PHY402

QUANTUM MECHANICS II

La-Net

COURSE CODE: PHY 402
COURSE TITLE: Quantum Mechanics II
COURSE UNIT: 3 UNITS
Here are five comprehensive series titles that fully cover the scope of the attached PHY 402 course:

Series 1: Perturbation Methods in Quantum Mechanics

Series 2: Quantum Scattering Theory and Elastic Potential Scattering

Series 3: Symmetries and Selection Rules in Quantum Mechanics

Series 4: Quantum Models of Atomic, Molecular, Solid-State, and Nuclear Phenomena

Series 5: Relativistic Wave Equations and Quantum Motion in Electromagnetic Fields

Series 2: Scattering Theory in Quantum Mechanics

Part 2.1: Fundamentals of Scattering

2.1.1 Classical versus quantum scattering
2.1.2 Scattering amplitude and differential cross-section
2.1.3 Physical interpretation of scattering experiments

Part 2.2: Elastic Potential Scattering

2.2.1 Concept of elastic scattering
2.2.2 Potential scattering models
2.2.3 Applications in atomic and nuclear systems

Part 2.3: Partial Wave Analysis

2.3.1 Expansion in spherical harmonics
2.3.2 Phase shifts and resonance phenomena
2.3.3 Applications in low-energy scattering

Part 2.4: Born Approximation and Green's Function Methods

2.4.1 First Born approximation
2.4.2 Higher-order corrections
2.4.3 Green's function approach to scattering problems

Introduction

In quantum mechanics, scattering experiments provide one of the most direct ways of probing the structure and interactions of particles. By studying how particles deflect when they encounter a potential, physicists gain valuable information about the forces at play and the nature of matter at microscopic scales. Scattering theory therefore forms a cornerstone of modern physics, linking theoretical models with experimental observations.

The aim of this Series is to introduce you to the principles and methods of quantum scattering, with particular emphasis on elastic potential scattering. You will learn how scattering amplitudes and cross-sections are defined, how partial wave analysis is applied, and how approximation methods such as the Born approximation and Green's function techniques are used to solve scattering problems.

We shall commence this Series by examining the fundamentals of scattering, comparing classical and quantum approaches and introducing the concepts of scattering amplitude and cross-section.

Next, we will explore elastic potential scattering, focusing on how potential models describe collisions and their applications in atomic and nuclear systems. Following that, we will move on to partial wave analysis, where we will study spherical harmonic expansions, phase shifts, and resonance phenomena. Finally, we will conclude with the Born approximation and Green's function methods, which provide powerful tools for solving complex scattering problems and connecting theory with experimental data.

Series Learning Outcomes

Series 2: Scattering Theory in Quantum Mechanics

Upon completing this Series, you should be able to:

- **SLO 2.1** define the basic concepts of scattering in quantum mechanics and distinguish them from classical scattering,
- **SLO 2.2** explain the meaning of scattering amplitude and differential cross-section and interpret their physical significance,
- **SLO 2.3** describe the principles of elastic potential scattering and apply potential models to atomic and nuclear systems,
- **SLO 2.4** demonstrate the use of partial wave analysis by expanding scattering states in spherical harmonics and identifying phase shifts,
- **SLO 2.5** analyse resonance phenomena in low-energy scattering using partial wave methods,
- **SLO 2.6** apply the Born approximation to calculate scattering amplitudes for weak potentials, and
- **SLO 2.7** evaluate the role of Green's function methods in solving scattering problems and connecting theory with experimental data.

2.1 Fundamentals of Scattering

Scattering is one of the most important tools in quantum mechanics because it allows us to probe the structure and interactions of particles. By studying how particles deflect when they encounter a potential, we gain insight into the forces acting at microscopic scales. Unlike classical scattering, quantum scattering requires us to consider the wave nature of particles, leading to concepts such as scattering amplitudes and cross-sections.

2.1.1 Classical versus quantum scattering

In **classical scattering**, particles are treated as point-like objects that follow definite trajectories when they interact with a potential. The deflection angle depends on the impact parameter and the nature of the force.

In **quantum scattering**, particles are described by wave functions. Instead of definite trajectories, we calculate probabilities for particles to scatter into different directions.

- Classical scattering: deterministic paths.
- Quantum scattering: probabilistic outcomes.

Fill in the blank: In quantum scattering, particles are described by ______ functions rather than definite trajectories.

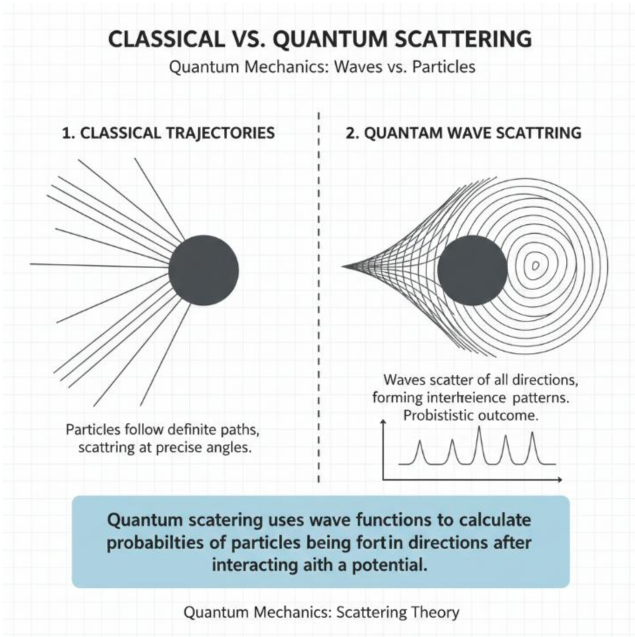


Figure 2.1 Caption: Comparison of classical and quantum scattering.

2.1.2 Scattering amplitude and differential cross-section

The **scattering amplitude** is a complex quantity that encodes the probability amplitude for a particle to scatter into a particular direction.

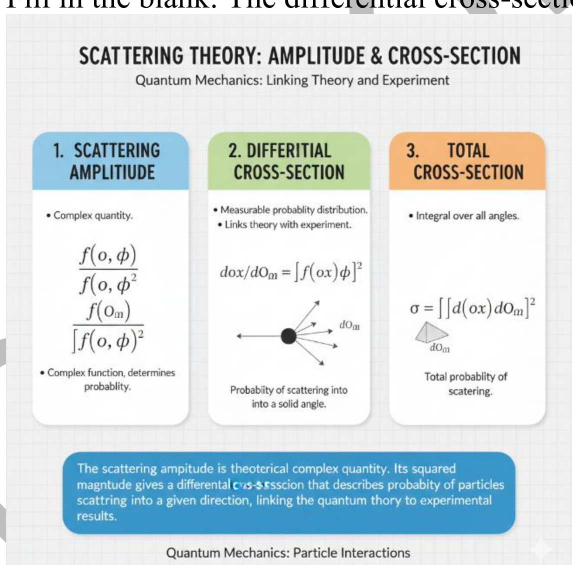
The **differential cross-section** is defined as:

$d\sigma d\Omega=|f(\theta,\phi)|2$

where $f(\theta,\phi)$ is the scattering amplitude.

Physically, the differential cross-section tells us how likely a particle is to scatter into a small solid angle $d\Omega$.

Fill in the blank: The differential cross-section is the square of the ______ amplitude.



Box 2.1 Placeholder: Key features of scattering amplitude and cross-section.

2.1.3 Physical interpretation of scattering experiments

Scattering experiments are used to study the structure of matter.

By measuring cross-sections, physicists infer the nature of forces and potentials.

Elastic scattering preserves the kinetic energy of the particles, while inelastic scattering involves energy transfer.

Examples include Rutherford's experiment, which revealed the nuclear structure of atoms.

Fill in the blank: Rutherford's scattering experiment revealed the existence of the atomic ______.

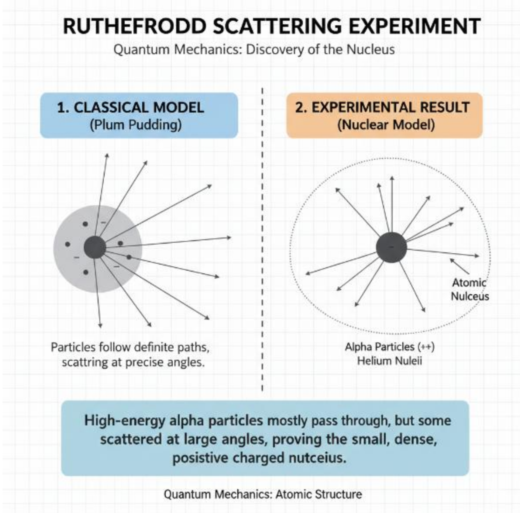


Figure 2.2 Caption: Rutherford's experiment and its role in discovering the atomic nucleus.

Pilot questions 2.1

What is the main difference between classical and quantum scattering?

Define scattering amplitude.

Write down the formula for the differential cross-section.

What does the differential cross-section physically represent?

Which famous experiment revealed the existence of the atomic nucleus?

2.2 Elastic Potential Scattering

Elastic potential scattering is a central topic in quantum scattering theory. In this process, particles interact with a potential but emerge with the same total kinetic energy they had before the collision. Unlike inelastic scattering, no energy is transferred to internal degrees of freedom, so the scattering is purely a redirection of motion.

2.2.1 Concept of elastic scattering

Elastic scattering occurs when the incident particle collides with a target and is deflected without any loss of kinetic energy.

The wave function of the scattered particle retains the same energy as the incoming wave.

Only the direction of motion changes, not the magnitude of the momentum.

Elastic scattering is often the simplest case to analyse and forms the basis for more complex scattering processes.

Fill in the blank: In elastic scattering, the total kinetic energy of the particle is ______ after the collision.

