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:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

Schrödinger's equation

$$H = \frac{P^2}{2m} + V(X)$$

Energy of a particle

$$\langle x|\psi(t)\rangle = \psi(x,t)$$

Definition of wavefunction

$$\langle x|P|\psi(t)\rangle = -i\hbar \frac{\partial}{\partial x}\psi(x,t)$$

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

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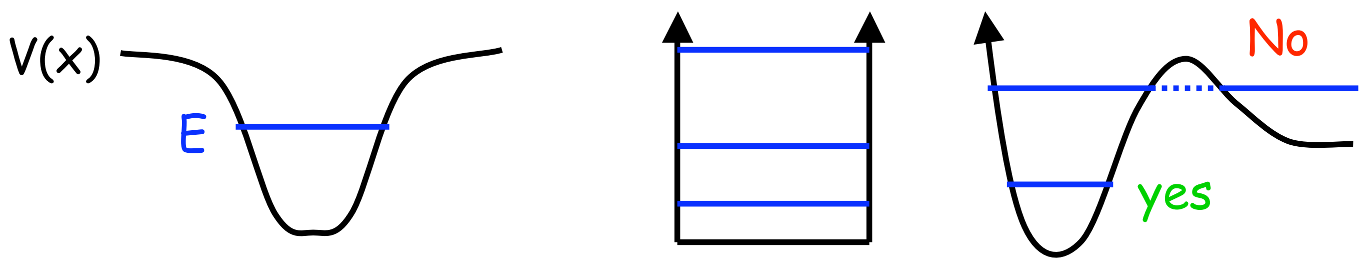
1. Bound-state problems:

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



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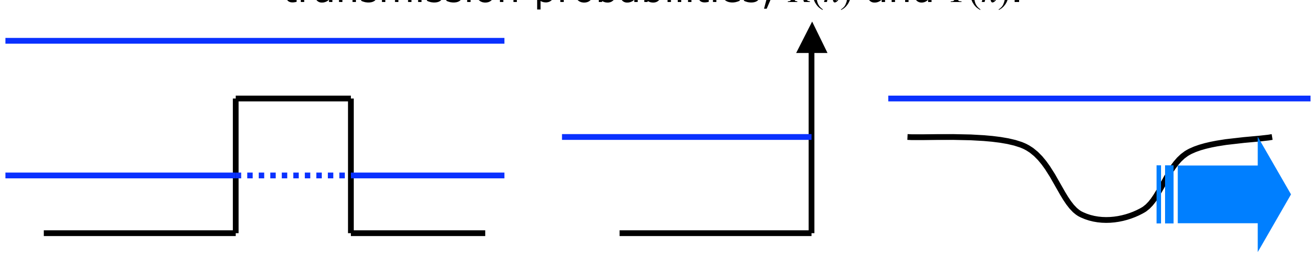
2. Scattering problems:

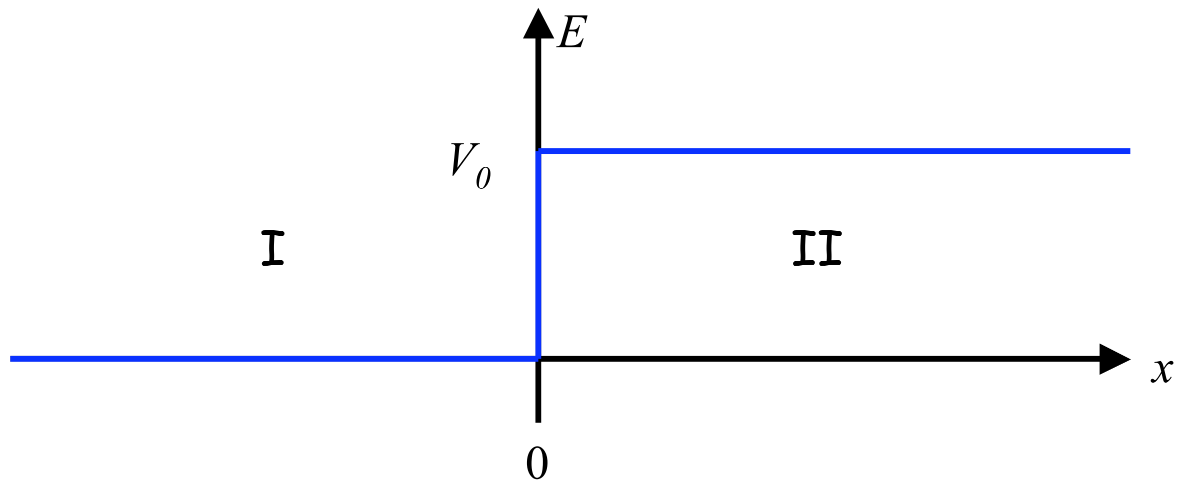
- $V(x) < \mathrm{E}$ in region extending to infinity in at least one direction
- Energy spectrum is continuous
- Typical problem:
  - For a given incident k find reflection and transmission probabilities, $R(k)$ and $T(k)$.



