Lecture 14: Motion in 1D

Phy851/fall 2009
Simple Problems in 1D

- To describe the motion of a particle in 1D, we need the following four QM elements:

  \[ i\hbar \frac{d}{dt} \psi(t) = H \psi(t) \]  
  \[ H = \frac{P^2}{2m} + V(X) \]  
  \[ \langle x | \psi(t) \rangle = \psi(x, t) \]  
  \[ \langle x | P | \psi(t) \rangle = -i\hbar \frac{\partial}{\partial x} \psi(x, t) \]

  - Schrödinger's equation
  - Energy of a particle
  - Definition of wavefunction
  - Action of momentum operator in x-basis

- Putting them together yields the Schrödinger wave equation:

  \[ i\hbar \frac{d}{dt} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t) \]
Bound States vs Scattering States

- Problems dealing with motion in 1D fall into one of two categories

1. **Bound-state problems:**
   - \( V(x) < E \) over finite region only
   - Energy levels are discrete
   - Typical problem:
     - Find Energy eigenvalues: \( \{E_n\} \); \( n=1,2,3,... \)
     - Find corresponding Energy eigenstates: \( \{|E_n\}\} \)
     - Find time evolution of an arbitrary state

2. **Scattering problems:**
   - \( V(x) < E \) in region extending to infinity in at least one direction
   - Energy spectrum is continuous
   - Typical problem:
     - For a given incident \( k \) find reflection and transmission probabilities, \( R(k) \) and \( T(k) \).
Example: Scattering from a Step Potential

• Consider the potential:

\[ V(x) = \begin{cases} 
0 & x < 0 \\
V_0 & x > 0 
\end{cases} \]

• Goal: find eigenstates

• Strategy:
  - Divide into regions of constant V
  - Make suitable Ansatz for each region
  - Use boundary conditions to connect regions
General Solution for Constant V

• Solving the energy eigenvalue equation:

Start with the basic equation

\[ H | \psi_E \rangle = E | \psi_E \rangle \]

Specify the Hamiltonian

\[ \left( \frac{P^2}{2M} + V \right) | \psi_E \rangle = E | \psi_E \rangle \]

Hit with \( \langle k | \) from left

\[ \langle k | \left( E - \frac{P^2}{2M} - V \right) | \psi_E \rangle = 0 \]

Use \( \langle k | P = \hbar k \langle k | \)

\[ \left( E - \frac{\hbar^2 k^2}{2M} - V \right) \langle k | \psi_E \rangle = 0 \]

• Solution:

Either

\[ \left( E - \frac{\hbar^2 k^2}{2M} - V \right) = 0 \]

or

\[ \langle k | \psi_E \rangle = 0 \]

For given \( E \) can only be satisfied for two \( k \) values, so \( \langle k | \psi \rangle \) must be zero for all other \( k \):

\[ E - \frac{\hbar^2 k^2}{2M} - V = 0 \]

\[ k = \pm \frac{\sqrt{2M(E - V)}}{\hbar} \]

\[ \langle k | \psi_E \rangle = c_+ \delta (k - \frac{\sqrt{2m(E-V)}}{\hbar}) + c_- \delta (k + \frac{\sqrt{2m(E-V)}}{\hbar}) \]
Wavefunction for constant $V$

- We have found:

$$\langle k | \psi_E \rangle = c_+ \delta\left(k - \frac{\sqrt{2m(E-V)}}{\hbar}\right) + c_- \delta\left(k + \frac{\sqrt{2m(E-V)}}{\hbar}\right)$$

- Closure tells us that:

$$|\psi\rangle = \int dk \langle k | k \rangle \langle k | \psi \rangle$$

$$|\psi\rangle = \int dk |k\rangle \left[ c_+ \delta\left(k - \frac{\sqrt{2m(E-V)}}{\hbar}\right) + c_- \delta\left(k + \frac{\sqrt{2m(E-V)}}{\hbar}\right) \right]$$

$$|\psi\rangle = c_+ |k_E\rangle + c_- | - k_E\rangle$$

$$k_E = \frac{\sqrt{2m(E-V)}}{\hbar}$$

- Hit with $\langle x |$ to construct the wavefunction:

$$\langle x | \psi_E \rangle = c_+ \langle x | k_E \rangle + c_- \langle x | - k_E \rangle$$

$$\psi_E(x) = c_+ e^{ik_Ex} + c_- e^{-ik_Ex}$$

$c_+$ and $c_-$ will be set by boundary conditions
Energy Eigenstate Wave Function for Step Potential:

So we have for each region:

$$\psi_E(x) = c_+ e^{ik_1E x} + c_- e^{-ik_2E x}$$

Applying this for each region gives

$$\psi_I(x) = a_1 e^{ik_1E x} + b_1 e^{-ik_1E x} \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{II}(x) = a_2 e^{ik_2E x} + b_2 e^{-ik_2E x} \quad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

Q: How do we find the coefficients?

