One-Dimensional Quantum Mechanics

Free Particle $H = P^2/2m$

- The eigenstates are clearly $|p\rangle$, the momentum states
  - Alas, these are not properly normalizable.
    We should use normalizable superpositions
    $$|\psi\rangle = \int dp\, \tilde{\psi}(p)\, |p\rangle$$
    which are approximate eigenstates if $\tilde{\psi}(p)$ is peaked near one value
  - Time dependence is pretty easy in this basis
    $$|\Psi(t)\rangle = e^{-iHt/\hbar}|\psi\rangle = \int dp\, \tilde{\psi}(p)\, e^{-ip^2t/2\hbar m}|p\rangle$$
  - The spatial wavefunction is the Fourier transform
    $$\langle x|\Psi(t)\rangle = \Psi(x,t) = \int dp\, \tilde{\psi}(p)\, e^{-ip^2t/2\hbar m}\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$
- Now is as good a time as any to talk about wave velocities
  - Any wave can be written as a Fourier integral
    $$\Psi(x,t) = \int \frac{dk}{\sqrt{2\pi}}\, \phi(k)\, e^{i(kx-\omega t)}$$
    In our QM case, $k = p/\hbar$, and $\phi(k) = \sqrt{\hbar}\,\tilde{\psi}(\hbar k)$, $\omega = \hbar k^2/2m$.
  - The <u>phase velocity</u> is the velocity of a given peak or trough of a single wave number k. Evidently this moves along at $v_p = \omega/k$ (the phase is $k(x - v_p t)$)
  - If we have a narrow spread in wavenumber k, the Fourier components travel at almost the same speed.
    The "beat" causes an envelope of modulated amplitude to

travel along through the individual modes

+ In math, we say $k \approx k_0$ and then $\omega(k) \approx \omega_0 + \omega_0'(k-k_0)$

+ Then
$$\Psi(x,t) \approx \int \frac{dk}{2\pi}\, \phi(k)\, e^{i[kx - \omega_0 t - \omega_0'(k-k_0)t]}$$
$$= e^{-i(\omega_0 - \omega_0' k_0)t} \int \frac{dk}{\sqrt{2\pi}}\, \phi(k)\, e^{ik(x-\omega_0' t)}$$

+ Compare to
$$\Psi(x,0) = \int \frac{dk}{\sqrt{2\pi}}\, \phi(k)\, e^{ikx}$$

We see
$$\Psi(x,t) \approx e^{-i(\omega_0 - \omega_0' k)t}\, \Psi(x - \omega_0' t, 0)$$

+ The first part is a physically meaningless phase (it is like the time evolution of a stationary state)
+ The second says that the group envelope moves at a <u>group velocity</u> $v_g = d\omega/dk|_{k_0}$.

• For nonrelativistic QM, $v_g = \hbar k/m = p/m$ = the classical velocity
the phase velocity $v_p = \omega/k = \hbar k/2m = \frac{1}{2}$ that
which velocity tells you about $\langle x \rangle$? Think about Ehrenfest

• <u>Delta-Function Potential</u>

$$H = P^2/2m - \alpha\,\delta(x), \quad \alpha > 0.$$

– Different kinds of stationary states
(Supposing that $V(x) \to 0$ as $x \to \pm\infty$)

• $E > 0$. These are <u>scattering states</u> (like free particle)
+ Allow any value of energy, ie. continuous eigenvalues + delta-function normalization for stationary states
+ [illegible] boundary conditions [illegible] by [illegible] "[illegible]"

+ We choose boundary conditions at $x \to \pm\infty$ by considering "right-moving" and "left-moving" aka "incoming" and "outgoing" waves. These have wavefunctions

$$\Psi \sim e^{ipx/\hbar} e^{-ip^2 t/2m\hbar} \text{ (right-moving) or } \Psi \sim e^{-ipx} e^{-ip^2 t/2m\hbar} \text{ (left)}$$

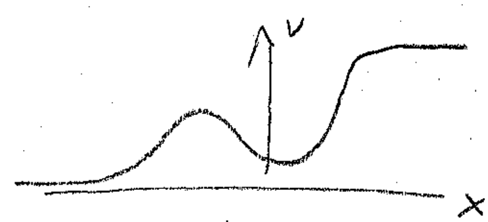
for positive p

- $E<0$ These are <u>bound states</u>
  + Only allow discrete energy eigenvalues. Stationary states are orthonormal
  + Vanishing wavefunctions as $x \to \pm\infty$, confined or bound to potential
- A potential may have both types and both are needed for completeness:

$$\mathbb{1} = \sum_{n=1}^{N} |E_n\rangle\langle E_n| + \int dz\, |E_z\rangle\langle E_z|$$

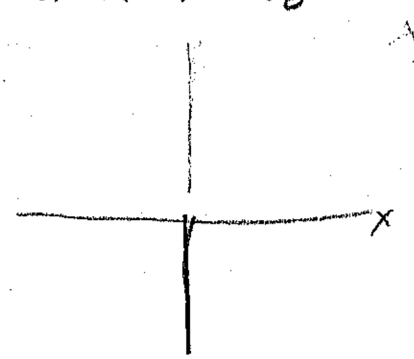
where N is total # of bound states and z is a parameter controlling scattering state energy

- An asymmetric potential may have states that are hybrid bound + scattering. Have continuous eigenvalues but do not reach everywhere



- In most "real" cases $V \to 0$ at infinity. But if $V \to V_0$ constant, just shift the discussion above

— Bound states of the delta-function well



- With $E<0$, Schrödinger is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi \quad \text{away from } x=0$$

$$\kappa = \sqrt{-2mE}/\hbar > 0$$

+ The general solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

+ For $x<0$, need $A=0$ to have normalizability

For $x>0$, need $B=0$

$$\langle x|\psi\rangle = \psi(x) = \begin{cases} Be^{\kappa x}, & x<0 \\ Ae^{-\kappa x}, & x>0 \end{cases}$$

- How does the delta function come in?

