Quantum Mechanics and Atomic Physics

Lecture 5: Potential Wells: Part I

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

Prof. Eva Halkiadakis
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.

- Introduced a “particle-in-a-box”
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 $x \rightarrow \infty$
Newtonian example, con’t

- What if car is released from $x_0$ with some non-zero speed?

- Total energy
  $E = \frac{mv_0^2}{2} + mgh(x_0)$

- Now car is in a new bound energy state

Reed: Chapter 3
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 $V(x,t) = V(x)$:

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

Assume $\Psi(x,t) = \Psi(x) \Phi(t)$

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

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 $x$,

Depending only on $t$. 

$\frac{1}{\Psi(x)} \frac{d^2 \Psi(x)}{dx^2}$

$\frac{d \Phi(t)}{dt}$
Time-Independent Potentials, con’t

- “Separation of variables”
- Left hand side = Right hand side
  - Each must be a constant, and the same constant

\[
\begin{align*}
\frac{i \hbar}{\psi(x)} \frac{d}{dt} \phi(t) &= \bar{E} \\
\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) &= \bar{E}
\end{align*}
\]
Solve (1):
\[ \frac{d\phi}{\phi} = \frac{E}{i\hbar} dt = -i \frac{E}{\hbar} dt \]
\[ \int \frac{d\phi}{\phi} = -i \frac{E}{\hbar} \int dt \]
\[ \ln \phi = -i \frac{E}{\hbar} t \]
\[ \Rightarrow \phi(t) = e^{-i E t / \hbar} \]

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.

Multiply (2) by \( \psi(x) \):
\[ -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \]

Does this look familiar? It’s the time-independent S.E.
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 $E>0$
Real Example: Electron trapped in a “box”

FIGURE 3.5  Schematic diagram of an electron trapped in a one-dimensional “box” made of electrodes and grids in an evacuated tube. From An Introduction to Quantum Physics by A. P. French and Edwin F. Taylor. Copyright © 1978 by the Massachusetts Institute of Technology. Used by permission of W. W. Norton & Company, Inc.
In the outside regions: $x<0, x>L$

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

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

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: \(0 \leq x \leq L\)

\[ \text{In } 0 \leq x \leq L, \quad V = 0 \]

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

Define \( k^2 = \frac{2mE}{h^2} \)

\[ \Rightarrow \frac{d^2 \psi}{dx^2} = -k^2 \psi \]

**General Solution:**

\[ \psi = A \sin kx + B \cos kx \]

- 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:
  \[ \Psi(0) = \Psi(L) = 0 \]

\[ \Psi(0) = 0 \implies \Psi = A \sin kx \]

\[ KL = n \pi \implies k = \frac{n \pi}{L} \]

Energy Eigenvalues \( E_n \)

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

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

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

\[ n = 0 \] leads to a null solution

We just derived the quantization of energy!
Normalized Wavefunction

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

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

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

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

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

\[ \Rightarrow \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad 0 \leq x \leq L \quad n = 1, 2, 3, \ldots \]

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 Probablility 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
Why do we not detect a wavy nature in everyday life?

- For a microscopic object

- Let’s evaluate the quantum number for an electron with energy \( E = 20 \text{eV} \) trapped in a potential well of \( L = 1 \text{Å} \)

\[
E = 20 \text{eV} = 3.20 \times 10^{-18} \text{J}
\]

\[
L = 1 \text{Å} = 10^{-10} \text{m}
\]

\[
E = \frac{\pi^2 \hbar^2}{2mL^2} n^2
\]

\[
\Rightarrow n = \sqrt{\frac{2mL^2E}{\pi^2 \hbar^2}} = \sqrt{\frac{2 \times (9.11 \times 10^{-31} \text{J} \cdot \text{s}) \times (1 \times 10^{-10} \text{m})^2 \times (3.20 \times 10^{-18} \text{J})}{(3.14159)^2 \times (1.055 \times 10^{-34} \text{J} \cdot \text{s})^2}}
\]

\[
\approx 0.73 \approx 1
\]
Now for a macroscopic object

- Let’s evaluate the quantum number for an object of mass $m = 1\text{kg}$, energy $E = 1\text{J}$ trapped in a potential well of width $L = 1\text{m}$.

$$n = \sqrt{\frac{2mL^2E}{\pi^2\hbar^2}}$$

$$= \sqrt{\frac{2(1\text{kg})(1\text{m})^2(1\text{J})}{\pi^2(1.055\times10^{-34}\text{J}\cdot\text{s})^2}}$$

$$n \approx 4.3 \times 10^{33}$$

This value of $n$ is so large that we would never be able to distinguish the quantized nature of energy levels.

