PHYS 621 Lecture Notes 10

Uncertainty Relations

Suppose $\hat{A} = \hat{A}^{\dagger}$, $\hat{B} = \hat{B}^{\dagger}$, $[\hat{A}, \hat{B}] \neq 0$.

$$\langle [\hat{A}, \hat{B}] \rangle = \langle (\hat{A}\hat{B} - \hat{B}\hat{A}) \rangle$$

$$\langle (\Delta \hat{A})^2 \rangle = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle$$

$$\langle (\Delta \hat{B})^2 \rangle = \langle (\hat{B} - \langle \hat{B} \rangle)^2 \rangle$$

Consider a state $|\psi\rangle$, and define:

$$|\phi\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle$$

$$|\chi\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle$$

$$\|\phi\|^2 = \langle \phi | \phi \rangle = \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle = \langle (\Delta \hat{A})^2 \rangle$$

$$\|\chi\|^2 = \langle \chi | \chi \rangle = \langle \psi | (\hat{B} - \langle \hat{B} \rangle)^2 | \psi \rangle = \langle (\Delta \hat{B})^2 \rangle$$

$$|\langle \phi | \chi \rangle|^2 = |\langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) | \psi \rangle|^2$$

$$= |\langle \psi | \left(\frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{2} \{ \hat{A} - \langle \hat{A} \rangle, \hat{B} - \langle \hat{B} \rangle \} \right) | \psi \rangle$$

$$[\hat{A}, \hat{B}] = (\hat{A}\hat{B} - \hat{B}\hat{A}) \qquad \{\hat{A}, \hat{B}\} = (\hat{A}\hat{B} + \hat{B}\hat{A})$$

Since $[\hat{A},\hat{B}]$ is anti-Hermitian $\rightarrow$ pure imaginary exp. value

and $\{\hat{A},\hat{B}\}$ is Hermitian $\rightarrow$ real expectation values,

$$|\langle\phi|\chi\rangle|^2 = |\langle\psi|\tfrac{1}{2}[\hat{A},\hat{B}]|\psi\rangle|^2$$

$$+|\langle\psi|\tfrac{1}{2}\{\underbrace{\hat{A}-\langle\hat{A}\rangle}_{\Delta\hat{A}},\underbrace{\hat{B}-\langle\hat{B}\rangle}_{\Delta\hat{B}}\}|\psi\rangle|^2$$

$$\geq \tfrac{1}{4}|\langle\psi|[\hat{A},\hat{B}]|\psi\rangle|^2$$

By the Cauchy Inequality,

$$||\phi||^2\,||\chi||^2 \geq |\langle\phi|\chi\rangle|^2$$

$$\rightarrow \langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \tfrac{1}{4}|\langle\psi|[\hat{A},\hat{B}]|\psi\rangle|^2$$

If $\hat{A}=\hat{x}$, $\hat{B}=\hat{p}$, $[\hat{x},\hat{p}]=i\hbar$

$$\rightarrow \boxed{\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle \geq \frac{\hbar^2}{4}}$$

or, $\boxed{\Delta x\,\Delta p \geq \hbar/2}$

Comparing w/ the Gaussian wavepacket,

we learn that $\psi_{p_0}(x, t=0)$ is a

minimum-uncertainty wavepacket w/ $\Delta x \, \Delta p = \hbar/2$.

$$\boxed{\psi(x) = \frac{1}{(\pi d^2)^{1/4}} e^{i p_0 x/\hbar} \, e^{-(x-\bar{x})^2/2d^2}}$$

→ Heisenberg's Uncertainty principle:

It is impossible to simultaneously have a measurement of a particle's position and momentum.

☆ we also learn that only commuting observables <u>can</u> be simultaneously measured.

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One-Dimensional Problems in a Potential $V(x)$.

The setup:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$\hat{x}^\dagger = \hat{x} \rightarrow V(\hat{x}) = (V(\hat{x}))^\dagger$$

$$\hat{p}^\dagger = \hat{p} \rightarrow \frac{\hat{p}^2}{2m} = \left(\frac{\hat{p}^2}{2m}\right)^\dagger$$

$$\hat{H} = \hat{H}^\dagger \qquad \text{Hermitian Hamiltonian}$$

In position space:

$$\langle x| V(\hat{x}) |x'\rangle = V(x')\, \delta(x-x')$$

$$\langle x| \frac{\hat{p}^2}{2m} |x'\rangle = \frac{1}{2m} \delta(x-x') \left(-i\hbar \frac{\partial}{\partial x'}\right)^2$$

Then, $i\hbar \frac{\partial}{\partial t} \underbrace{\langle x|\psi(t)\rangle}_{\psi(x,t)} = \int dx' \langle x|\hat{H}|x'\rangle \underbrace{\langle x'|\psi(t)\rangle}_{\psi(x',t)}$