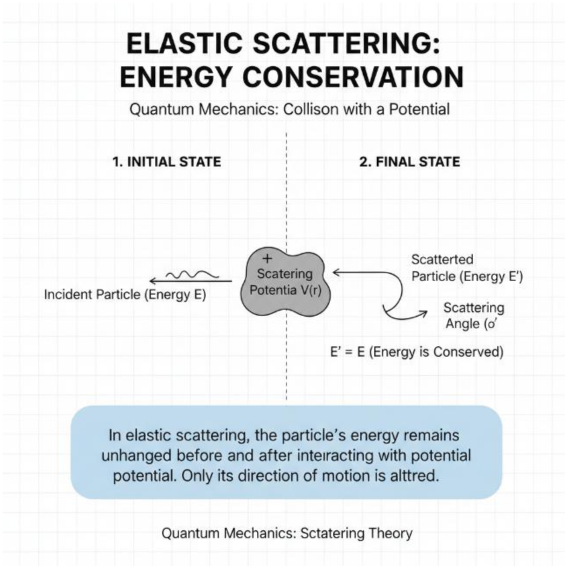


Figure 2.3 Caption: Elastic scattering preserves kinetic energy while changing direction.

2.2.2 Potential scattering models

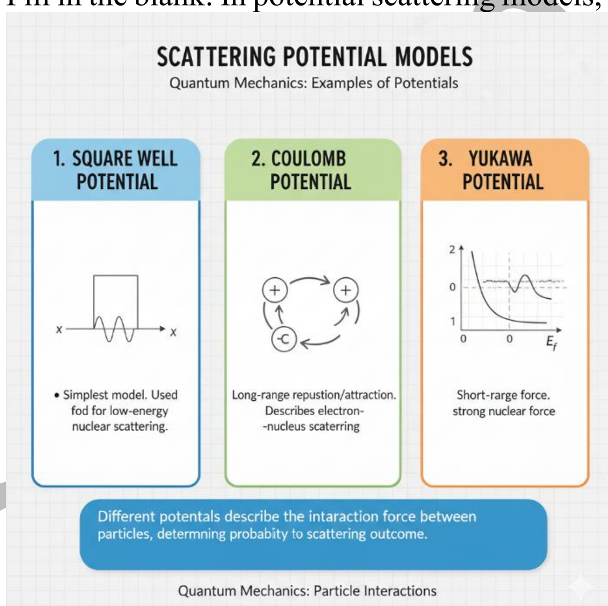
In quantum mechanics, elastic scattering is often studied using **potential scattering models**, where the interaction is represented by a potential function V(r).

Common potentials include square wells, Coulomb potentials, and Yukawa potentials.

The Schrödinger equation is solved with the potential to obtain scattering amplitudes and cross-sections.

These models help us understand how different forces influence scattering behaviour.

Fill in the blank: In potential scattering models, the interaction is represented by a ______ function.



Box 2.2 Placeholder: Examples of potential scattering models.

2.2.3 Applications in atomic and nuclear systems

Elastic potential scattering has wide applications in physics:

Atomic systems: Electron scattering from atoms reveals information about atomic orbitals and charge distributions.

Nuclear systems: Neutron scattering from nuclei provides insights into nuclear structure and forces.

Condensed matter: Elastic scattering of electrons in crystals helps determine lattice structures.

Fill in the blank: Elastic scattering of neutrons from nuclei provides insights into ______ structure.

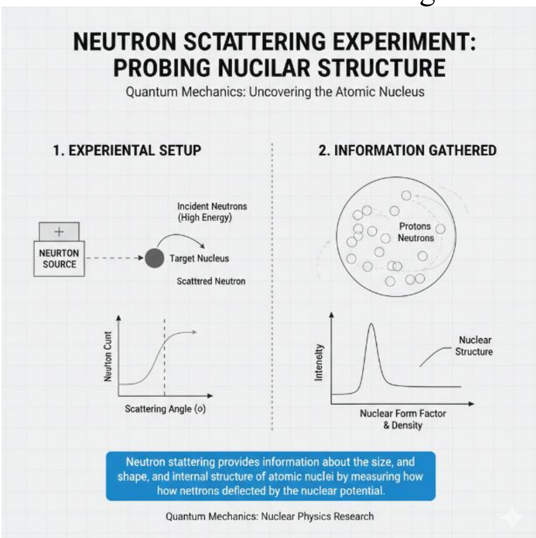


Figure 2.4 Caption: Neutron scattering reveals nuclear structure through elastic scattering.

Pilot questions 2.2

What is elastic scattering, and how does it differ from inelastic scattering?

In elastic scattering, what happens to the total kinetic energy of the particle?

What are potential scattering models, and why are they useful?

Give two examples of potentials used in scattering models.

How is elastic scattering applied in atomic and nuclear systems?

2.3 Partial Wave Analysis

Partial wave analysis is a powerful method in quantum scattering theory. It allows us to express the scattering wave function as a sum of spherical harmonics, each corresponding to a different angular momentum component. This approach is particularly useful for central potentials, where the interaction depends only on the distance between particles.

2.3.1 Expansion in spherical harmonics

In quantum mechanics, the scattered wave function can be expanded in terms of **spherical harmonics**, which are functions that describe angular dependence.

The incident plane wave is expressed as a sum of spherical waves.

Each spherical wave corresponds to a particular angular momentum quantum number l.

This expansion simplifies the analysis of scattering by reducing the problem to radial equations.

Fill in the blank: In partial wave analysis, the angular dependence of the wave function is expressed using ______ harmonics.

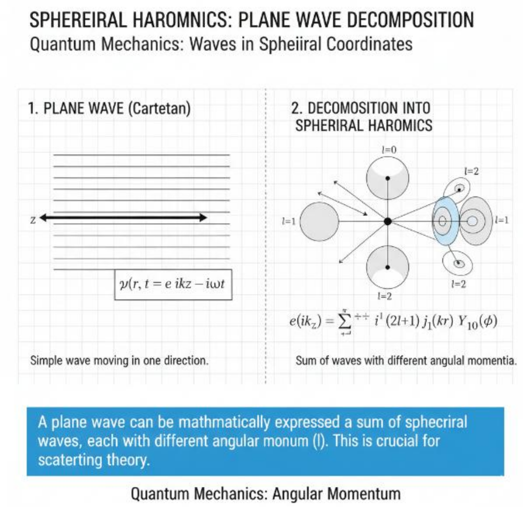


Figure 2.5 Caption: Expansion of a plane wave into spherical harmonics.

2.3.2 Phase shifts and resonance phenomena

The effect of the potential on each partial wave is characterised by a **phase shift** δl.

- Phase shifts measure how much the wave is delayed or advanced due to the scattering potential.
- Resonance occurs when the phase shift changes rapidly near a particular energy, indicating strong interaction.
- Resonances are associated with temporary formation of quasi-bound states.

Fill in the blank: A rapid change in phase shift near a particular energy indicates a ______ phenomenon.

Box 2.3 Placeholder: Key features of phase shifts and resonance.

- Phase shifts: measure scattering effects.
- Resonance: strong interaction, quasi-bound states. AI prompt suggestion: "Generate an infographic summarising phase shifts and resonance phenomena."

2.3.3 Applications in low-energy scattering

Partial wave analysis is especially useful in **low-energy scattering**, where only a few partial waves contribute significantly.

- At very low energies, the s-wave (l=0) dominates.
- Higher partial waves (p-wave, d-wave, etc.) become important at higher energies.
- This method explains phenomena such as neutron scattering at low energies and electron scattering in gases.

Fill in the blank: At very low energies, the dominant contribution to scattering comes from the ______ wave.

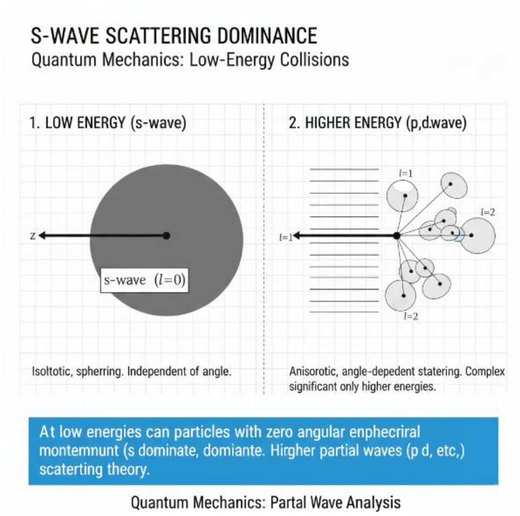


Figure 2.6 Caption: Low-energy scattering dominated by s-wave contribution.

Pilot questions 2.3

What is the purpose of partial wave analysis in quantum scattering?
Which mathematical functions are used to express angular dependence in partial wave analysis?
What does a phase shift represent in scattering theory?
What physical phenomenon is indicated by a rapid change in phase shift?
Which partial wave dominates scattering at very low energies?

2.4 Born Approximation and Green's Function Methods

The Born approximation and Green's function methods are two important approaches in quantum scattering theory. They provide practical ways of calculating scattering amplitudes when exact solutions are difficult to obtain. These methods are particularly useful for weak potentials and for connecting theoretical models with experimental data.

2.4.1 First Born approximation

The **Born approximation** is a method used when the scattering potential is weak.

The scattering amplitude is approximated by the Fourier transform of the potential:

$f(\theta)\approx -\frac{2m}{4\pi\hbar^2}\int e^{-iq\cdot r}V(r)\, d^3r$

where q is the momentum transfer.

This approximation is valid when the potential does not strongly distort the incident wave.

It is widely used in atomic and nuclear scattering problems.

Fill in the blank: The Born approximation is most accurate when the scattering potential is ______.

