Measurement Expectation: Statistics Lesson

- Ensemble & probable outcome of a single measurement or the average outcome of a large # of measurements

\[
\langle x \rangle = \frac{n_1x_1 + n_2x_2 + n_3x_3 + \ldots n_ix_i}{n_1 + n_2 + n_3 + \ldots n_i} = \frac{\sum_{i=1}^{n} n_ix_i}{N} = \frac{\int xP(x)dx}{\int P(x)dx}
\]

For a general Fn \( f(x) \)

\[
\langle f(x) \rangle = \frac{\sum_{i=1}^{n} n_if(x_i)}{N} = \frac{\int \psi^*(x)f(x)\psi(x)dx}{\int P(x)dx}
\]

Sharpness of a distribution:

- scatter around the average

\[
\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N}}
\]

\[
\sigma = \sqrt{(x^2) - (\bar{x})^2}
\]

\( \sigma \) = small \( \rightarrow \) Sharp distr.

Uncertainty \( \Delta X = \sigma \)
Particle in the Box, n=1, find $<x>$ & $\Delta x$?

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$$

$$<x> = \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{2}{L} \int_0^L x \sin^2\left(\frac{\pi x}{L}\right) dx$$

, change variable $\theta = \left(\frac{\pi x}{L}\right)$

$$\Rightarrow <x> = \frac{2}{L} \int_0^1 \theta \sin^2\theta , \text{ use } \sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$$

$$= \frac{2L}{\pi^2} \left[ \frac{\theta}{2} - \frac{\sin 2\theta}{4} \right]$$

$$\Rightarrow <x> = \frac{L}{\pi^2} \left(\frac{\pi^2}{2}\right) = \frac{L}{2} \text{ (same result as from graphing } \psi^2(x))$$

Similarly $<x^2> = \int_0^L x^2 \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{L^2}{2\pi^2}$

and $\Delta x = \sqrt{<x^2> - <x>^2} = \sqrt{\frac{L^2}{3} - \frac{L^2}{2\pi^2}} = 0.18L$

$\Delta x = 20\%$ of $L$, Particle not sharply confined in Box

---

Table 5.2 Common Observables and Associated Operators

<table>
<thead>
<tr>
<th>Observable</th>
<th>Symbol</th>
<th>Associated Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>position</td>
<td>$x$</td>
<td>$x$</td>
</tr>
<tr>
<td>momentum</td>
<td>$p$</td>
<td>$\hbar \frac{\partial}{i \partial x}$</td>
</tr>
<tr>
<td>potential energy</td>
<td>$U$</td>
<td>$U(x)$</td>
</tr>
<tr>
<td>kinetic energy</td>
<td>$K$</td>
<td>$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$</td>
</tr>
<tr>
<td>hamiltonian</td>
<td>$H$</td>
<td>$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)$</td>
</tr>
<tr>
<td>total energy</td>
<td>$E$</td>
<td>$i\hbar \frac{\partial}{\partial t}$</td>
</tr>
</tbody>
</table>
The Case of a Rusty “Twisted Pair” of Naked Wires & How Quantum Mechanics Saved ECE Majors!

- Twisted pair of Cu Wire (metal) in virgin form
- Does not stay that way for long in the atmosphere
  - Gets oxidized in dry air quickly $\text{Cu} \rightarrow \text{Cu}_2\text{O}$
  - In wet air $\text{Cu} \rightarrow \text{Cu(OH)}_2$ (the green stuff on wires)
- Oxides or Hydride are non-conducting ..so no current can flow across the junction between two metal wires
- No current means no circuits $\rightarrow$ no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news!

Potential Barrier

Consider George as a “free Particle/Wave” with Energy $E$ incident from Left
Free particle are under no Force; have wavefunctions like

$$\Psi = A \, e^{i(kx - wt)} \quad \text{or} \quad B \, e^{i(-kx - wt)}$$
Tunneling Through A Potential Barrier

- Classical & Quantum Pictures compared: When E>U & when E<U
- Classically, an particle or a beam of particles incident from left encounters barrier:
  - when E > U → Particle just goes over the barrier (gets transmitted)
  - When E<U → particle is stuck in region I, gets entirely reflected, no transmission (T)
- What happens in a Quantum Mechanical barrier? No region is inaccessible for particle since the potential is (sometimes small) but finite

Beam Of Particles With E < U Incident On Barrier From Left

Region I
Region III

Incident Beam
Reflected Beam
Transmitted Beam

Description Of Wave Functions in Various regions: Simple Ones first

In Region I: \(\Psi_I(x,t) = Ae^{ik(x-L)} + Be^{i(-kL-x)}\) = incident + reflected Waves

with \(E = \hbar \omega = \frac{\hbar k^2}{2m}\)

Define Reflection Coefficient: \(R = \frac{|B|^2}{|A|^2}\) = frac of incident wave intensity reflected back

In Region III: \(\Psi_III(x,t) = Fe^{i(kx)} + Ge^{i(-kx)}\) = transmitted

Note: \(Ge^{i(-kx)}\) corresponds to wave incident from right!