A: We need to specify boundary conditions:
   - 4 unknowns required 4 boundary condition eqs.
Boundary conditions at $\pm \infty$

- In scattering problems, we need to specify the asymptotic forms of the wavefunction for $x \to \pm \infty$.
  - i.e. specify $c_+$ and $c_-$ for the left-most and right-most regions

- For 1-d scattering, the most common approach is:
  - For left-most region, take:
    \[ \psi_{in}(X) = e^{ik_{in}x} + r e^{-ik_{in}x} \]
  - For right-most region, take:
    \[ \psi_{out} = t e^{ik_{out}x} \]

- For step-potential, this translates to:
  \[ \psi_I(x) = e^{ik_1x} + r e^{-ik_1x} \]
  \[ \psi_{II}(x) = t e^{ik_2x} \]
Boundary conditions at a Potential discontinuity

- The remaining unknown constants are determined from `continuity conditions' applied to each Potential discontinuity

allow $\Psi(x)$ and its derivatives to be discontinuous and see if the eigenvalue equation can still be satisfied

- Let $x=0$ be the location of the discontinuity:
- Let $\psi(x)$ be a continuous smooth function
- Define:

\[
\Psi(x) = \psi(x) + \alpha U(x) + \beta x U(x) + \frac{\gamma}{2} x^2 U(x) + \ldots
\]

\[
U(x) = \begin{cases} 
0 & x < 0 \\
1 & x > 0 
\end{cases} \quad \text{`Unit Step-function'}
\]

- Differentiation gives:

\[
\Psi'(x) = \psi'(x) + \alpha \delta(x) + \beta U(x) + \gamma x U(x) + \ldots
\]

\[
\Psi''(x) = \psi''(x) + \alpha \delta'(x) + \beta \delta(x) + \gamma U(x) + \ldots
\]

\[
\vdots \quad \vdots
\]

Recall that:

\[
U''(x) = \delta(x)
\]
Continuity conditions

\[ \Psi(x) = \psi(x) + \alpha U(x) + \beta x U(x) + \frac{\gamma}{2} x^2 U(x) + \ldots \]

\[ \Psi'(x) = \psi'(x) + \alpha \delta(x) + \beta U(x) + \gamma x U(x) + \ldots \]

\[ \Psi''(x) = \psi''(x) + \alpha \delta'(x) + \beta \delta(x) + \gamma U(x) + \ldots \]

\[ \vdots \quad \vdots \]

- Taking the limit as \( x \to 0 \) from the left gives:
  \[ \Psi(0^-) = \psi(0) \]

- Taking the limit as \( x \to 0 \) from the right gives:
  \[ \Psi(0^+) = \psi(0) + \alpha \]

- Thus \( \alpha \) is the discontinuity in \( \Psi(x) \) at \( x=0 \):
  \[ \Psi(0^+) - \Psi(0^-) = \alpha \]

- Likewise:
  \[ \Psi'(0^+) - \Psi'(0^-) = \beta \]

  \[ \Psi''(0^+) - \Psi''(0^-) = \gamma \]

  - And so on ...
Plugging into the Energy Eigenvalue Equation

- Projecting the Energy Eigenvalue equation onto $\langle x \rangle$ gives:

$$\left[ E + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V(x) \right] \psi(x, t) = 0$$

- Theorem:

  - the wavefunction and its first derivative must be everywhere continuous.
  - **Exception:** where there is a $\psi(x-x_0)$ or $\psi'(x-x_0)$ in the potential.
    - $\delta(x-x_0)$ potential $\rightarrow$ discontinuity in $\psi'(x)$ at $x=x_0$
    - $\delta'(x-x_0)$ potential $\rightarrow$ discontinuity in $\psi(x)$ at $x=x_0$

- Conclusions:
  - There is nothing on the L.h.s. to cancel the delta functions on the R.h.s. unless $V(x)$ contains a $\psi(x)$ and/or a $\psi'(x)$ term.
  - Unless this is the case, we must have $\alpha=0$ and $\beta=0$