DETAILED STUDY MATERIALS: QUANTUM MECHANICS - PARTICLE IN A BOX AND STATIONARY STATES

This document provides a detailed study of key concepts in Quantum Mechanics, focusing on the "Particle in a Box" model and stationary states under various potentials. It includes theoretical explanations and outlines common numerical problems encountered in these topics.

I. PARTICLE IN A BOX

The "Particle in a Box" model is a fundamental problem in quantum mechanics used to illustrate quantization of energy and wave-particle duality. It considers a particle confined to a specific region of space by impenetrable potential barriers.

A. Setting up the Schrödinger Equation for a One-Dimensional Box

Consider a particle of mass 'm' confined to a one-dimensional region of length 'L' along the x-axis (from x=0 to x=L). The potential V(x) is defined as:

- V(x) = 0, for 0 < x < L (inside the box)
- V(x) = \u221e, for x \u2264 0 and x \u2265 L (outside the box)

The time-independent Schrödinger equation is given by:

\u2212\u210F\u00b2/(2m) \u2202\u00b2\u03c8(x)/\u2202x\u00b2 + V(x)\u03c8(x) = E\u03c8(x)

Since V(x) is infinite outside the box, the wave function \u03c8(x) must be zero in those regions. For the region inside the box (0 < x < L), V(x) = 0, so the equation simplifies to:

\u2212\u210F\u00b2/(2m) d\u00b2\u03c8(x)/dx\u00b2 = E\u03c8(x)

Rearranging, we get: d\u00b2\u03c8(x)/dx\u00b2 = \u2212k\u00b2\u03c8(x), where k\u00b2 = 2mE/\u210F\u00b2.

B. Solution of the Schrödinger Equation

The general solution to d\u00b2\u03c8(x)/dx\u00b2 = \u2212k\u00b2\u03c8(x) is:

\u03c8(x) = A sin(kx) + B cos(kx)

Boundary conditions are applied to find A, B, and the allowed values of E:

1. At x = 0, \u03c8(0) = 0: A sin(0) + B cos(0) = 0 \u2192 B = 0. So, \u03c8(x) = A sin(kx).
2. At x = L, \u03c8(L) = 0: A sin(kL) = 0. Since A cannot be zero (otherwise \u03c8(x)=0 everywhere), sin(kL) must be zero. This implies kL = n\u03c0, where n is a positive integer (n = 1, 2, 3, ...).

Thus, k_n = n\u03c0/L.

C. Eigenvalues and Eigenfunctions

Substituting k_n back into the expression for k\u00b2:

k_n\u00b2 = (n\u03c0/L)\u00b2 = 2mE_n/\u210F\u00b2

This gives the quantized energy levels (eigenvalues):

\u2212 E_n = n\u00b2\u03c0\u00b2\u210F\u00b2 / (2mL\u00b2), for n = 1, 2, 3, ...

The corresponding wave functions (eigenfunctions) are:

\u03c8_n(x) = A sin(n\u03c0x/L)

To find A, we use the normalization condition (\u222b||\u03c8_n(x)||\u00b2dx = 1). This yields A = \u221a(2/L).

\u2212 \u03c8_n(x) = \u221a(2/L) sin(n\u03c0x/L), for 0 < x < L.

D. Comparison with Free Particle Eigenfunctions and Eigenvalues

For a free particle (V(x) = 0 everywhere), the Schrödinger equation is:

\u2212\u210F\u00b2/(2m) d\u00b2\u03c8(x)/dx\u00b2 = E\u03c8(x)

The solutions are plane waves: \u03c8(x) = A exp(ikx), where k = \u221a(2mE)/\u210F. The energy E can take any non-negative value, meaning the energy spectrum is continuous. There are no boundary conditions to quantize energy.

In contrast, for the particle in a 1D box:

- The energy levels are discrete and quantized (E_n).
- The wave functions are standing waves (sine functions), not propagating waves.
- The lowest possible energy (ground state) is E_1 = \u03c0\u00b2\u210F\u00b2 / (2mL\u00b2) (zero-point energy), whereas a free particle can have E=0.