This piece does not exist in the scattering picture we are thinking of now (G=0)

So \(\Psi(x,t) = Fe^{i(kx)}\) represents transmitted beam. Define \(T = \frac{|F|^2}{|A|^2}\)

Unitarity Condition \(\Rightarrow R + T = 1\) (particle is either reflected or transmitted)
Wave Function Across The Potential Barrier

In Region II of Potential U

\[ \frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} (U - E) \psi(x) = 0 \]

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

\[ = \alpha^2 \psi(x) \]

with \( \alpha = \frac{\sqrt{2m(U - E)}}{\hbar} \); \( U > E \Rightarrow \alpha^2 > 0 \)

Solutions are of form \( \psi(x) = e^{ikx} \)

\[ \Psi_2(x,t) = Ce^{-ikx} + De^{-ikx} \quad 0 < x < L \]

To determine C & D ⇒ apply matching cond.

\[ \Psi_2(x,t) = \text{continuous} \text{ across barrier (x=0,L)} \]

\[ \frac{d\Psi_2(x,t)}{dx} = \text{continuous} \text{ across barrier (x=0,L)} \]

Continuity Conditions Across Barrier

At \( x = 0 \), continuity of \( \psi(x) \) ⇒

\[ A + B = C + D \quad (1) \]

At \( x = 0 \), continuity of \( \frac{d\psi(x)}{dx} \) ⇒

\[ ikA - ikB = \alpha C - \alpha D \quad (2) \]

Similarly at \( x = L \) continuity of \( \psi(x) \) ⇒

\[ C e^{-\alpha L} + D e^{+\alpha L} = F e^{ikL} \quad (3) \]

at \( x = L \), continuity of \( \frac{d\psi(x)}{dx} \) ⇒

\[ -(\alpha C) e^{-\alpha L} + (\alpha D) e^{+\alpha L} = ikF e^{ikL} \quad (4) \]

Four equations & four unknowns

Can determine A,B,C,D but if you

Divide thruout by A in all 4 equations : ⇒ ratio of amplitudes → relations for R & T

That's what we need any way
Potential Barrier when $E < U$

Expression for Transmission Coef $T(E)$:

Depends on barrier Height $U$, barrier Width $L$ and particle Energy $E$

$$T(E) = \left[ 1 + \frac{1}{4} \left( \frac{E^2}{E(U-E)} \right) \sinh^2(\alpha L) \right]^{-1}$$

and $R(E) = 1 - T(E)$ ....... what's not transmitted is reflected

Above equation holds only for $E < U$

For $E > U$, $\alpha =$ imaginary

Sinh($\alpha L$) becomes oscillatory

This leads to an Oscillatory $T(E)$ and Transmission resonances occur where

For some specific energy ONLY, $T(E) = 1$

At other values of $E$, some particles are reflected back ... even though $E > U$!!

That’s the Wave nature of the Quantum particle

Ceparated in Coppertino

Solved Example 6.1 (...that I made such a big deal about yesterday)

Q: Two wires are separated by insulating Oxide layer. Modeling the Oxide layer as a square barrier of height $U = 10.6$ eV, estimate the transmission coeff for an incident beam of electrons of $E = 7.5$ eV when the layer thickness is

(a) 5.0 nm

(b) 1.0 nm

Q: If a 1.0 mA current in one of the terminal wires is incident on Oxide layer, how much of this current passes thru the Oxide layer on to the adjacent wire if the layer thickness is 1.0 nm?