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:

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

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

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

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:

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

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

$$|\psi\rangle = c_+ |k_E\rangle + c_- |-k_E\rangle \qquad k_E = \frac{\sqrt{2m(E-V)}}{\hbar}$$

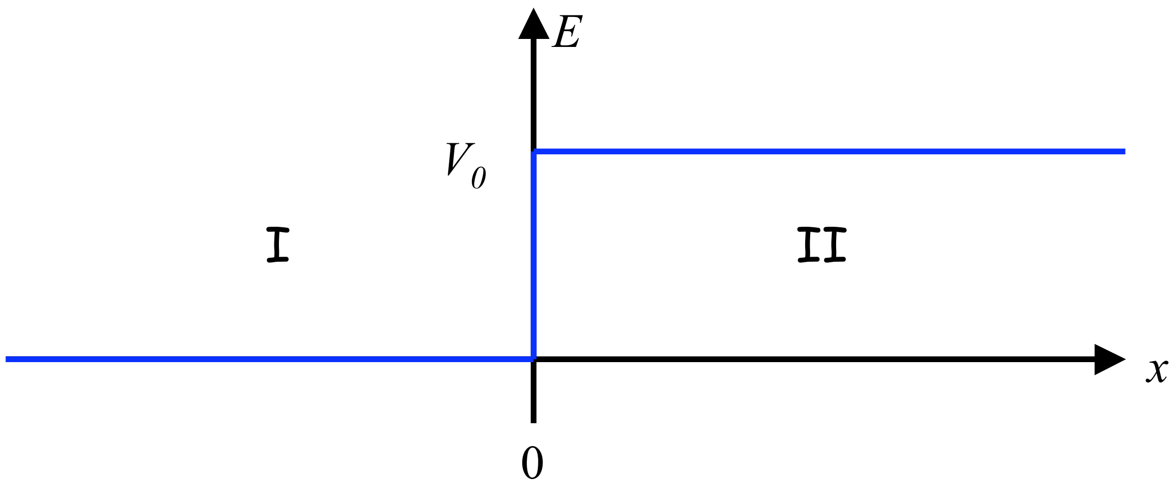
- Hit with $\langle x|$ to construct the wavefunction:

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

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

c_+ and c_- will be set by boundary conditions

Energy Eigenstate Wave Function for Step Potential:



- So we have for each region:

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

- Applying this for each region gives

$$\psi_I(x) = a_1 e^{ik_1 x} + b_1 e^{-ik_1 x} \qquad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{II}(x) = a_2 e^{ik_2 x} + b_2 e^{-ik_2 x} \qquad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

- Q: How do we find the coefficients?

- A: We need to specify boundary conditions:
  - 4 unknowns required 4 boundary condition eqs.

Boundary conditions at ±∞

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

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- For 1-d scattering, the most common approach is:
  - For left-most region, take:

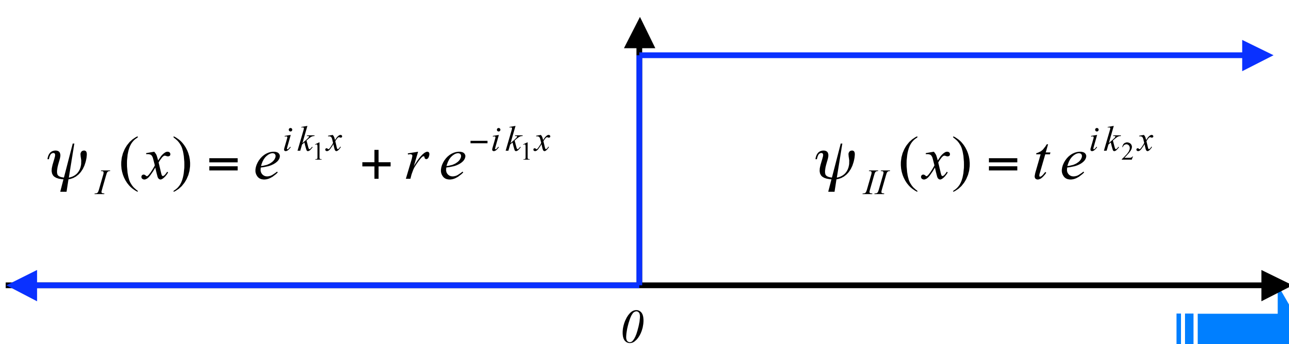
$$\psi_{in}(X) = e^{ik_{in}x} + r\,e^{-ik_{in}x}$$

  - For right-most region, take:

$$\psi_{out} = t\,e^{ik_{out}x}$$

- For step-potential, this translates to:

$$\psi_I(x) = e^{ik_1x} + r\,e^{-ik_1x} \qquad \psi_{II}(x) = t\,e^{ik_2x}$$



Boundary conditions at a Potential discontinuity

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

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- ***Strategy*:** 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:

$$\Psi(x) = \psi(x) + \alpha U(x) + \beta x U(x) + \frac{\gamma}{2} x^2 U(x) + \dots$$

$$U(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}$$

`Unit Step-function'

  - Differentiation gives:

$$\Psi'(x) = \psi'(x) + \alpha\delta(x) + \beta U(x) + \gamma x U(x) + \dots$$

$$\Psi''(x) = \psi''(x) + \alpha\delta'(x) + \beta\,\delta(x) + \gamma U(x) + \dots$$

$$\vdots \qquad\qquad \vdots$$

Recall that:

$U'(x)=\delta(x)$

Continuity conditions

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

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

$$\Psi''(x) = \psi''(x) + \alpha\delta'(x) + \beta\,\delta(x) + \gamma U(x) + \ldots$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

- Taking the limit as *x* → *0* from the *left* gives:

$$\Psi(0^-) = \psi(0)$$

- Taking the limit as *x* → *0* from the *right* gives:

$$\Psi(0^+) = \psi(0) + \alpha$$

- Thus α 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 ⟨*x*| gives:

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

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

- This gives:

$$[E - V(x)]\left(\psi(x) + \alpha U(x) + \beta x U(x) + \frac{\gamma}{2}x^2 U(x) + \ldots\right)$$

$$= -\frac{\hbar^2}{2M}\left(\psi''(x) + \alpha\delta'(x) + \beta\delta(x) + \gamma U(x) + \ldots\right)$$

- 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 $\beta=0$

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 → discontinuity in $\psi'(x)$ at $x=x_0$
    - $\delta'(x-x_0)$ potential → discontinuity in $\psi(x)$ at $x=x_0$