For example, the difference in energy between two consecutive states, $n_1 = 4.3 \times 10^{33}$ and $n_2 = 4.3 \times 10^{33} + 1$ is around $10^{-34}\text{J}$! This is much too small to be detected.

This also shows that quantum predictions must agree with classical results in the limit of large quantum numbers: Bohr’s correspondence principle.
Bohr’s correspondence principle

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

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

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

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

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

Classically: continuum of energies so \(\Delta E/E = 0\)
Bohr’s correspondence principle, con’t

Let’s evaluate the probability to find a particle in \( x_1 \leq x \leq x_2 \)

\[
P = \int_{x_1}^{x_2} \psi^* \psi \, dx = \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \left( \frac{n \pi x}{L} \right) \, dx
\]

\[
= \frac{2}{L} \int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos \left( \frac{2n \pi x}{L} \right) \right) \, dx
= \frac{1}{L} \left[ x - \frac{L}{2n \pi} \sin \left( \frac{2n \pi x}{L} \right) \right]_{x_1}^{x_2}
\]

\[
= \frac{x_2 - x_1}{L} - \frac{1}{2n \pi} \left( \sin \left( \frac{2n \pi x_2}{L} \right) - \sin \left( \frac{2n \pi x_1}{L} \right) \right)
\]

Bounded: \(-2 \leq \ldots \leq 2\)

So, \( \lim_{n \to \infty} P = \frac{x_2 - x_1}{L} \)

Indeed this is the classical expectation!
You can go back to the problem from last time and convince yourself this works.
Example

- Probabilities for a particle in a box:
  - A particle is known to be in the ground state of a infinite square well with length L. Calculate the probability that this particle will be found in the middle half of the well, between \( x = \frac{L}{4} \) and \( x = \frac{3L}{4} \).
    - Classically: we expect \( 1/2 \) - a classical particle spends equal time in all parts of the well
    - Plug in equation on previous page: \( x_1 = \frac{L}{4}, \ x_2 = \frac{3L}{4} \) and \( n = 1 \)
Ground state $n=1$: $\psi_1 = \sqrt{2/L} \sin \frac{\pi x}{L}$

$$P = \int_{\psi_1}^{3\psi_1} \psi_1^* \psi_1 \, dx = \frac{2}{L} \int_{\psi_1}^{3\psi_1} \sin^2 \frac{\pi x}{L} \, dx$$

$$= \frac{2}{L} \int_{\psi_1}^{3\psi_1} \frac{1}{2} \left(1 - \cos \frac{2\pi x}{L}\right) \, dx$$

$$= \frac{1}{L} \left[ x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{\psi_1}^{3\psi_1}$$

$$= \frac{1}{L} \left[ \frac{3L}{4} - \frac{L}{4} - \frac{L}{2\pi} \left( \sin \frac{3\pi}{2} - \sin \frac{\pi}{2} \right) \right]$$

$$= \frac{1}{L} \left[ \frac{L}{2} - \frac{L}{2\pi} (-1 - 1) \right] = \frac{1}{2} + \frac{1}{\pi} \approx 0.82 = 82\%.$$
Full Wavefunction for Infinite Potential Well

In summary,

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

\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \ldots \]
The Finite Square Well

- Mass \( m \) in a potential well of finite depth
  - This is a more realistic case than infinite square well: e.g. electron trapped in surface of metal which needs a few eV to escape (as in photoelectric effect)

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

- \( V=V_0 \) for \(|x| > L\)
  - Outside the well

- For \( E < V_0 \) we are seeking bound energy states (bottom of the well is at \( V=0 \))

More on this next time....
Summary/Announcements

- Introduction to concept of Potential Wells
- The Infinite Square Well
- The Finite Square Well (to be continued…)

Next time:
- More on Potential Wells

Next homework due on Monday Sept 24! (on Chapter 2)

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