E. Properties of Particle in a Box Wave Functions

- **Normalization:** The wave functions are normalized such that the total probability of finding the particle in the box is 1: \u222b\u2080\u1d67 |\u03c8_n(x)|\u00b2 dx = 1.
- **Orthogonality:** Wave functions for different energy levels are orthogonal: \u222b\u2080\u1d67 \u03c8_m*(x)\u03c8_n(x) dx = 0 for m \u2260 n. This property is crucial for expanding arbitrary wave functions in terms of energy eigenfunctions.
- **Probability Distribution:** The probability density is given by |\u03c8_n(x)|\u00b2 = (2/L) sin\u00b2(n\u03c0x/L). This shows that the probability is not uniform across the box. For higher 'n', the probability distribution becomes more complex with nodes (zero probability) and antinodes (maximum probability).

F. Expectation Values and the Uncertainty Principle

Expectation values represent the average value of an observable quantity for a particle in a given state \u03c8_n(x).

- **Expectation value of position :** = \u222b\u2080\u1d67 \u03c8_n*(x) x \u03c8_n(x) dx = L/2. The average position is always the center of the box, regardless of the energy level 'n'.
- **Expectation value of position squared :** = \u222b\u2080\u1d67 \u03c8_n*(x) x\u00b2 \u03c8_n(x) dx = L\u00b2/3 - L\u00b2/(2n\u00b2\u03c0\u00b2).

- **Expectation value of momentum :** = \u222b\u2080\u1d67 \u03c8_n*(x) (\u2212i\u210F d/dx) \u03c8_n(x) dx = 0. This is because the particle is confined, and its momentum is not directed. The wave function is a superposition of states with momentum +p and -p.
- **Expectation value of momentum squared :** = \u222b\u2080\u1d67 \u03c8_n*(x) (\u2212\u210F\u00b2 d\u00b2/dx\u00b2) \u03c8_n(x) dx = (n\u00b2\u03c0\u00b2\u210F\u00b2) / L\u00b2 = 2mE_n.

Significance to the Uncertainty Principle: Heisenberg's Uncertainty Principle states that \u0394x \u0394p_x \u2265 \u210F/2. Here, \u0394x\u00b2 = - \u00b2 and \u0394p_x\u00b2 = - \u00b2.

For the particle in a box, both \u0394x and \u0394p_x are non-zero for all energy levels 'n'. Even in the ground state (n=1), the particle has an uncertain position and momentum. The product \u0394x \u0394p_x is found to be greater than \u210F/2, satisfying the uncertainty principle. As 'n' increases, E_n and increase, meaning \u0394p_x increases (particle is more "certain" about its momentum magnitude). However, the wave function becomes more complex, increasing \u0394x. The principle holds: confining a particle increases the uncertainty in both position and momentum.

G. Extension to Two and Three Dimensions

The particle in a box problem can be extended to higher dimensions. For a rectangular box of dimensions Lx, Ly, Lz:

- **2D Box:** V(x,y) = 0 for 0
- Energy eigenvalues: E_{n_x,n_y} = (\u03c0\u00b2\u210F\u00b2 / 2m) * (n_x\u00b2/Lx\u00b2 + n_y\u00b2/Ly\u00b2).
- Eigenfunctions: \u03c8_{n_x,n_y}(x,y) = \u221a(4/(LxLy)) sin(n_x\u03c0x/Lx) sin(n_y\u03c0y/Ly).
- **3D Box:** V(x,y,z) = 0 for 0
- Energy eigenvalues: E_{n_x,n_y,n_z} = (\u03c0\u00b2\u210F\u00b2 / 2m) * (n_x\u00b2/Lx\u00b2 + n_y\u00b2/Ly\u00b2 + n_z\u00b2/Lz\u00b2).
- Eigenfunctions: \u03c8_{n_x,n_y,n_z}(x,y,z) = \u221a(8/(LxLyLz)) sin(n_x\u03c0x/Lx) sin(n_y\u03c0y/Ly) sin(n_z\u03c0z/Lz).