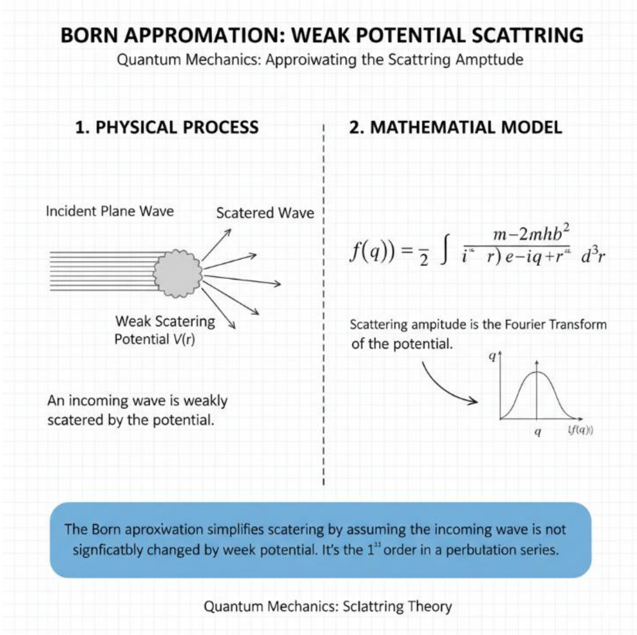


Figure 2.7 Caption: Born approximation applied to weak potential scattering.

2.4.2 Higher-order corrections

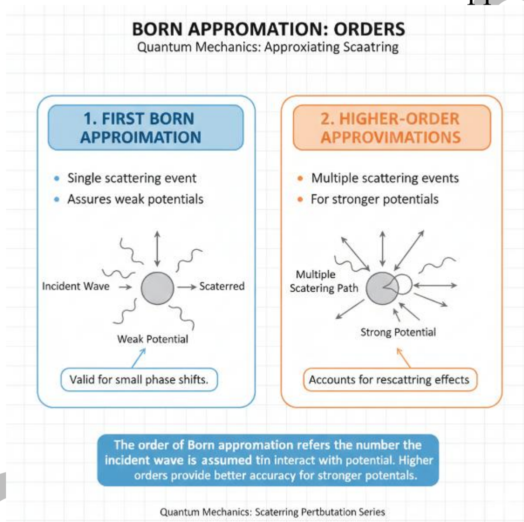
When the potential is not sufficiently weak, higher-order terms must be considered.

The second Born approximation includes corrections from multiple scattering events.

These higher-order terms improve accuracy but increase mathematical complexity.

In practice, the first Born approximation is often sufficient for many physical problems.

Fill in the blank: The second Born approximation accounts for multiple ______ events.



Box 2.4 Placeholder: Key differences between first and higher-order Born approximations.

2.4.3 Green's function approach to scattering problems

The **Green's function method** provides a general framework for solving scattering problems.

A Green's function represents the response of a system to a point source.

In scattering theory, it is used to express the wave function in terms of the incident wave and the scattered contribution.

This approach is powerful because it connects boundary conditions, potentials, and scattering amplitudes in a unified way.

Fill in the blank: In scattering theory, Green's functions represent the response of a system to a ______ source.

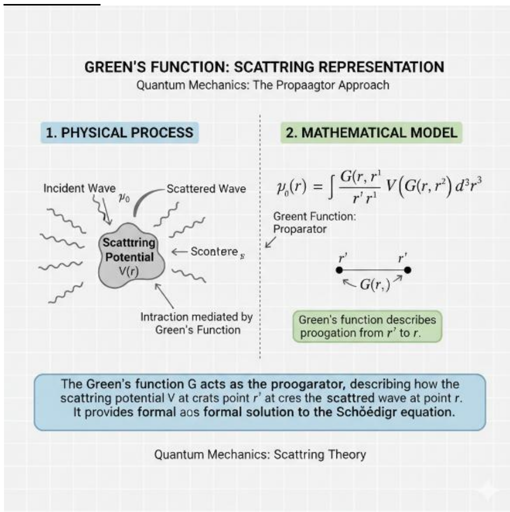


Figure 2.8 Caption: Green's function approach to scattering problems.

Pilot questions 2.4

What is the Born approximation, and when is it valid?
Write down the expression for the scattering amplitude in the first Born approximation.
What does the second Born approximation account for?
What is the role of Green's functions in scattering theory?
How does the Green's function method connect potentials and scattering amplitudes?

Series Summary

In this Series, we explored the principles and methods of quantum scattering, focusing on elastic potential scattering. We began with the **fundamentals of scattering**, comparing classical and quantum approaches and introducing the concepts of scattering amplitude and differential cross-section. We then examined **elastic potential scattering**, where particles interact with a potential but retain their kinetic energy, and studied potential scattering models with applications in atomic and nuclear systems. Following that, we moved on to **partial wave analysis**, which uses spherical harmonics to describe angular dependence, introduces phase shifts, and explains resonance phenomena, particularly in low-energy scattering. Finally, we concluded with the **Born approximation and Green's function methods**, which provide practical tools for calculating scattering amplitudes and connecting theoretical models with experimental data. Together, these topics give learners a comprehensive understanding of scattering theory in quantum mechanics.

Glossary of Terms

Scattering amplitude: A complex quantity that encodes the probability amplitude for a particle to scatter into a particular direction. **Differential cross-section**: A measure of the likelihood of scattering into a given solid angle, obtained from the square of the scattering amplitude. **Elastic scattering**: Scattering in which the total kinetic energy of the particles remains unchanged. **Potential scattering model**: A representation of scattering interactions using a potential function such as a square well or Coulomb potential. **Partial wave analysis**: A method of expanding the scattering wave function into spherical harmonics, each corresponding to a different angular momentum. **Phase shift**: A measure of how much a wave is delayed or advanced due to the scattering potential. **Resonance**: A phenomenon where rapid changes in phase shift indicate strong interaction and temporary quasi-bound states. **Born approximation**: An approximation method valid for weak potentials, where the scattering amplitude is given by the Fourier transform of the potential. **Green's function**: A mathematical tool representing the response of a system to a point source, used to solve scattering problems.

Concept Check Questions 2

Objective Questions

- (SLO 2.1) In quantum scattering, particles are described by ______ functions rather than definite trajectories.
- (SLO 2.2) The differential cross-section is the square of the ______ amplitude.
- (SLO 2.3) In elastic scattering, the total kinetic energy of the particle is ______ after the collision.
- (SLO 2.4) In partial wave analysis, angular dependence is expressed using ______ harmonics.
- (SLO 2.6) The Born approximation is most accurate when the scattering potential is ______.

Short-Answer Questions

(SLO 2.1) Explain the difference between classical and quantum scattering.
(SLO 2.2) What does the differential cross-section physically represent?
(SLO 2.3) Give two examples of potential scattering models.
(SLO 2.5) What physical phenomenon is indicated by a rapid change in phase shift?
(SLO 2.7) What role do Green's functions play in scattering theory?

Long-Answer Questions

(SLO 2.3, 2.4) Analyse how elastic potential scattering is modelled using potentials and how partial wave analysis simplifies the problem.
(SLO 2.5) Discuss resonance phenomena in scattering, explaining their physical significance and connection to quasi-bound states.
(SLO 2.6) Evaluate the usefulness of the Born approximation in atomic and nuclear scattering problems.
(SLO 2.7) Examine how Green's function methods unify boundary conditions, potentials, and scattering amplitudes in quantum mechanics.

Answers to Pilot Questions 2

Part 2.1 Fundamentals of Scattering

- Classical scattering involves deterministic paths, quantum scattering involves probabilistic wave functions.
- Scattering amplitude is the probability amplitude for scattering into a given direction.
- $d\sigma d\Omega=|f(\theta,\phi)|2$.
- It represents the likelihood of scattering into a small solid angle.
- Rutherford's experiment revealed the atomic nucleus.

Part 2.2 Elastic Potential Scattering

- Elastic scattering preserves kinetic energy, inelastic scattering involves energy transfer.
- The total kinetic energy remains unchanged.
- Potential scattering models represent interactions using a potential function.
- Examples: square well potential, Coulomb potential.
- Elastic scattering is used in atomic systems (electron scattering) and nuclear systems (neutron scattering).

Part 2.3 Partial Wave Analysis

- It simplifies scattering problems by expanding wave functions into spherical harmonics.
- Spherical harmonics.

Phase shifts represent the effect of the potential on each partial wave.
Resonance.
The s-wave dominates at very low energies.

Part 2.4 Born Approximation and Green's Function Methods

The Born approximation is valid for weak potentials.
$f(\theta)\approx-2m4\pi\hbar2\int e-iq\cdot rV(r)\ d3r.$
Multiple scattering events.
Green's functions represent the response of a system to a point source.
They connect potentials, boundary conditions, and scattering amplitudes.

References and Attributions 2

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Series 5: Relativistic Wave Equations and Quantum Motion in Electromagnetic Fields

Here is a proposed outline:

Series 3: Symmetry Principles and Selection Rules in Quantum Mechanics

Part 3.1: Fundamentals of Symmetry in Quantum Mechanics
- 3.1.1 Concept of symmetry and invariance
- 3.1.2 Role of symmetry in physical laws
- 3.1.3 Examples of symmetry operations (parity, rotation, translation)

Part 3.2: Conservation Laws and Symmetry Operators
- 3.2.1 Noether's theorem and conservation principles
- 3.2.2 Commutation relations and conserved quantities
- 3.2.3 Applications in angular momentum and parity conservation

Part 3.3: Selection Rules in Quantum Transitions
- 3.3.1 Concept of selection rules
- 3.3.2 Electric dipole transitions and parity considerations

Introduction

Symmetry plays a fundamental role in quantum mechanics. It provides deep insights into the behaviour of physical systems and determines which processes are allowed or forbidden. Selection rules, which arise directly from symmetry principles, guide us in predicting transitions between quantum states, such as those observed in atomic and molecular spectra. Together, symmetry and selection rules form a powerful framework that connects abstract mathematical concepts with experimental observations.

The aim of this Series is to help you understand how symmetry principles shape the laws of quantum mechanics and how selection rules emerge from these symmetries. You will learn how symmetry operations are defined, how they lead to conservation laws, and how they restrict possible transitions in atomic, molecular, and nuclear systems.

We shall begin this Series by studying the **fundamentals of symmetry in quantum mechanics**, introducing the concepts of invariance and symmetry operations such as parity, rotation, and translation. Next, we will explore **conservation laws and symmetry operators**, focusing on Noether's theorem, commutation relations, and applications in angular momentum and parity conservation. Following this, we will examine **selection rules in quantum transitions**, including electric dipole transitions, parity considerations, and angular momentum rules. Finally, we will conclude with **applications of symmetry and selection rules**, where we will see how these principles explain atomic spectra, molecular spectroscopy, and phenomena in nuclear and particle physics.