What becomes of the remaining current?

$$T(E) = \left[ 1 + \frac{1}{4} \left( \frac{U^2}{E(U-E)} \right) \sinh^2(\alpha L) \right]^{-1}$$

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$
Then transform the systems orthogonal dimensions (in 1-Dimension (x) → three orthogonal dimensions (r ← x,y,z)

Then transform the systems
- Particle in 1D rigid box → 3D rigid box
- 1D Harmonic Oscillator → 3D Harmonic Oscillator
  - Keep an eye on the number of different integers needed to specify system 1 → 3 (corresponding to 3 available degrees of freedom x,y,z)

\[ \hat{r} = \hat{x} + \hat{y} + \hat{z} \]

Learn to extend S. Eq and its solutions from “toy” examples in 1-Dimension (x) → three orthogonal dimensions (r ← x,y,z)

\[ T(E) = \left[ 1 + \frac{1}{4} \left( \frac{E - E_1}{E_1} \right)^2 \right]^{\frac{1}{2}} \]

\[ \text{Use } \hbar = 1.973 \text{ keV } \AA^1, m_0 = 511 \text{ keV } \AA^2 \]

\[ \alpha = \sqrt{\frac{2 m_r (U - E)}{\hbar}} = \sqrt{\frac{2 \times 511 \text{ kev } / c^2 (3.0 \times 10^{-11} \text{ kev})}{1.973 \text{ keV } \AA^2}} = 0.8875 \AA^{-1} \]

Substitute in expression for \( T = T(E) \)

\[ T = \left[ 1 + \frac{1}{4} \left( \frac{U - E}{U_0 - E_0} \right)^2 \right]^{\frac{1}{2}} \text{H}^2(0.8875 \AA^{-1})(50 \AA) \]

\[ = 0.953 \times 10^{-6} \text{ (small)} \]

However, for \( L = 10 \AA, T = 6.57 \times 10^{-7} \)

Reacting barrier width by \( \times 3 \) leads to Trans. Go up enhancement by 3: factor of magnitude 10

1 mA current \( = \frac{Q}{N} = \frac{N_0}{1} \Rightarrow N = 6.25 \times 10^4 \text{ electrons} \)

\( N_r = \frac{N_0}{N} = (6.25 \times 10^4 \text{ electrons}) \times \frac{1}{1} \]

For \( L = 10 \AA, T = 6.57 \times 10^{-7} \) ⇒ \( N_r = 4.11 \times 10^4 \Rightarrow I_r = 65.7 \mu A \)
The Quantum Mechanics In 3D: Particle in 3D Box

Time Dependent Schrödinger Eqn:

\[-\frac{\hbar^2}{2m} \nabla^2 \Psi(x, y, z, t) + U(x, y, z) \Psi(x, y, z, t) = i\hbar \frac{\partial \Psi(x, y, z, t)}{\partial t} \quad \text{...In 3D}\]

\[\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\]

So \[\frac{\hbar^2}{2m} \nabla^2 = \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) + \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2}\right) + \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2}\right) = [K]\]

\[= [K_x] + [K_y] + [K_z]\]

so \([H] \Psi(x, t) = [E] \Psi(x, t)\) is still the Energy Conservation Eq

Stationary states are those for which all probabilities are constant in time and are given by the solution of the TDSE in separable form:

\[\Psi(x, y, z, t) = \Psi(r, t) = \psi(r)e^{i\omega t}\]

This statement is simply an extension of what we derived in case of 1D time-independent potential.
Particle in 3D Rigid Box: Separation of Orthogonal Spatial (x,y,z) Variables

TISE in 3D: \[ \frac{\hbar^2}{2m} \nabla^2 \psi(x,y,z) + U(x,y,z) \psi(x,y,z) = E \psi(x,y,z) \]

x,y,z independent of each other, write \( \psi(x,y,z) = \psi_1(x) \psi_2(y) \psi_3(z) \)

and substitute in the master TISE, after dividing throughout by \( \psi = \psi_1(x) \psi_2(y) \psi_3(z) \)

and noting that U(r)=0 for (0<x,y,z<L) \( \Rightarrow \)

\[ \left( \frac{\hbar^2}{2m} \frac{\partial^2 \psi_1(x)}{\partial x^2} \right) + \left( \frac{\hbar^2}{2m} \frac{\partial^2 \psi_2(y)}{\partial y^2} \right) + \left( \frac{\hbar^2}{2m} \frac{\partial^2 \psi_3(z)}{\partial z^2} \right) = E = \text{Const} \]

This can only be true if each term is constant for all x,y,z \( \Rightarrow \)

\[ \frac{\hbar^2}{2m} \frac{\partial^2 \psi_1(x)}{\partial x^2} = E \psi_1(x) \quad \frac{\hbar^2}{2m} \frac{\partial^2 \psi_2(y)}{\partial y^2} = E \psi_2(y) \quad \frac{\hbar^2}{2m} \frac{\partial^2 \psi_3(z)}{\partial z^2} = E \psi_3(z) \]