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \int dx'\, \delta(x-x') \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x'^2} \psi(x',t) + V(x')\psi(x',t)\right]$$

Integrating over x':

$$\boxed{i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)}$$

This is the Schrödinger Eq. for the wavefunction

Separation of variables: Suppose $\Psi(x,t) = \phi(t)\psi(x)$

$$\begin{cases} i\hbar\, \dot{\phi}_E(t) = E\,\phi(t) \\ -\frac{\hbar^2}{2m}\psi_E''(x) + V(x)\,\psi_E(x) = E\,\psi_E(x) \end{cases}$$

Solution! $\phi_E(t) = e^{-iEt/\hbar}$

$$\Psi_E(x,t) = e^{-iEt/\hbar}\,\psi(x)$$

This is a stationary state:

Probability density $\rho_E(x,t) = |\Psi_E(x,t)|^2 = |\psi_E(x)|^2$

– independent of t.

The time-independent Schrödinger equation simplifies if we define

$$\epsilon = \frac{2mE}{\hbar^2}, \quad U(x) = \frac{2m}{\hbar^2}V(x)$$

Then $$\boxed{\psi_E''(x) = -(\epsilon - U(x))\,\psi_E(x)}$$

Next we discuss some general properties of this equation and the Eigenvalue problem.

General Properties of Solutions

Consider $U(x) = U_0$ constant.

The system is equivalent to the free particle with $U_0 = 0$:

Solutions oscillate: $\psi_E(x) = A e^{ikx}$

$$\psi_E''(x) = -k^2 \psi_E(x) = -(\epsilon - U_0)\psi_E(x)$$

$$\rightarrow \epsilon = k^2 + U_0$$

Energy $E = \frac{\hbar^2}{2m}\epsilon = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{2m} U_0$

General time-dependent solution:

$$\Psi(x,t) = \int \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-i\left(\frac{\hbar}{2m}(k^2+U_0)t\right)} f(k)$$

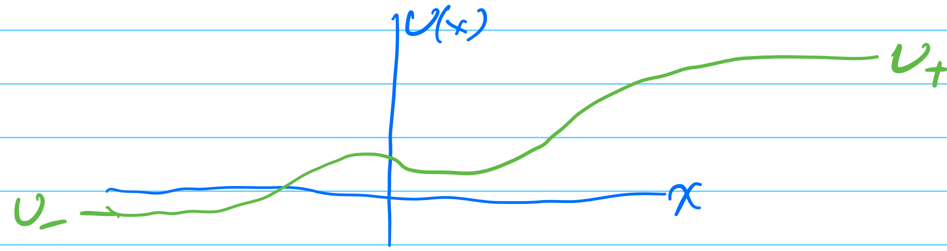
$$= e^{-i\frac{\hbar U_0 t}{2m}} \underbrace{\int \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-i\frac{\hbar k^2}{2m}t} f(k)}$$

Every solution differs from a $U_0 = 0$ solution by the same time-dependent phase.

Hence, $\langle \psi_1(t) | \hat{A} | \psi_2(t) \rangle$ is identical to the equivalent $U_0 = 0$ case, for all $\hat{A}$ and all $|\psi_1\rangle$, $|\psi_2\rangle$.

Let $\lim_{x\to+\infty} U(x) = U_+$, $\lim_{x\to-\infty} U(x) = U_-$,

Assume $U_+ > U_-$.



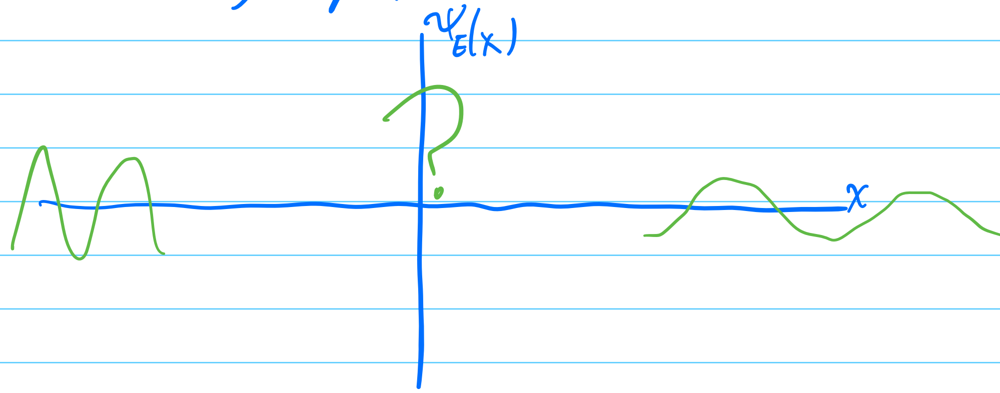
1) Consider stationary solutions with $\epsilon > U_+ > U_-$

As $x \to \pm\infty$ there are two solutions to the second order diff. eq.:

$$\psi(x) \sim e^{ik_\pm x} \quad \text{and} \quad \psi(x) \sim e^{-ik_\pm x}$$

$$k_+ = \sqrt{\epsilon - U_+} \quad , \quad k_- = \sqrt{\epsilon - U_-}$$

Real and imaginary parts are sinusoidal



These are non-normalizable states, but can be superposed to give normalizable wavepackets.