Series Learning Outcomes

Series 3: Symmetry Principles and Selection Rules in Quantum Mechanics

By the end of this Series, you should be able to:

- **SLO 3.1** define the concept of symmetry and invariance in quantum mechanics and illustrate examples of symmetry operations such as parity, rotation, and translation,
- **SLO 3.2** explain how conservation laws arise from symmetry principles, applying Noether's theorem and commutation relations to identify conserved quantities,
- **SLO 3.3** analyse the role of symmetry operators in angular momentum and parity conservation,
- **SLO 3.4** describe the concept of selection rules and apply them to electric dipole transitions, parity considerations, and angular momentum changes,
- **SLO 3.5** evaluate spin and angular momentum selection rules in atomic and molecular transitions,
- **SLO 3.6** apply symmetry principles and selection rules to interpret atomic spectra, molecular spectroscopy, and nuclear transitions, and
- **SLO 3.7** assess the broader significance of symmetry and selection rules in connecting theoretical models with experimental observations.

3.1 Fundamentals of Symmetry in Quantum Mechanics

Symmetry is one of the most powerful ideas in physics. In quantum mechanics, symmetry principles help us understand why certain physical laws hold and why some transitions are allowed while others are forbidden. By studying symmetry, we uncover the deep connections between mathematics and physical reality.

3.1.1 Concept of symmetry and invariance

A system is said to possess **symmetry** if it remains unchanged under a certain transformation.

- **Invariance** means that the physical properties of the system do not change when the transformation is applied.
- Examples include rotational symmetry (system unchanged when rotated), translational symmetry (unchanged when shifted), and parity symmetry (unchanged when coordinates are inverted).
- Symmetry principles are closely tied to conservation laws.

Fill in the blank: A system possesses symmetry if it remains ______ under a transformation.

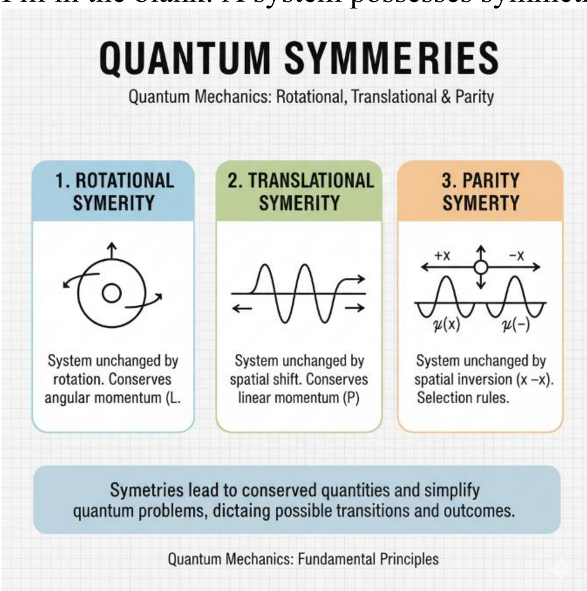


Figure 3.1 Caption: Examples of symmetry operations in quantum mechanics.

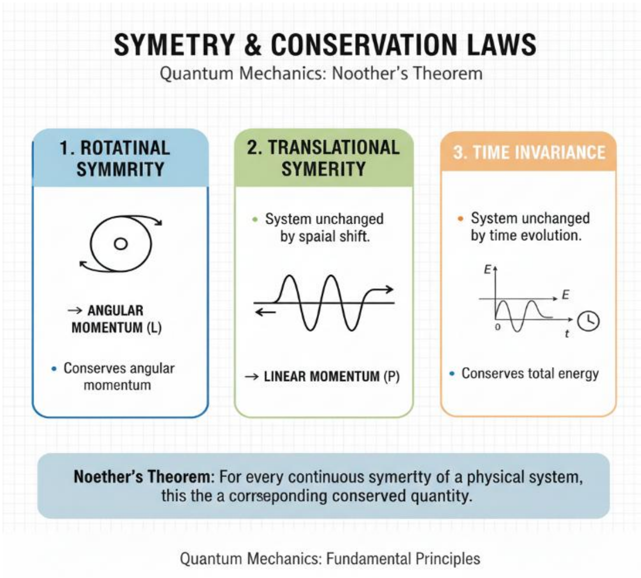
3.1.2 Role of symmetry in physical laws

Symmetry principles explain why physical laws are universal and consistent.

- Rotational symmetry → conservation of angular momentum.
- Translational symmetry → conservation of linear momentum.
- Time invariance → conservation of energy.

These connections are formalised in **Noether's theorem**, which states that every continuous symmetry corresponds to a conservation law.

Fill in the blank: According to Noether's theorem, every continuous symmetry corresponds to a ______ law.



Box 3.1 Placeholder: Key links between symmetry and conservation laws.

3.1.3 Examples of symmetry operations

Symmetry operations are mathematical transformations that leave the system unchanged.

- **Parity (P)**: Inversion of spatial coordinates $(x,y,z)\rightarrow(-x,-y,-z)$.
- **Rotation (R)**: Rotation of the system around an axis.
- **Translation (T)**: Shifting the system in space without altering its properties.

These operations form the basis of symmetry groups, which are used to classify physical systems.

Fill in the blank: The inversion of spatial coordinates is known as the ______ operation.

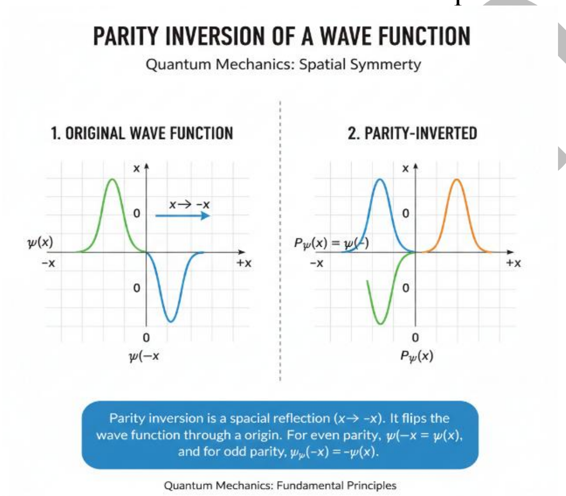


Figure 3.2 Caption: Parity operation applied to a quantum system.

Pilot questions 3.1

- What does it mean for a system to possess symmetry?
- Define invariance in the context of quantum mechanics.
- State Noether's theorem in simple terms.
- Give one example of a symmetry operation and its corresponding conservation law.
- What is the parity operation in quantum mechanics?

3.2 Conservation Laws and Symmetry Operators

Symmetry principles are not just abstract ideas; they have direct consequences in the form of **conservation laws**. In quantum mechanics, these laws are expressed through symmetry operators, which act on wave functions and reveal quantities that remain unchanged during physical processes.

3.2.1 Noether's theorem and conservation principles

Noether's theorem is a cornerstone of modern physics. It states that every continuous symmetry corresponds to a conservation law.

Translational symmetry → conservation of **linear momentum**.

Rotational symmetry → conservation of **angular momentum**.

Time invariance → conservation of **energy**.

This theorem provides a deep link between mathematics and physics, showing that conservation laws are not arbitrary but arise naturally from symmetry.

Fill in the blank: Noether's theorem states that every continuous symmetry corresponds to a _______ law.

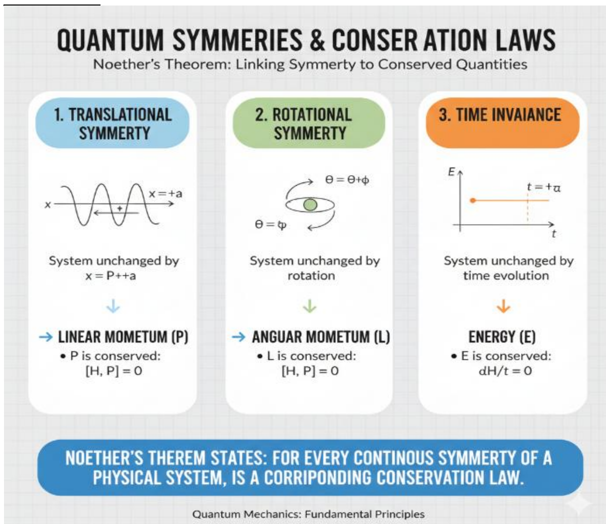


Figure 3.3 Caption: Noether's theorem connects symmetry with conservation principles.

3.2.2 Commutation relations and conserved quantities

In quantum mechanics, conserved quantities are associated with operators that commute with the Hamiltonian.

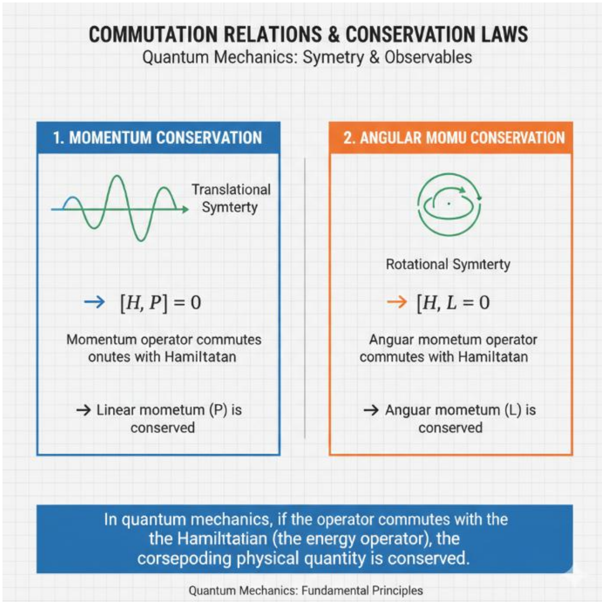
If an operator A^ commutes with the Hamiltonian H^, i.e. [H^,A^]=0, then the corresponding physical quantity is conserved.

Examples:

[H^,p^]=0 → momentum conserved.