With \( E_1 + E_2 + E_3 = E = \text{Constant} \) (Total Energy of 3D system)

Each term looks like particle in 1D box (just a different dimension)

So wavefunctions must be like \( \psi_1(x) \propto \sin k_x x \quad \psi_2(y) \propto \sin k_y y \quad \psi_3(z) \propto \sin k_z z \)

Particle in 3D Rigid Box: Separation of Orthogonal Variables

Wavefunctions are like \( \psi_1(x) \propto \sin k_x x \quad \psi_2(y) \propto \sin k_y y \quad \psi_3(z) \propto \sin k_z z \)

Continuity Conditions for \( \psi_i \) and its first spatial derivatives \( \Rightarrow \)

\( n_i \pi = k_i L \)

 Leads to usual Quantization of Linear Momentum \( \hat{p} = \hbar \)k \( \ldots \) in 3D

\[ p_x = \left( \frac{\pi \hbar}{L} \right) n_x \quad p_y = \left( \frac{\pi \hbar}{L} \right) n_y \quad p_z = \left( \frac{\pi \hbar}{L} \right) n_z \] \( n_x, n_y, n_z = 1,2,3,\ldots\infty \)

Note: by usual Uncertainty Principle argument neither of \( n_x, n_y, n_z = 0 \) (why?)

Particle Energy \( E = K+U = K + 0 = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \)

Energy is again quantized and brought to you by integers \( n_x, n_y, n_z \) (independent) and \( \psi(r) \propto A \sin k_x x \sin k_y y \sin k_z z \) (A = Overall Normalization Constant)

\[ \Psi(\vec{r},t) = \psi(\vec{r}) e^{-i\frac{Et}{\hbar}} = A [ \sin k_x x \sin k_y y \sin k_z z ] e^{-i\frac{Et}{\hbar}} \]
Particle in 3D Box: Wave function Normalization Condition

\[ \Psi(\vec{r}, t) = \psi(\vec{r}) e^{\frac{i E t}{\hbar}} = A \left[ \sin k_x x \sin k_y y \sin k_z z \right] e^{\frac{i E t}{\hbar}} \]

\[ \Psi^*(\vec{r}, t) = \psi^*(\vec{r}) e^{\frac{i E t}{\hbar}} = A \left[ \sin k_x x \sin k_y y \sin k_z z \right] e^{\frac{i E t}{\hbar}} \]

\[ \Psi^*(\vec{r}, t) \Psi(\vec{r}, t) = A^2 \left[ \sin^2 k_x x \sin^2 k_y y \sin^2 k_z z \right] \]

Normalization Condition: \( 1 = \iiint_{x,y,z} P(r) \, dx \, dy \, dz \Rightarrow \)

\[ 1 = A^2 \int_{x=0}^{L} \sin^2 k_x x \, dx \int_{y=0}^{L} \sin^2 k_y y \, dy \int_{z=0}^{L} \sin^2 k_z z \, dz = A^2 \left( \frac{L}{2} \right) \left( \frac{L}{2} \right) \left( \frac{L}{2} \right) \]

\[ \Rightarrow A = \left[ \frac{2}{L} \right]^\frac{3}{2} \text{ and } \Psi(\vec{r}, t) = \left[ \frac{2}{L} \right]^\frac{3}{2} \left[ \sin k_x x \sin k_y y \sin k_z z \right] e^{\frac{i E t}{\hbar}} \]

Particle in 3D Box: Energy Spectrum & Degeneracy

\[ E_{n_1,n_2,n_3} = \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) ; \quad n_i = 1, 2, 3 \ldots \infty, n_i \neq 0 \]

Ground State Energy \( E_{111} = \frac{3\pi^2 \hbar^2}{2mL^2} \)

Next level \( \Rightarrow \) 3 Excited states \( E_{211} = E_{121} = E_{112} = \frac{6\pi^2 \hbar^2}{2mL^2} \)

Different configurations of \( \psi(\vec{r}) = \psi(x,y,z) \) have same energy \( \Rightarrow \) degeneracy

\[ \begin{array}{c|c|c} \hline \hline n^2 & \text{Degeneracy} & \text{Landau Level} \\ \hline 4k_0 & 12 & \text{None} \\ \frac{3}{2}k_0 & 11 & 3 \\ \frac{1}{2}k_0 & 10 & 3 \\ k_0 & 9 & 3 \\ 2k_0 & 6 & 3 \\ & & \text{None} \\ \hline \end{array} \]