These wavepackets can escape towards $x \to \pm\infty$.
→ Unbound states

2) Solutions with $U_- < E < U_+$:

$E - U(x) > 0$ as $x \to -\infty$
- Unbound solution

$E - U(x) < 0$ as $x \to +\infty$ — Classically forbidden region: $E < V(x)$

$\psi_E''(x) \approx -(E - U_+)\psi_E(x)$ as $x \to +\infty$

$= \underbrace{(U_+ - E)}_{>0} \psi_E(x)$

Solutions: $\psi_E(x) \sim e^{\kappa x}$, $\psi_E(x) \sim e^{-\kappa x}$

with $\kappa = \sqrt{U_+ - E}$

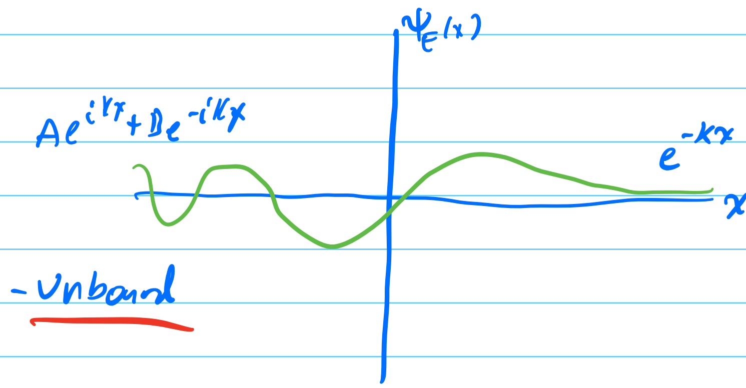
As $x \to +\infty$, $e^{\kappa x} \to \infty$ nonphysical solution

- wavepackets would be non-normalizable.

So, only the $\psi_E(x) \sim e^{-\kappa x}$ solution is physical

As $x \to -\infty$, this solution will become a particular linear combination of the e^{ikx} and e^{-ikx} solutions

→ only one solution for each E with $U_- < E < U_+$.



3) Solutions with $\epsilon < U_- < U_+$

$\epsilon - U(x) < 0$ as $x \to \pm\infty$

For general ϵ:

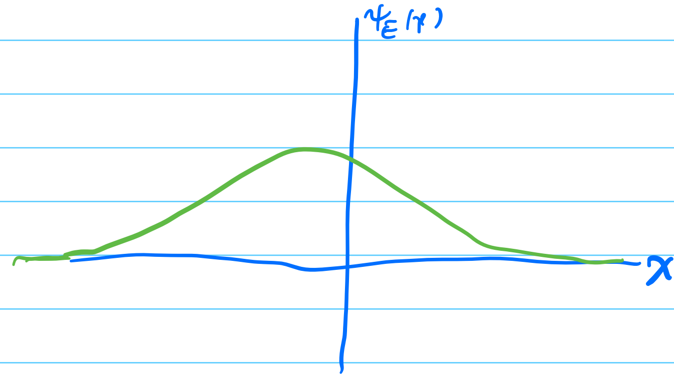
The solution that behaves as $\psi_E(x) \sim e^{-\kappa_+ x}$ as $x \to +\infty$ matches onto a solution that behaves as a linear combination of $\psi_E(x) \sim e^{\kappa_- x}$ and $\psi_E(x) \sim e^{-\kappa_- x}$ as $x \to -\infty$.

These solutions are unphysical unless the $e^{-\kappa_- x}$ part is absent.

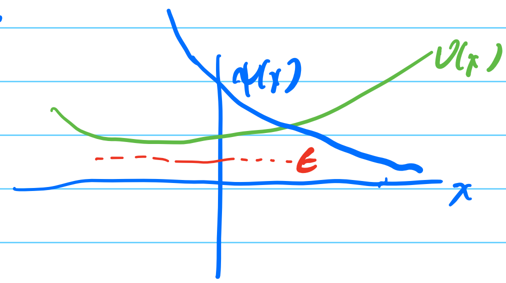
This may happen only for certain values of ϵ.

For these values of ϵ, the solutions fall exponentially at $x \to \pm\infty$

— Bound states



★ There are no physical solutions with $\epsilon < U(x)$ for all x, because those solutions would be either exponentially growing as $x \to -\infty$ or $x \to +\infty$.



★ If $U(x)$ has a global minimum U_{min}, then physical solutions must have $\epsilon > U_{min}$.