Concept of Degenerate Energy Levels: Degeneracy occurs when two or more different quantum states have the same energy. In a 2D or 3D box, if the dimensions are not all equal (e.g., Lx \u2260 Ly), different combinations of quantum numbers (n_x, n_y, n_z) can result in the same total energy. For example, in a cubic box (Lx=Ly=Lz=L), the states (n_x=1, n_y=2, n_z=1) and (n_x=2, n_y=1, n_z=1) would have the same energy if the terms involving n_x and n_y in the energy formula are equal, which can happen for different quantum numbers if the dimensions differ.

II. STATIONARY STATES UNDER SPECIAL POTENTIALS

Stationary states are states whose probability density |\u03c8(x,t)|\u00b2 is independent of time. These states can be represented as \u03c8(x,t) = \u03c8(x) exp(-iEt/\u210F), where \u03c8(x) is an energy eigenfunction and E is the corresponding energy eigenvalue.

A. The Potential Step

Consider a particle encountering a potential step:

- V(x) = 0 for x < 0
- V(x) = V_0 for x \u2265 0

Let the particle's energy be E.

1. **Case 1: E > V_0**

   In this case, the particle has enough energy to overcome the step. Classically, it would continue moving, possibly with reduced speed. Quantum mechanically:

   - Region x < 0: \u2212\u210F\u00b2/(2m) d\u00b2\u03c8_1/dx\u00b2 = E\u03c8_1 \u2192 k_1 = \u221a(2mE)/\u210F. Wave function is a sum of incident and reflected waves: \u03c8_1(x) = A exp(ik_1x) + B exp(\u2212ik_1x).
   - Region x \u2265 0: \u2212\u210F\u00b2/(2m) d\u00b2\u03c8_2/dx\u00b2 = (E-V_0)\u03c8_2 \u2192 k_2 = \u221a(2m(E-V_0))/\u210F. Wave function is a transmitted wave: \u03c8_2(x) = C exp(ik_2x). (No reflected wave from the right).

   Applying boundary conditions (\u03c8_1(0)=\u03c8_2(0) and d\u03c8_1/dx|_{x=0} = d\u03c8_2/dx|_{x=0}), we can calculate the reflection coefficient (R) and transmission coefficient (T).

Reflection Coefficient (R): Fraction of incident probability current reflected. R = |B/A|\u00b2 = (\u2009k_1 \u2212 k_2\u2009 / k_1 + k_2)\u00b2 = (1 \u2212 \u221a(1 \u2212 V_0/E))\u00b2 / (1 + \u221a(1 \u2212 V_0/E))\u00b2.

Transmission Coefficient (T): Fraction of incident probability current transmitted. T = 1 - R = 4k_1k_2/(k_1+k_2)\u00b2 = 4\u221a(1 \u2212 V_0/E) / (1 + \u221a(1 \u2212 V_0/E))\u00b2.

3. **Case 2: E < V_0**

   Classically, the particle would be reflected. Quantum mechanically, there's a non-zero probability of transmission.

   - Region x < 0: Same as above, k_1 = \u221a(2mE)/\u210F. \u03c8_1(x) = A exp(ik_1x) + B exp(\u2212ik_1x).
   - Region x \u2265 0: E-V_0 is negative. Let \u03ba = \u221a(2m(V_0-E))/\u210F. The equation becomes d\u00b2\u03c8_2/dx\u00b2 = \u03ba\u00b2\u03c8_2. The solution must be normalizable, so we only allow a decaying exponential: \u03c8_2(x) = C exp(\u2212\u03ba x).

   Applying boundary conditions yields R = 1 and T = 0. This means there is no steady-state transmission (the wave function decays exponentially and becomes negligible far from the boundary). However, if we consider a finite barrier, tunneling can occur.