[H^,L^]=0 → angular momentum conserved.

Fill in the blank: A physical quantity is conserved if its operator commutes with the ______.



Box 3.2 Placeholder: Key commutation relations in quantum mechanics.

3.2.3 Applications in angular momentum and parity conservation

Two important examples of conservation laws in quantum mechanics are:

- **Angular momentum conservation**: Arises from rotational symmetry. It explains why atomic orbitals are classified by quantum numbers l and m.
- **Parity conservation**: Arises from invariance under spatial inversion. In many systems, parity is conserved, meaning the wave function remains unchanged under inversion.

Fill in the blank: Conservation of angular momentum arises from ______ symmetry.

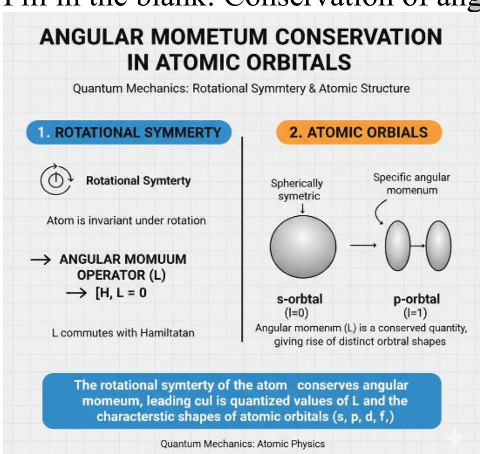


Figure 3.4 Caption: Angular momentum conservation explained by rotational symmetry.

Pilot questions 3.2

- State Noether's theorem in your own words.
- What conservation law arises from translational symmetry?
- What condition must an operator satisfy to represent a conserved quantity?
- Give one example of a commutation relation that leads to conservation.
- Which symmetry principle leads to conservation of angular momentum?

3.3 Selection Rules in Quantum Transitions

Selection rules are the guidelines that determine which transitions between quantum states are allowed and which are forbidden. They arise directly from symmetry principles and conservation laws. By applying these rules, physicists can predict the spectral lines observed in atomic and molecular systems.

3.3.1 Concept of selection rules

Selection rules specify the conditions under which a transition between two quantum states can occur.

- They are derived from the properties of symmetry operators acting on wave functions.
- Allowed transitions satisfy certain conservation laws (e.g. angular momentum, parity).
- Forbidden transitions violate these conditions and therefore have zero or negligible probability.

Fill in the blank: Selection rules determine which quantum state transitions are ______ and which are forbidden.

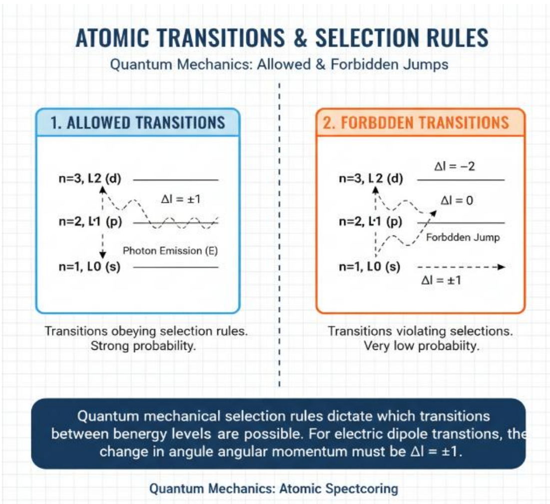


Figure 3.5 Caption: Selection rules govern transitions between quantum states.

3.3.2 Electric dipole transitions and parity considerations

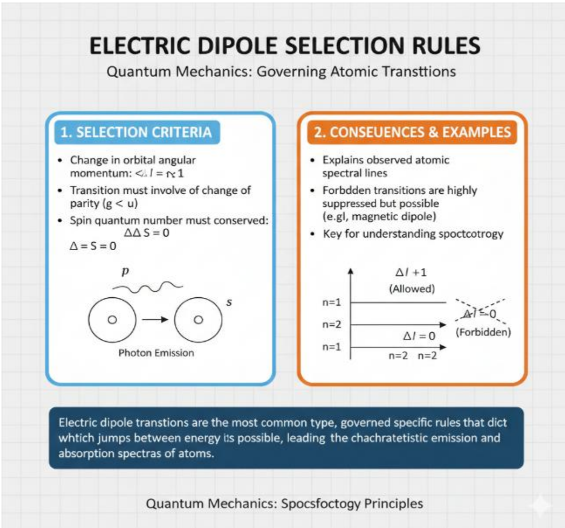
The most common selection rules are those for **electric dipole transitions**.

- For an electric dipole transition, the change in orbital angular momentum quantum number must satisfy:

$\Delta l = \pm 1$

- Parity plays a crucial role: transitions are only allowed between states of opposite parity.
- These rules explain why some spectral lines appear while others do not.

Fill in the blank: For electric dipole transitions, the change in orbital angular momentum quantum number must be $\Delta l = \pm$ ___.



Box 3.3 Placeholder: Key electric dipole selection rules.

3.3.3 Spin and angular momentum selection rules

Spin and total angular momentum also impose restrictions on transitions.

The spin quantum number s usually remains unchanged in electric dipole transitions.

For total angular momentum j:

$\Delta j=0,\pm 1$ but not $j=0 \rightarrow j=0$

These rules ensure conservation of angular momentum during transitions.

Fill in the blank: In electric dipole transitions, the spin quantum number usually remains ______.

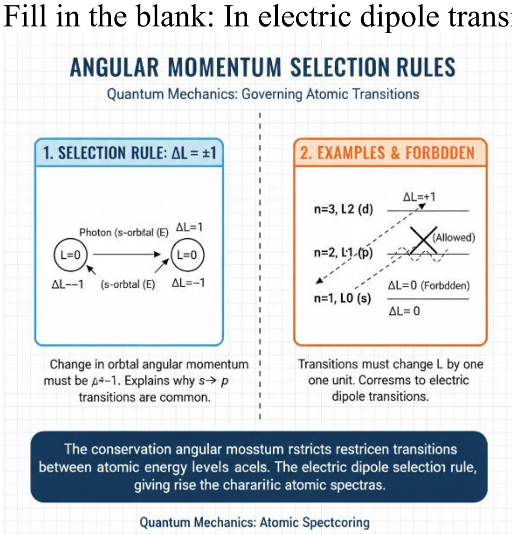


Figure 3.6 Caption: Angular momentum selection rules in quantum transitions.

Pilot questions 3.3

What are selection rules in quantum mechanics?

What condition must be satisfied for an electric dipole transition to occur?

How does parity affect selection rules?

State the rule for changes in total angular momentum quantum number j.

Why do selection rules explain the presence or absence of certain spectral lines?

3.4 Applications of Symmetry and Selection Rules

Symmetry principles and selection rules are not just theoretical constructs; they have direct applications in explaining observable phenomena across atomic, molecular, nuclear, and particle physics. By applying these rules, scientists can predict spectral lines, transition probabilities, and even the stability of certain states.

3.4.1 Atomic spectra and transition probabilities

In atomic physics, symmetry and selection rules explain why certain spectral lines appear and others do not.

- Electric dipole selection rules determine allowed transitions between atomic orbitals.
- Parity and angular momentum conservation restrict possible transitions.
- Transition probabilities are calculated using matrix elements that respect these rules.

Fill in the blank: Selection rules explain why certain ______ lines appear in atomic spectra while others are absent.

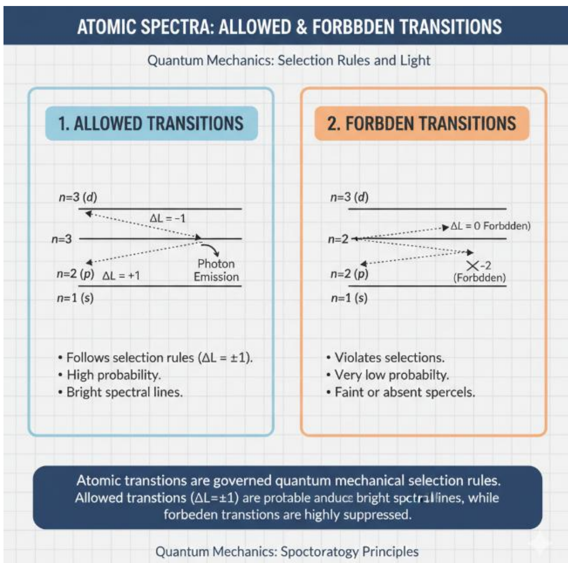


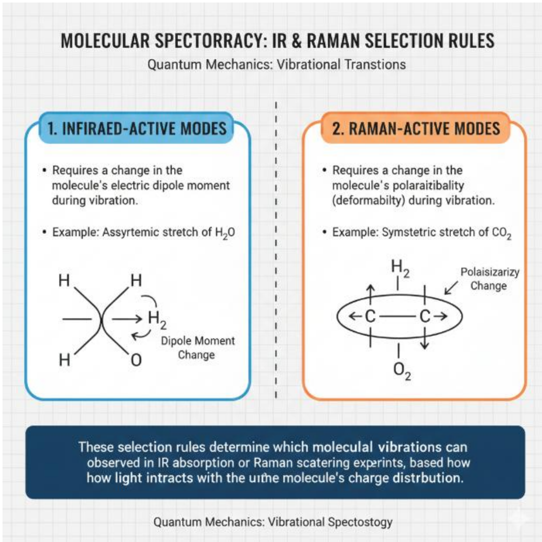
Figure 3.7 Caption: Selection rules determine atomic spectral lines.

3.4.2 Molecular spectroscopy and vibrational transitions

In molecular systems, symmetry governs vibrational and rotational transitions.

- Vibrational modes are classified according to symmetry groups.
- Only vibrations that change the dipole moment are infrared-active.
- Raman spectroscopy relies on different symmetry considerations, involving changes in polarizability.

Fill in the blank: In infrared spectroscopy, only vibrational modes that change the ______ moment are active.



Box 3.4 Placeholder: Key applications of symmetry in molecular spectroscopy.

