Quantum Mechanics and Atomic Physics

Lecture 5: Potential Wells: Part I

http://www.physics.rutgers.edu/ugrad/361

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Last time

Boundary Conditions

1. $\Psi$ must be square integrable: $\int \Psi^*(x,t) \Psi(x,t) dx = 1$

2. The wavefunction $\Psi$ must be a continuous function!
   - This means forcing two solutions at the boundary to agree:
     $\Psi^<(\text{boundary}) = \Psi^>(\text{boundary})$

3. If $V(x)$ is continuous or finitely discontinuous across a boundary, then the first derivative of $\Psi$, $d\Psi/dx$, must be made continuous across the boundary. But if $V(x)$ is infinitely discontinuous across the boundary, then $d\Psi/dx$ cannot be specified across the boundary.

Now, let’s introduce a “particle-in-a-box” ....
Example: “particle-in-a-box”

- Consider a particle of mass \( m \) which can move freely along the \( x \) axis anywhere from \( x=\pm a/2 \) to \( x=\mp a/2 \), but is strictly prohibited from being found outside this region. The particle bounces back and forth between the walls at \( x=\pm a/2 \) of a (1-dim) box. Assume the walls to be completely impenetrable, no matter how energetic the particle is (this is an idealization!).

- The wave function of the particle is:

\[
\psi(x,t) = \begin{cases} 
A \cos \frac{\pi x}{a} e^{-i \frac{E t}{\hbar}} & \text{for } \frac{-a}{2} \leq x \leq \frac{a}{2} \\
0 & \text{else}
\end{cases}
\]
Example, con’t

- Verify that it is a solution to the S.E. in the region $-a/2 \leq x \leq +a/2$ and determine the value of the lowest energy state.

Since there are no forces acting on particle, $V = \text{constant in the region}$.

$i$: We can take $V=0$ in the region.

So,

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = i \hbar \frac{\partial \psi}{\partial t}, \quad -\frac{a}{2} < x < +\frac{a}{2}$$

$$\Rightarrow \frac{\partial \psi}{\partial x} = -\frac{\pi}{a} A \sin \frac{\pi x}{a} e^{-iEt/\hbar}$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\left(\frac{\pi}{a}\right)^2 A \cos \frac{\pi x}{a} e^{-iEt/\hbar} = -\left(\frac{\pi}{a}\right)^2 \psi$$

$$\frac{\partial \psi}{\partial t} = -i\frac{E}{\hbar} A \cos \frac{\pi x}{a} e^{-iEt/\hbar} = -i\frac{E}{\hbar} \psi$$

$$\Rightarrow \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 \psi = -i\hbar \frac{iE}{\hbar} \psi$$

$$\Rightarrow \frac{1}{2m} \left(\frac{\pi}{a}\right)^2 \psi = E \psi \Rightarrow E = \frac{\pi^2 \hbar^2}{2ma^2}$$
Example, con’t

- Plot the space dependence of the wave function (for fixed time).
Solutions to S.E. in 1-dimension:

Overview

- Examples of applications of solutions to the S.E. for a 1-dimensional potential function, $V(x)$
  - Modeling of real electronic devices (e.g. CCD chips)
  - Understanding nuclear phenomena (beyond the energy levels of the H-atom) such as alpha-decay

- In the next few lectures we will:
  - Examine potential wells
  - Solve the S.E. for the first time for an infinite well
  - Consider the finite well
    - Quantum tunneling
  - Consider potential barriers
    - A potential well turned inside-out
    - Important for understanding nuclear structure/scattering
Concept of a Potential Well: Classical Newtonian Example

- Let’s consider a car of mass $m$ on a roller coaster track
- $V(x) = mgh(x)$
- If released from rest, total energy $E = mgh(x_0)$
- If no friction/air resistance, it will remain in valley (or well) between $x_0$ and $x_1$.
  - Constrained in potential well
  - In a bound energy state
    - Total energy is less than $V(x)$ as $x \to \infty$

Reed: Chapter 3
Newtonian example, con’t

- What if car is released from $x_0$ with some non-zero speed?
- Total energy $E = mv_0^2/2 + mgh(x_0)$
- Now car is in a new bound energy state
Newtonian example, con’t

- Now, what if the track to the right of the release point is always lower than the vertical level of the release point?

- The car will eventually arrive at \( x = \infty \)

- This is an illustration of an unbound energy state

In classical mechanics the energy \( E \) is unrestricted - \( E \) does not appear in Newton’s second law.

In QM, it does enter explicitly in S.E. and for a given potential energy, the total energy \( E \) is a parameter of the solutions to S.E.
Time-Independent Potentials

Let’s revisit S.E. for a time-independent potential \( V(x,t) = V(x) \):

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \tilde{\Phi}(x,t)}{\partial x^2} + V(x) \tilde{\Phi}(x,t) = i\hbar \frac{\partial \tilde{\Phi}(x,t)}{\partial t}
\]

Assume \( \tilde{\Phi}(x,t) = \Psi(x) \phi(t) \)

\[
-\frac{\hbar^2}{2m} \phi(t) \frac{d^2 \Psi(x)}{dx^2} + V(x) \Psi(x) \phi(t) = i\hbar \Psi(x) \frac{d\phi(t)}{dt}
\]

Divide by \( \Psi(x) \phi(t) \):

\[
-\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{d^2 \Psi(x)}{dx^2} + V(x) = i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt}
\]

Depends only on \( x \)

\[
\text{Depends only on} \ t.
\]
Time-Independent Potentials, con’t

- “Separation of variables”

- Left hand side = Right hand side
  - Each must be a constant, and the same constant

\[ i \hbar \frac{1}{\Phi(k)} \frac{d\Phi(k)}{dt} = E \] \hspace{1cm} (1)

\[ -\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{d^2\Psi(x)}{dx^2} + V(x) = E \] \hspace{1cm} (2)
Does this look familiar? It’s the time-independent S.E.

