4E : The Quantum Universe

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Particle Beams and Flux Conservation

If we write the particle wavefunction for incident as $\psi_{I+} = Ae^{ikIx}$ and reflected as $\psi_{I-} = Be^{-ikIx}$

The particle flux arriving at the barrier, defined as number of particles per unit length per unit time

$S_{I+} = |\psi_{I+}^* \psi_{I+}| V_{I+} = |\psi_{I+}^* \psi_{I+}| \left(\frac{p}{m}\right)$ and $S_{I-} = |\psi_{I-}^* \psi_{I-}| \left(\frac{p}{m}\right)$; (for non-relativistic case)

Since the wavefunction in region III $\psi_{III+} = \psi_{III} = Fe^{ikI_{III}x}$ and $S_{III+} = |\psi_{III+}^* \psi_{III+}| \left(\frac{p_{III}}{m}\right)$

The general expression for flux probabilities : number of particles passing by any point per unit time:

Transmission Probability $T = \frac{|\psi_{III+}^* \psi_{III+}| V_{III+}}{|\psi_{I+}^* \psi_{I+}| V_{I+}} = \left(\frac{F}{A}\right)^* \left(\frac{F}{A}\right) \left(\frac{V_{III+}}{V_{I+}}\right)$

Reflection Probability $R = \frac{|\psi_{I-}^* \psi_{I-}| V_{I-}}{|\psi_{I+}^* \psi_{I+}| V_{I+}} = \left(\frac{B}{A}\right)^* \left(\frac{B}{A}\right) \left(\frac{V_{I-}}{V_{I+}}\right)$

The general expression for conservation of particle flux remains: $1 = T + R$
Where does this generalization become important?

- Particle with energy $E$ incident from left on a potential step $U$, with $E > U$
- Particle momentum, wavelength and velocities are different in region I and II
- Is the reflection probability = 0 ?
Where does this generalization become important?
QM in 3 Dimensions

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

\[ \vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \]

- 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)
Quantum Mechanics In 3D: Particle in 3D Box

Extension of a Particle In a Box with rigid walls

1D $\rightarrow$ 3D

$\Rightarrow$ Box with Rigid Walls ($U=\infty$) in X,Y,Z dimensions

U(r)=0 for $(0<x,y,z,L)$

Ask same questions:
- Location of particle in 3d Box
- Momentum
- Kinetic Energy, Total Energy
- Expectation values in 3D

To find the Wavefunction and various expectation values, we must first set up the appropriate TDSE & TISE
The Schrödinger Equation in 3 Dimensions: Cartesian Coordinates

Time Dependent Schrodinger Eqn:

\[-\frac{\hbar^2}{2m} \nabla^2 \Psi(x, y, z, t) + U(x, y, z)\Psi(x, t) = i\hbar \frac{\partial \Psi(x, y, z, t)}{\partial t} \] ....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 \[\hat{H}\Psi(x, t) = \hat{E}\Psi(x, t)\] 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:

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

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 \((0<x,y,z,<L)\) \(\Rightarrow\)

\[
\left(-\frac{\hbar^2}{2m} \frac{1}{\psi_1(x)} \frac{\partial^2 \psi_1(x)}{\partial x^2}\right) + \left(-\frac{\hbar^2}{2m} \frac{1}{\psi_2(y)} \frac{\partial^2 \psi_2(y)}{\partial y^2}\right) + \left(-\frac{\hbar^2}{2m} \frac{1}{\psi_3(z)} \frac{\partial^2 \psi_3(z)}{\partial z^2}\right) = E = \text{Constant}
\]

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

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_1(x)}{\partial x^2} = E_1\psi_1(x); \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_2(y)}{\partial y^2} = E_2\psi_2(y); \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_3(z)}{\partial z^2} = E_3\psi_3(z)
\]