3.4.3 Nuclear and particle physics applications

Symmetry and selection rules also extend to nuclear and particle physics.

Nuclear transitions are governed by angular momentum and parity conservation.

In particle physics, conservation of quantum numbers (such as baryon number, lepton number, and isospin) restricts possible reactions.

Symmetry principles explain why certain decays are forbidden and why others dominate.

Fill in the blank: In particle physics, conservation of quantum numbers such as ______ number restricts possible reactions.

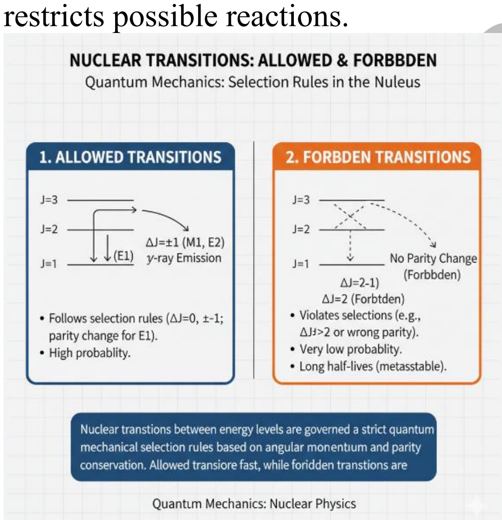


Figure 3.8 Caption: Nuclear and particle transitions governed by symmetry rules.

Pilot questions 3.4

How do selection rules explain atomic spectral lines?

What condition must be satisfied for a vibrational mode to be infrared-active?

What symmetry principle underlies Raman-active transitions?

Which conservation laws govern nuclear transitions?

Give one example of a quantum number conserved in particle physics.

Series Summary

In this Series, we examined how symmetry principles underpin the laws of quantum mechanics and how selection rules emerge from these symmetries. We began with the **fundamentals of symmetry**, introducing invariance and symmetry operations such as parity, rotation, and translation. Next, we studied **conservation laws and symmetry operators**, focusing on Noether's theorem, commutation relations, and applications in angular momentum and parity conservation. We then explored **selection rules in quantum transitions**, including electric dipole transitions, parity considerations, and angular momentum restrictions. Finally, we applied these principles to real systems, showing how symmetry and selection rules explain atomic spectra, molecular spectroscopy, and nuclear and particle physics phenomena. Together, these topics provide a unified framework for understanding why certain transitions are allowed and others forbidden, linking theory with experimental observations.

Glossary of Terms

Symmetry: A property of a system that remains unchanged under a transformation. **Invariance**: The condition of a system being unaffected by a symmetry operation. **Noether's theorem**: A principle stating that every continuous symmetry corresponds to a conservation law. **Symmetry operator**: A mathematical operator that represents a symmetry transformation. **Parity (P)**: A symmetry operation involving inversion of spatial coordinates. **Selection rules**: Guidelines that determine which quantum transitions are allowed or forbidden. **Electric dipole transition**: A transition governed by dipole moment changes, subject to angular momentum and parity rules. **Angular momentum conservation**: A law arising from rotational symmetry. **Infrared-active mode**: A vibrational mode that changes the dipole moment and can be observed in infrared spectroscopy. **Raman-active mode**: A vibrational mode that changes polarizability and can be observed in Raman spectroscopy.

Concept Check Questions 3

Objective Questions

- (SLO 3.1) A system possesses symmetry if it remains ______ under a transformation.
- (SLO 3.2) Noether's theorem states that every continuous symmetry corresponds to a ______ law.
- (SLO 3.3) Conservation of angular momentum arises from ______ symmetry.
- (SLO 3.4) For electric dipole transitions, the change in orbital angular momentum quantum number must be $\Delta l = \pm$ ___.
- (SLO 3.6) In infrared spectroscopy, only vibrational modes that change the ______ moment are active.

Short-Answer Questions

(SLO 3.1) Define invariance in the context of quantum mechanics.
(SLO 3.2) What condition must an operator satisfy to represent a conserved quantity?
(SLO 3.4) How does parity affect selection rules?
(SLO 3.5) State the rule for changes in total angular momentum quantum number j.
(SLO 3.6) What symmetry principle underlies Raman-active transitions?

Long-Answer Questions

(SLO 3.2, 3.3) Analyse how Noether's theorem connects symmetry principles to conservation laws, with examples.
(SLO 3.4, 3.5) Discuss the role of parity and angular momentum in determining selection rules for atomic transitions.
(SLO 3.6) Evaluate the importance of symmetry in molecular spectroscopy, comparing infrared and Raman selection rules.

(SLO 3.7) Assess how symmetry and selection rules unify theoretical models with experimental observations in nuclear and particle physics.

Answers to Pilot Questions 3

Part 3.1 Fundamentals of Symmetry

A system possesses symmetry if it remains unchanged under a transformation.
Invariance means the system's properties do not change under a symmetry operation.
Noether's theorem states that every continuous symmetry corresponds to a conservation law.
Rotational symmetry → conservation of angular momentum.
Parity is the inversion of spatial coordinates.

Part 3.2 Conservation Laws and Symmetry Operators

Noether's theorem links continuous symmetries to conservation laws.
Translational symmetry → conservation of linear momentum.
An operator must commute with the Hamiltonian.
Example: $[\hat{H},\hat{L}]=0$ → angular momentum conserved.
Rotational symmetry leads to conservation of angular momentum.

Part 3.3 Selection Rules in Quantum Transitions

Selection rules determine allowed and forbidden transitions.
$\Delta l=\pm 1$.
Transitions are only allowed between states of opposite parity.
$\Delta j=0,\pm 1$, but not $j=0 \rightarrow j=0$.
They explain why some spectral lines appear and others do not.

Part 3.4 Applications of Symmetry and Selection Rules

They explain atomic spectral lines by restricting allowed transitions.
Vibrational modes must change the dipole moment.
Raman-active transitions depend on changes in polarizability.
Nuclear transitions are governed by angular momentum and parity conservation.
Example: baryon number conservation in particle physics.

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COURSE CODE: PHY 402
COURSE TITLE: Quantum Mechanics II
COURSE UNIT: 3 UNITS

Here are five comprehensive series titles that fully cover the scope of the attached PHY 402 course:

Series 1: Perturbation Methods in Quantum Mechanics

Series 2: Quantum Scattering Theory and Elastic Potential Scattering

Series 3: Symmetries and Selection Rules in Quantum Mechanics

Series 4: Quantum Models of Atomic, Molecular, Solid-State, and Nuclear Phenomena

Series 5: Relativistic Wave Equations and Quantum Motion in Electromagnetic Fields

Here is a proposed outline:

Series 4: Quantum Models of Matter and Nuclear Phenomena

Part 1: Quantum Models of Atomic Systems
- 4.1.1 Hydrogen atom and Schrödinger solutions
- 4.1.2 Multi-electron atoms and approximation methods
- 4.1.3 Atomic spectra and fine structure

Part 2: Quantum Models of Molecular Systems
- 4.2.1 Molecular bonding and orbital theory
- 4.2.2 Vibrational and rotational spectra
- 4.2.3 Applications in spectroscopy and chemical physics

Part 3: Quantum Models in Solid-State Physics
- 4.3.1 Free electron and band theory
- 4.3.2 Bloch's theorem and crystal lattices
- 4.3.3 Applications in semiconductors and superconductors

Part 4: Quantum Models of Nuclear Phenomena
- 4.4.1 Nuclear shell model
- 4.4.2 Collective models and nuclear excitations
- 4.4.3 Applications in nuclear reactions and decay processes

Introduction

Quantum mechanics provides the foundation for understanding the behaviour of matter across different scales, from atoms and molecules to solids and nuclei. Each of these systems exhibits unique phenomena, yet they can all be described using quantum models that reveal the underlying principles governing their structure and interactions.

The aim of this Series is to introduce you to the quantum models that explain atomic, molecular, solid-state, and nuclear phenomena. You will learn how the Schrödinger equation is applied to atomic systems, how molecular bonding and spectra are described, how band theory explains the properties of solids, and how nuclear models account for the structure and reactions of nuclei.

We shall begin this Series by examining **quantum models of atomic systems**, focusing on the hydrogen atom, multi-electron atoms, and atomic spectra. Next, we will explore **quantum models of molecular systems**, including bonding theories, vibrational and rotational spectra, and their applications in spectroscopy. Following that, we will study **quantum models in solid-state physics**, where concepts such as band theory, Bloch's theorem, and applications in semiconductors and superconductors are introduced. Finally, we will conclude with **quantum models of nuclear phenomena**, covering the nuclear shell model, collective models, and applications in nuclear reactions and decay processes.

Series Learning Outcomes

Series 4: Quantum Models of Matter and Nuclear Phenomena

By the end of this Series, you should be able to:

SLO 4.1 describe the quantum models of atomic systems, including the hydrogen atom, multi-electron atoms, and atomic spectra,
SLO 4.2 explain the principles of molecular quantum models, focusing on bonding theories, vibrational and rotational spectra, and their applications in spectroscopy,
SLO 4.3 analyse quantum models in solid-state physics, including free electron theory, band theory, Bloch's theorem, and their applications in semiconductors and superconductors,
SLO 4.4 evaluate nuclear quantum models such as the shell model and collective models, and apply them to nuclear excitations, reactions, and decay processes,
SLO 4.5 integrate knowledge of atomic, molecular, solid-state, and nuclear quantum models to interpret experimental phenomena across different physical systems.

