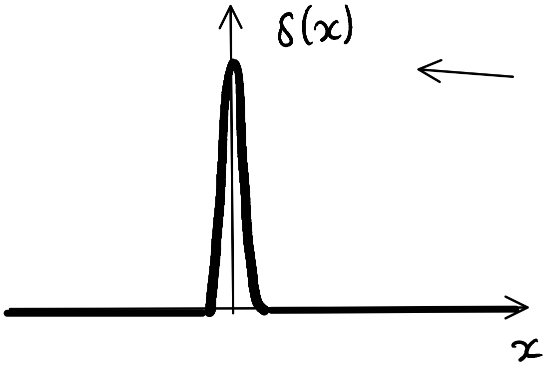


A classical bound state, but a quantum scattering state.

The two kinds of solutions to the Schrödinger equation correspond to bound and scattering states. Since in quantum mechanics "tunneling" allows particle to "leak" through any finite potential barrier, only potential at infinity matters.

$$\begin{cases} E < [V(-\infty) \text{ and } V(+\infty)] \Rightarrow \text{bound state} \\ E > [V(-\infty) \ \underline{\underline{\text{or}}} \ V(+\infty)] \Rightarrow \text{scattering state} \end{cases}$$

The delta-function potential



The Dirac delta-function

It is infinitely high, infinitesimally narrow spike whose area is 1.

$$\delta(x) \equiv \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}$$

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1$$

Property of the delta-function:

$$f(x)\,\delta(x-a) = f(a)\,\delta(x-a)$$

[The product is zero anywhere except a].

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)\int_{-\infty}^{\infty} \delta(x-a)\,dx = f(a)$$

This is the most important property of the delta-function:

$$\boxed{\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)}$$

We consider a potential:

$$V(x) = -\alpha\delta(x)$$

α: some positive constant

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$$

Bound states $(E<0)$
Scattering states $(E>0)$

First, we look at the bound states

(1) $x<0$ $\quad V(x)=0 \Rightarrow \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = k^2\psi$

$$k = \frac{\sqrt{-2mE}}{\hbar}$$

E is negative by assumption and k is real and positive.

$$\psi(x) = \underbrace{\cancel{Ae^{-kx}}}_{\substack{A=0 \text{ since} \\ \psi\to\infty \text{ if } x\to-\infty}} + Be^{kx}$$

$$\psi(x) = Be^{kx}$$

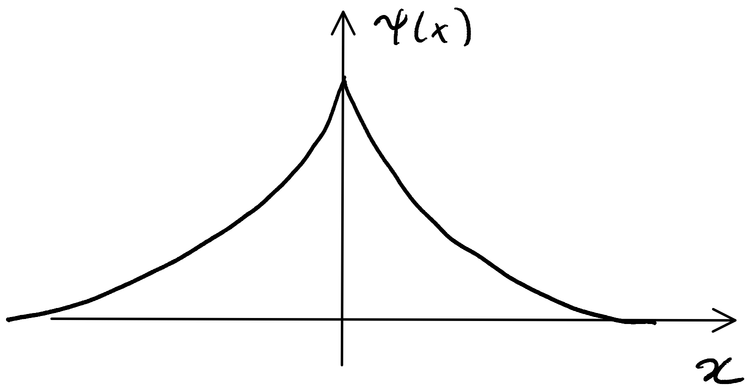
(2) $x>0$ $\quad V(x)=0 \quad \psi(x) = Fe^{-kx} + \underbrace{\cancel{Ge^{kx}}}_{\substack{G=0 \text{ since} \\ \psi\to\infty \quad x\to\infty}}$

$$\psi(x) = Fe^{-kx}$$

Now we need to stitch two solutions. The boundary conditions at x=0 are:

$$\begin{cases} 1. & \psi \text{ is always continuous} \\ 2. & d\psi/dx \text{ is continuous except at points where the potential is infinite.} \end{cases}$$

#1 gives $F = B \Rightarrow \psi(x) = \begin{cases} Be^{\kappa x} & (x \leq 0) \\ Be^{-\kappa x} & (x \geq 0) \end{cases}$



#2 tells us nothing

Normalizing: $\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 2|B|^2 \int_0^{\infty} e^{-2\kappa x}\,dx$

$$= \frac{|B|^2}{k} = 1$$

$$B = \sqrt{k}$$

We still need to find E ... to be continued.