Let's consider basic properties of (position basis) Schrödinger eqn

+ It's 2nd order in space, so ψ is continuous everywhere

+ Suppose we integrate the Schrödinger eqn from $x = a-\epsilon$ to $a+\epsilon$

Then $$-\frac{\hbar^2}{2m}\int_{a-\epsilon}^{a+\epsilon} dx\, \frac{d^2\psi}{dx^2} + \int_{a-\epsilon}^{a+\epsilon} dx\, V(x)\psi(x) = E\int_{a-\epsilon}^{a+\epsilon} dx\, \psi(x) \quad \text{as } \epsilon \to 0$$

The RHS $\to 0$ because $\psi(x)$ is continuous.

If $V(x)$ is continuous + finite, so is $\frac{d\psi}{dx}$

But if $V(a)$ jumps to an infinite value, this breaks down

For the delta function

$$\left.\frac{d\psi}{dx}\right|_{0^+} - \left.\frac{d\psi}{dx}\right|_{0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0) \quad (\star)$$

- Back to the bound state wavefunction:
  + Continuity of ψ at $x=0$ requires $A=B$
  + The b.c. $(\star)$ requires

$$(-A\kappa) - (A\kappa) = -2A\kappa = \frac{-2m\alpha}{\hbar^2}A \Rightarrow \kappa = \frac{m\alpha}{\hbar^2}$$

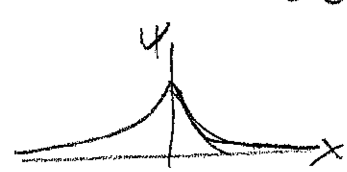
  + There is one bound state with $E = \frac{-\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$

  This is regardless of how "deep" the potential goes.

  Evidently, it can only hold one bound state b/c the well is thin

  + Normalization as usual

$$A = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar}$$



- Scattering States

• Schrödinger eqn is now

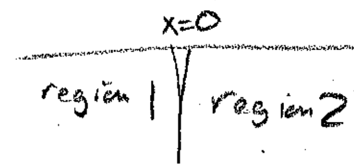
$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad , \quad k = \frac{\sqrt{2mE}}{\hbar}$$

+ The solution (away from $x=0$) is

$$\langle x|\psi\rangle = \psi(x) = Ae^{ikx} + Be^{-ikx}$$

with different coefficients for $x<0$, $x>0$

+ The boundary conditions apparently give



$$A_1 + B_1 = A_2 + B_2$$

$$ik(A_2 - B_2) - ik(A_1 - B_1) = -\frac{2m\alpha}{\hbar^2}(A_1 + B_1)$$

+ Note that k is a free parameter. So also is one of the coefficients $A_{1,2}$ or $B_{1,2}$ (to represent normalization). What do the equations tell us?

• These are non-normalizable states, so we should really build wave packets. As we saw, those have a group velocity representing movement of a particle. We should ask if the potential can <u>scatter</u> – in this case reflect – the particle

+ Note that the $e^{\pm ikx}$ wavefunctions are right-moving / left-moving

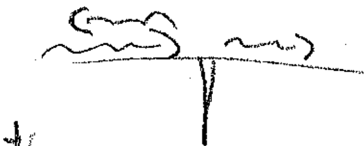
+ Let's imagine a packet coming in from the left (region 1)
In region 2, there should be only an outgoing wave $B_2 = 0$

+ Then we solve

$$2ikB_1 = -\frac{2m\alpha}{\hbar^2}(A_1 + B_1) \Rightarrow B_1 = \frac{im\alpha/\hbar^2 k}{1 - im\alpha/\hbar^2 k}A_1$$

$$A_2 = A_1 + B_1 = \frac{1}{1 - im\alpha/\hbar^2 k}A_1$$

- The physical meaning is that an incoming packet hits the well with some reflecting + some transmitted



+ The relative probability of reflection at a specific wavenumber/energy is the ratio

$$R = |B_1|^2/|A_1|^2 = \frac{1}{1+(\hbar^2 k/m\alpha)^2} = \frac{1}{1+2\hbar^2 E/m\alpha^2}$$

Reflection Coefficient. This is the ratio of probability densities (or particles) in reflected to incoming waves.

+ The relative probability of transmission is the transmission coefficient. By probability conservation, $T = 1-R$.
In this case, $T = |A_2|^2/|A_1|^2 = \frac{1}{1+(m\alpha/\hbar^2 k)^2} = \frac{1}{1+m\alpha^2/2\hbar^2 E}$

More generally, if the level of the potential changes on the right, we need to account for particle speed (so particle flux in = particle flux out).

Then $T = \left(k_2/k_1\right) |A_2|^2/|A_1|^2$. See future HW.

- What if $\alpha < 0$, so the well is a barrier? R and T are the same.

This means a quantum particle can tunnel through classically forbidding barriers — even infinitely tall ones.