4.1 Quantum Models of Atomic Systems

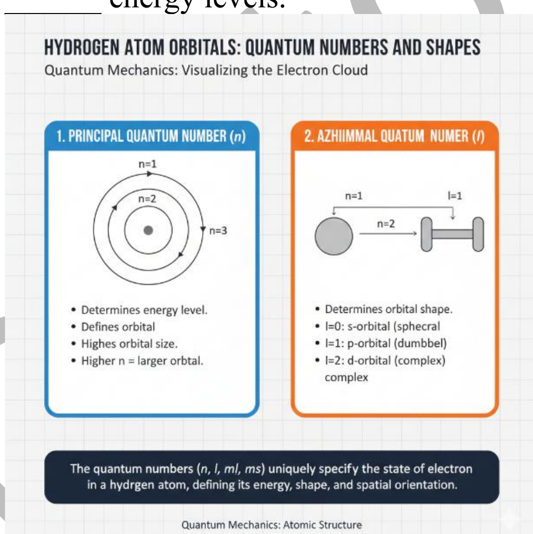
Atomic systems are the foundation of quantum mechanics. By studying them, we gain insight into how electrons behave, how energy levels are structured, and why atoms exhibit the spectra that we observe experimentally. This Part introduces the quantum models used to describe atomic systems, beginning with the hydrogen atom, extending to multi-electron atoms, and concluding with atomic spectra and fine structure.

4.1.1 Hydrogen atom and Schrödinger solutions

The **hydrogen atom** is the simplest atomic system, consisting of one proton and one electron. Because of its simplicity, it serves as the starting point for quantum models of atoms.
The behaviour of the electron in hydrogen is described by the **Schrödinger equation**, a fundamental equation in quantum mechanics that determines the allowed energy levels and wave functions of particles. Solving the Schrödinger equation for hydrogen reveals that electrons can only occupy discrete energy levels, each associated with a quantum number.

Principal quantum number (n): Determines the energy level of the electron.
Angular momentum quantum number (l): Determines the shape of the orbital.
Magnetic quantum number (m): Determines the orientation of the orbital.

Fill in the blank: The Schrödinger equation for hydrogen shows that electrons can only occupy _______ energy levels.



Caption: Hydrogen atom orbitals derived from Schrödinger solutions.

4.1.2 Multi-electron atoms and approximation methods

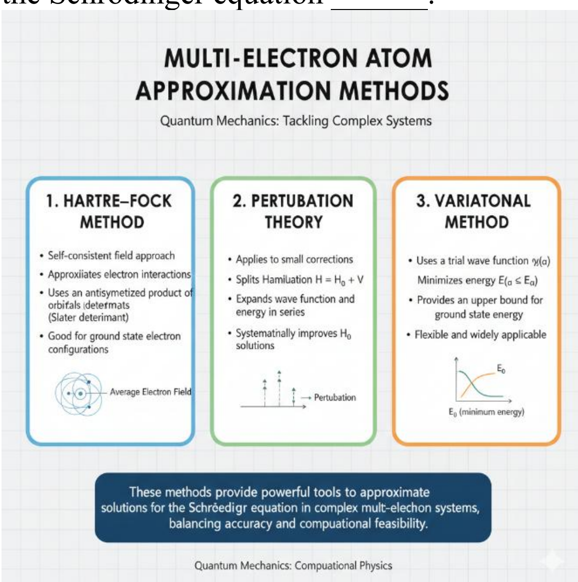
When we move beyond hydrogen to **multi-electron atoms**, the situation becomes more complex. Electrons interact not only with the nucleus but also with each other, making exact solutions impossible.

To handle this, physicists use **approximation methods**, such as:

- **Hartree–Fock method**: Approximates the wave function by considering electron interactions in an averaged way.
- **Perturbation theory**: Treats electron–electron interactions as small corrections to simpler models.
- **Variational method**: Uses trial wave functions to estimate the lowest energy state.

These methods allow us to predict the structure and behaviour of atoms with many electrons, such as helium, carbon, or iron.

Fill in the blank: In multi-electron atoms, electron–electron interactions make exact solutions of the Schrödinger equation ______.



Caption: Box 4.1: Common approximation methods for multi-electron atoms

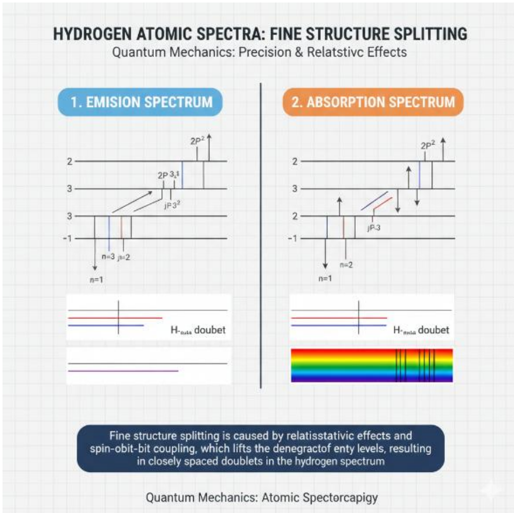
4.1.3 Atomic spectra and fine structure

Atoms emit or absorb light when electrons transition between energy levels. The resulting **atomic spectra** provide a fingerprint of each element.

- **Emission spectra**: Produced when electrons drop to lower energy levels, releasing photons.
- **Absorption spectra**: Produced when electrons absorb photons and move to higher energy levels.

In addition to these basic spectra, atoms exhibit **fine structure**, which arises from small corrections to energy levels due to relativistic effects and electron spin. Fine structure explains the splitting of spectral lines into closely spaced components.

Fill in the blank: Fine structure in atomic spectra arises from relativistic effects and ______ interactions.



Caption: Atomic spectra of hydrogen showing fine structure.

Pilot questions 4.1

- What makes the hydrogen atom an ideal starting point for quantum models?
- Which quantum numbers describe the energy, shape, and orientation of hydrogen orbitals?
- Why are approximation methods necessary for multi-electron atoms?
- Name two approximation methods used in atomic models.
- What causes fine structure in atomic spectra?

4.2 Quantum Models of Molecular Systems

Molecules are more complex than atoms because they involve interactions between multiple nuclei and electrons. Quantum models help us understand how molecules form, how they vibrate and rotate, and how these behaviours are reflected in their spectra. This Part introduces the key quantum models of molecular systems, focusing on bonding theories, vibrational and rotational spectra, and their applications in spectroscopy and chemical physics.

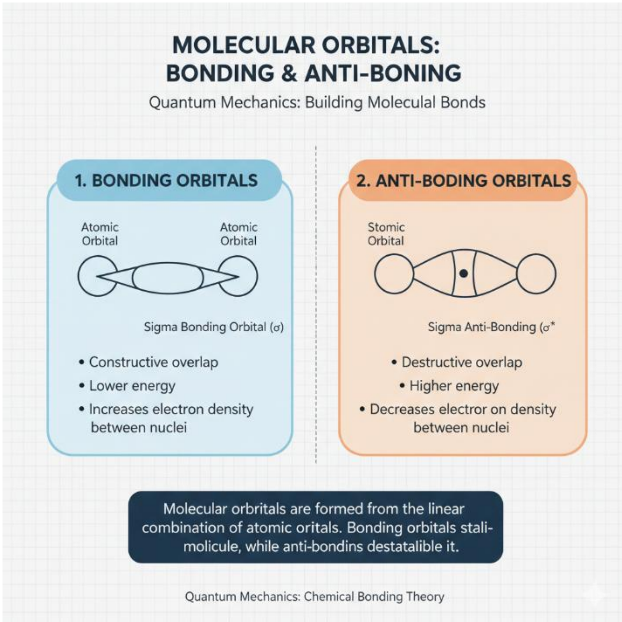
4.2.1 Molecular bonding and orbital theory

Molecular bonding is explained using **molecular orbital theory**, which describes how atomic orbitals combine to form molecular orbitals.

- **Bonding orbitals**: Lower energy orbitals formed when atomic orbitals combine constructively.
- **Anti-bonding orbitals**: Higher energy orbitals formed when atomic orbitals combine destructively.
- **Hybridisation**: Mixing of atomic orbitals to form new orbitals suited for bonding, such as sp, sp^2, and sp^3.

This theory explains why molecules are stable and how their shapes are determined.

Fill in the blank: When atomic orbitals combine constructively, they form ______ orbitals.



Caption: Formation of bonding and anti-bonding orbitals in molecular orbital theory.

4.2.2 Vibrational and rotational spectra

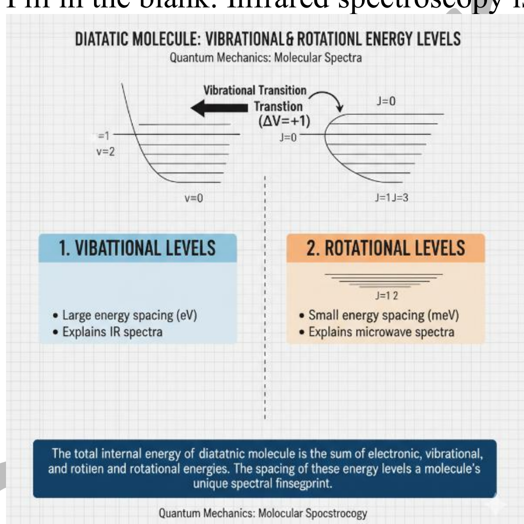
Molecules can vibrate and rotate, and these motions are quantised in quantum mechanics.

Vibrational spectra: Arise from transitions between quantised vibrational energy levels.

Rotational spectra: Arise from transitions between quantised rotational energy levels.

Infrared spectroscopy is used to study vibrational transitions, while microwave spectroscopy is used for rotational transitions.

Fill in the blank: Infrared spectroscopy is used to study ______ transitions in molecules.



Caption: Quantised vibrational and rotational energy levels in a diatomic molecule.

4.2.3 Applications in spectroscopy and chemical physics

Quantum models of molecular systems have wide applications in spectroscopy and chemical physics.

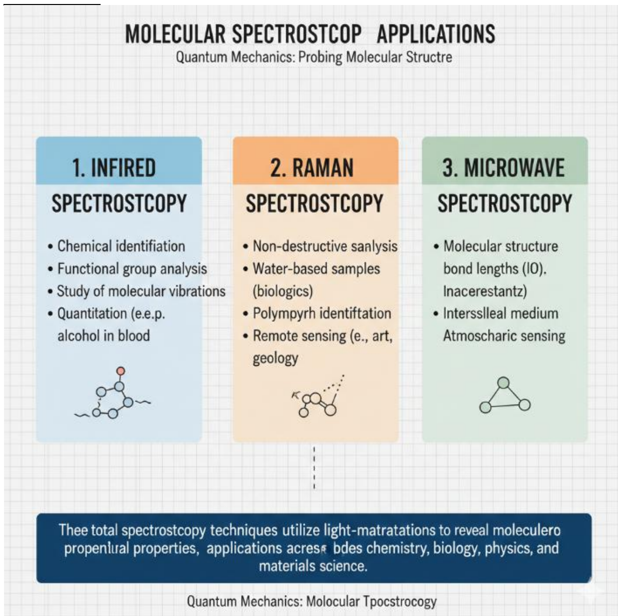
Infrared spectroscopy: Identifies functional groups in molecules by their vibrational frequencies.