We can ignore the constant of integration since it gets absorbed into the normalization anyway.

This equation has now been solved once and forever.
For any time-independent $V(x)$. We can pretty much ignore it from now on.

$$\frac{d\phi}{\phi} = \frac{E}{i\hbar} \, dt = -i \frac{E}{\hbar} \, dt$$

$$\int \frac{d\phi}{\phi} = -i \frac{E}{\hbar} \int dt$$

$$\ln \phi = -i \frac{E}{\hbar} t$$

$$\Rightarrow \phi(t) = e^{-iEt/\hbar}$$

Multiply (2) by $\psi(x)$:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)$$
The Infinite Potential Well

- A particle is trapped between walls so energetically high it would require an infinite amount of energy to get over them.

- Also called *infinite square well* or *infinite rectangular well*

- $V=0$ for $0 \leq x \leq L$
  - Inside the well

- $V=\infty$ for $x<0$, $x>L$
  - Outside the well

- Look for bound-state solutions with $E \geq 0$
In the outside regions: $x<0, x>L$

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

For $x<0, x>L$ $V = \infty$

So,

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

$E$ is assumed to be finite.

Equation is satisfied only if

$\psi = 0$
In the inside region: $0 \leq x \leq L$

In $0 \leq x \leq L$, $V = 0$

\[-\hbar^2 \frac{d^2 \psi}{2m \, dx^2} = E \psi\]

Define $\kappa^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \frac{d^2 \psi}{dx^2} = -\kappa^2 \psi$$

General solution:
$$\psi = A \sin \kappa x + B \cos \kappa x$$

- Let’s apply boundary conditions
  - 3rd condition cannot be applied since we have infinite potential discontinuities
  - We can apply conditions 1 and 2
Continuous Wavefunction

* Requirement of continuity:
  \[ \psi(0) = \psi(L) = 0 \]

1. \[ \psi(0) = 0 \Rightarrow \psi = A \cdot 0 + B = 0 \Rightarrow B = 0 \]
   So, \[ \psi = A \sin kx \]

2. \[ \psi(L) = 0 \Rightarrow kL = n \pi \Rightarrow L = \frac{n \pi}{k} \]

For \( n = 1, 2, 3, \ldots \):

\[ E_n = \frac{n^2 \pi^2 k^2}{2mL^2} \]

\[ \psi_n(x) = A \sin \frac{n \pi x}{L} \]

**Energy Eigenvalues** \( E_n \)

\( n \) is principle quantum number

**Ground state energy** corresponds to \( n = 1 \)

\( (n=0 \text{ leads to a null solution}) \)

**We just derived the quantization of energy!**
Normalized Wavefunction

* Requirement of normalization:

\[ \int \psi^* \psi \, dx = 1 = \int_0^L A^2 \sin^2 \left( \frac{n \pi x}{L} \right) \, dx \]

\[ = A^2 \int_0^L \frac{1}{2} \left( 1 - \cos \frac{2n \pi x}{L} \right) \, dx \]

\[ = \frac{1}{2} A^2 \left[ x - \frac{L}{2n \pi} \sin \frac{2n \pi x}{L} \right]_0^L \]

\[ = \frac{1}{2} A^2 L \]

\[ \implies A = \sqrt{\frac{2}{L}} \]

\[ \implies \psi_n (x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi x}{L} \right) \]

Eigenfunction: solution to the time-independent S.E.
Two key lessons

- The quantized energy levels $E_n$ (energy eigenvalues) resulted naturally by imposing the boundary conditions to the S.E.
  - Lead to the quantum numbers, $n$, allowing us to label the energy eigenvalues

- There is a wavefunction $\Psi_n$ (eigenfunction) corresponding to each eigenvalue
  - Gives the probability distribution of the system for a total energy $E_n$
Energy levels and Wavefunctions

- $n=1$ is ground state
- Number of extrema in wavefunction is equal to $n$
- Nodes are where $\Psi=0$
  - where we never expect to find the particle
  - Number of nodes for state $n$ is $n+1$
Wavefunctions and Probability Distributions

- Probability distributions $|\Psi_n|^2$
  - Peaks correspond to where there is a high probability to find the particle
  - Valleys correspond to low probability

Reed: Chapter 3
Bohr’s correspondence principle

\[ \lim_{n \to \infty} \text{Quantum Physics} = \text{Classical Physics} \]

\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2amL^2} \]

\[ \Rightarrow \Delta E = E_{n+1} - E_n \]

\[ \Delta E = \frac{\pi^2 \hbar^2}{2amL^2} \left[ (n+1)^2 - n^2 \right] \]

\[ = \frac{\pi^2 \hbar^2}{2amL^2} \left( 2n+1 \right) \]

\[ \frac{\Delta E}{E} = \frac{2n+1}{n^2} \Rightarrow \lim_{n \to \infty} \frac{\Delta E}{E} = \frac{2}{n} \to 0 \]

Classically: continuum of energies so \( \Delta E/E = 0 \)

More on this next time ....
Full Wavefunction for Infinite Potential Well

In summary,

\[ \Psi(x, t) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \cdot e^{-iE_n t / \hbar} \]

\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \ldots \]
Summary/Announcements

- Introduction to concept of Potential Wells
- The Infinite Square Well

- Next time:
  - Finite Square Well
  - More on Potential Wells

- Next homework due on Monday Sept 23! (on Chapter 2)

- MONDAY: First quiz on Chapter 1! Open book/open note (NO LAPTOPS OR OTHER ELECTRONIC DEVICES, except for calculator)