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 \(\psi_1(x) \propto \sin k_1 x\); \(\psi_2(y) \propto \sin k_2 y\); \(\psi_3(z) \propto \sin k_3 z\)
Particle in 3D Rigid Box: Separation of Orthogonal Variables

Wavefunctions are like \( \psi_1(x) \propto \sin k_1x \), \( \psi_2(y) \propto \sin k_2y \), \( \psi_3(z) \propto \sin k_3z \)

Continuity Conditions for \( \psi_i \) and its first spatial derivatives \( \Rightarrow n_i \pi = k_i L \)

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

\[
\begin{align*}
p_x &= \left( \frac{\pi \hbar}{L} \right) n_1 \\
p_y &= \left( \frac{\pi \hbar}{L} \right) n_2 \\
p_z &= \left( \frac{\pi \hbar}{L} \right) n_3
\end{align*}
\]

(\( n_1, n_2, n_3 = 1, 2, 3, \ldots \infty \))

Note: by usual Uncertainty Principle argument neither of \( n_1, n_2, n_3 \neq 0 ! \) (why?)

Particle Energy \( E = K + U = K + 0 = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) = \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \)

Energy is again quantized and brought to you by integers \( n_1, n_2, n_3 \) (independent) and \( \psi(\vec{r}) = A \sin k_1x \sin k_2y \sin k_3z \) (A = Overall Normalization Constant)

\[
\Psi(\vec{r},t) = \psi(\vec{r}) e^{-i \frac{E}{\hbar} t} = A [\sin k_1x \sin k_2y \sin k_3z] e^{-i \frac{E}{\hbar} t}
\]
Particle in 3D Box: Wave function Normalization Condition

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

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

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

Normalization Condition: \( 1 = \iiint P(r) dx \, dy \, dz \implies 1 = A^2 \int_{x=0}^{L} \sin^2 k_x x \, dx \int_{y=0}^{L} \sin^2 k_y y \, dy \int_{z=0}^{L} \sin^2 k_z z \, dz = A^2 \left( \frac{L}{2} \right) \left( \frac{L}{2} \right) \left( \frac{L}{2} \right) \)

\[ \implies A = \left[ \frac{2}{L} \right]^3 \quad \text{and} \quad \Psi(\vec{r},t) = \left[ \frac{2}{L} \right]^3 [\sin k_x x \sin k_y y \sin k_z z] e^{\frac{-iE}{\hbar} t} \]
Particle in 3D Box: Energy Spectrum & Degeneracy

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

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 \( \psi(r) = \psi(x,y,z) \) have same energy \( \Rightarrow \) degeneracy

\[ \begin{array}{|c|c|c|} \hline n^2 & \text{Degeneracy} & \text{None} \\ \hline 4E_0 & 12 & \text{None} \\ \frac{11}{3}E_0 & 11 & 3 \\ 3E_0 & 9 & 3 \\ 2E_0 & 6 & 3 \\ E_0 & 3 & \text{None} \\ \hline \end{array} \]
Degenerate States

\[ E_{211} = E_{121} = E_{112} = \frac{6\pi^2 \hbar^2}{2mL^2} \]
Probability Density Functions for Particle in 3D Box

Same Energy $\rightarrow$ Degenerate States
Can’t tell by measuring energy if particle is in 211, 121, 112 quantum state
Source of Degeneracy: How to “Lift” Degeneracy

- Degeneracy came from the threefold symmetry of a CUBICAL Box \((L_x = L_y = L_z = L)\)

- To Lift (remove) degeneracy \(\rightarrow\) change each dimension such that CUBICAL box \(\rightarrow\) Rectangular Box
  - \((L_x \neq L_y \neq L_z)\)
  - Then

\[
E = \left(\frac{n_1^2 \pi^2}{2mL_x^2}\right) + \left(\frac{n_2^2 \pi^2}{2mL_y^2}\right) + \left(\frac{n_3^2 \pi^2}{2mL_z^2}\right)
\]