B. Particle in a 1-D Potential Barrier of Finite Height and Finite Thickness

Consider a barrier V(x) = V_0 for 0 < x < a, and V(x) = 0 otherwise.

- **Case 1: E > V_0**

  The particle can be reflected or transmitted. The wave function is a sum of incident, reflected, and transmitted waves across the barrier. Coefficients R and T are calculated using boundary conditions at x=0 and x=a. T is generally less than 1 due to reflection.

- **Case 2: E < V_0**

  Classically, the particle would be reflected. Quantum mechanically, there is a non-zero probability of transmission, known as tunneling. The wave function inside the barrier decays exponentially but does not become zero. This non-zero amplitude on the other side leads to a transmitted wave.

  Tunneling Probability (for E < V_0 and a thick barrier):

The transmission coefficient T is approximately given by T \u2248 exp(\u22122\u03ba a), where \u03ba = \u221a(2m(V_0-E))/\u210F. This exponential dependence shows that tunneling probability decreases rapidly with barrier thickness 'a' and height (V_0-E).

C. Quantum Mechanical Tunneling

Quantum mechanical tunneling is a phenomenon where a particle can pass through a potential barrier even if its kinetic energy is less than the barrier height. This is a direct consequence of the wave nature of particles and the probabilistic interpretation of the wave function. It is essential in many physical processes, including nuclear fusion, radioactive decay, and the operation of scanning tunneling microscopes.

D. Particle in a Finite Potential Well (0 < E < V_0)

Consider a potential well of depth V_0 and width L:

- V(x) = \u2212V_0 for \u2212L/2 < x < L/2
- V(x) = 0 for |x| \u2265 L/2

For bound states, the particle's energy E is less than the height of the surrounding potential (E < 0, assuming V=0 outside). However, the problem is often formulated with V=0 outside and V=-V_0 inside, so 0 < E < V_0. The wave function must be continuous and have continuous derivatives at the boundaries.

Solution: The equation inside the well becomes \u2212\u210F\u00b2/(2m) d\u00b2\u03c8/dx\u00b2 = E\u03c8, leading to sinusoidal solutions (\u03c8 \u221d sin(kx)). Outside the well, it becomes \u2212\u210F\u00b2/(2m) d\u00b2\u03c8/dx\u00b2 = \u2212V_0\u03c8, leading to exponentially decaying solutions (\u03c8 \u221d exp(\u2212\u03ba x)).

Matching boundary conditions leads to a transcendental equation that determines the allowed energy levels. Unlike the infinite square well, a finite well has a finite number of bound states. The ground state energy is always greater than the ground state energy for an infinite well of the same width and deeper.

E. Bound States in Slowly Varying Potential

For a potential that varies slowly compared to the de Broglie wavelength of the particle, the WKB (Wentzel-Kramers-Brillouin) approximation can be used. This method allows us to find approximate wave functions and energy levels for complex potentials where exact solutions are difficult.

The WKB energy quantization condition for bound states in a potential V(x) is given by:

\u222b_{x_1}^{x_2} p(x) dx = (n + 1/2)\u03c0\u210F, where p(x) = \u221a(2m(E - V(x))) is the classical momentum, and x_1, x_2 are the classical turning points (where E = V(x)).

This approximation is valid when the potential does not change significantly over distances comparable to the wavelength. It correctly reproduces the energy levels of the harmonic oscillator and provides good estimates for other potentials.

NUMERICAL PROBLEMS OUTLINE

Typical numerical problems for these topics involve:

- Calculating specific energy eigenvalues and wave functions for a given particle mass and box dimensions.
- Computing probabilities of finding a particle in a specific region of the box.
- Calculating expectation values for position, momentum, and their squares.
- Verifying the uncertainty principle for given states.
- Calculating reflection and transmission coefficients for potential steps and barriers at specific energies and barrier parameters.
- Estimating tunneling probabilities for different barrier shapes and particle energies.
- Determining the number of bound states in a finite potential well and estimating their energies.

These calculations often involve numerical integration, solving transcendental equations, or applying approximation methods.