Raman spectroscopy: Provides complementary information by detecting changes in polarizability.

Microwave spectroscopy: Reveals molecular structure through rotational transitions.

These techniques are essential tools in chemistry, physics, and materials science.

Fill in the blank: Raman spectroscopy detects transitions that involve changes in molecular ______.



Caption: Box 4.2: Applications of molecular spectroscopy

Pilot questions 4.2

What is molecular orbital theory, and what types of orbitals does it describe?

What is hybridisation, and why is it important in molecular bonding?

Which type of spectroscopy is used to study vibrational transitions?

What type of transitions are detected in microwave spectroscopy?

How does Raman spectroscopy differ from infrared spectroscopy?

4.3 Quantum Models in Solid-State Physics

Solid-state physics applies quantum mechanics to explain the behaviour of electrons in solids. These models help us understand why materials conduct electricity, why some are insulators, and why others exhibit remarkable properties such as superconductivity.

4.3.1 Free electron and band theory

The **free electron model** treats conduction electrons in a solid as if they were free particles moving inside a box. While simple, it explains basic properties such as electrical conductivity and heat capacity.

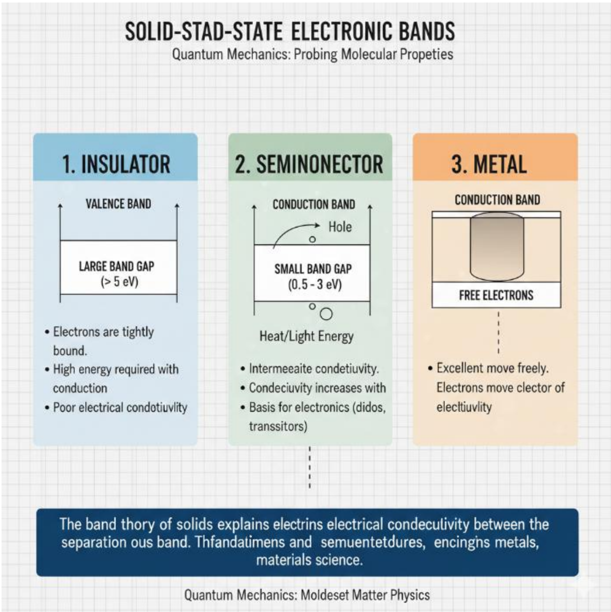
However, real solids have periodic arrangements of atoms, and this requires a more advanced model: **band theory**. Band theory shows that electrons occupy energy bands separated by gaps.

Conduction band: The band where electrons can move freely and conduct electricity.

Valence band: The band filled with electrons bound to atoms.

Band gap: The energy difference between the valence and conduction bands.

Fill in the blank: The energy difference between the valence band and the conduction band is called the ______.



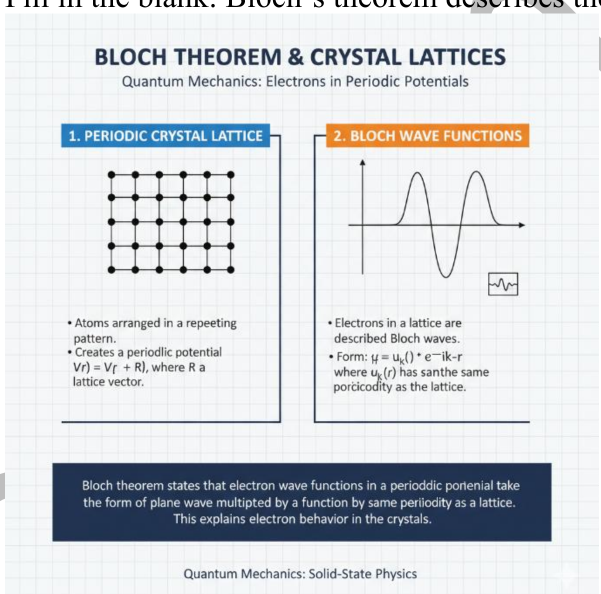
Caption: Band theory explains conduction and insulation in solids.

4.3.2 Bloch's theorem and crystal lattices

In a crystal lattice, atoms are arranged periodically. **Bloch's theorem** states that the wave function of an electron in a periodic potential can be written as a plane wave multiplied by a periodic function.

This theorem explains why electrons in crystals form energy bands and why their behaviour differs from free particles. It is fundamental to understanding semiconductors and metals.

Fill in the blank: Bloch's theorem describes the wave function of electrons in a ______ potential.



Caption: Bloch's theorem explains electron behaviour in periodic lattices.

4.3.3 Applications in semiconductors and superconductors

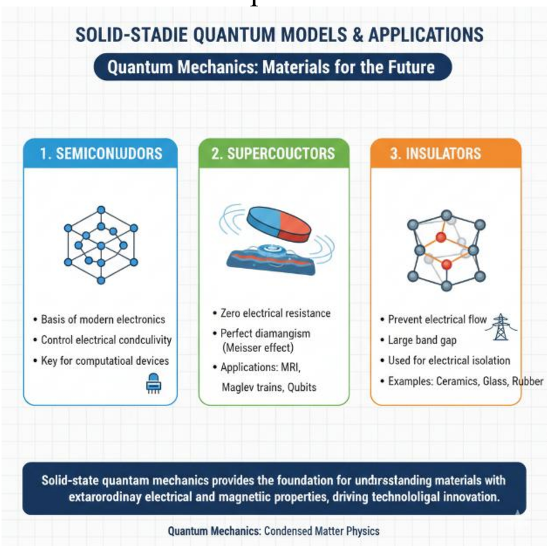
Quantum models of solids have practical applications in modern technology.

Semiconductors: Materials with a small band gap. Their conductivity can be controlled by doping, making them essential for electronics.

Superconductors: Materials that conduct electricity without resistance below a critical temperature. This phenomenon arises from quantum effects such as electron pairing (Cooper pairs).

Insulators: Materials with a large band gap, preventing electron conduction.

Fill in the blank: Superconductors conduct electricity without ______ below a critical temperature.



Caption: Box 4.3: Applications of solid-state quantum models

Pilot questions 4.3

What does the free electron model explain in solids?

What is the band gap in band theory?

State Bloch's theorem in simple terms.

How do semiconductors differ from insulators?

What property makes superconductors unique?

4.4 Quantum Models of Nuclear Phenomena

Nuclear systems are among the most complex in quantum mechanics. Unlike atoms and molecules, nuclei involve strong interactions between protons and neutrons, governed by the nuclear force. Quantum models of nuclear phenomena help us understand nuclear structure, excitations, and reactions, as well as processes such as radioactive decay.

4.4.1 Nuclear shell model

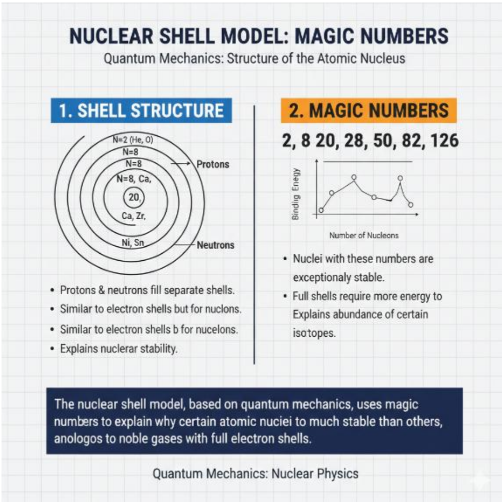
The **nuclear shell model** is analogous to the atomic shell model, but it applies to protons and neutrons inside the nucleus.

Protons and neutrons (collectively called **nucleons**) occupy discrete energy levels within the nucleus.

Shell closures at certain numbers of nucleons (called **magic numbers**) lead to particularly stable nuclei.

This model explains nuclear properties such as spin, parity, and binding energy.

Fill in the blank: Nuclei with closed shells at magic numbers are especially ______.



Caption: Nuclear shell model illustrating nucleon energy levels and magic numbers.

4.4.2 Collective models and nuclear excitations

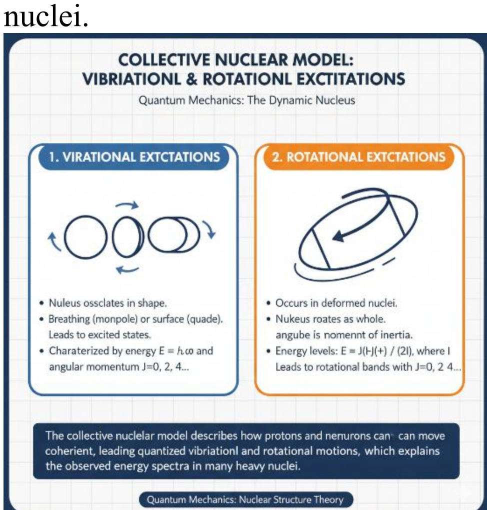
While the shell model explains many nuclear properties, it does not account for collective behaviours. The **collective model** describes nuclei as systems that can vibrate and rotate.

Vibrational excitations: Nuclei oscillate around their equilibrium shape.

Rotational excitations: Nuclei rotate as a whole, especially in deformed nuclei.

These collective motions explain patterns in nuclear spectra that the shell model alone cannot.

Fill in the blank: Rotational excitations occur when nuclei rotate as a whole, especially in ______ nuclei.



Caption: Collective nuclear excitations include vibrations and rotations.

4.4.3 Applications in nuclear reactions and decay processes

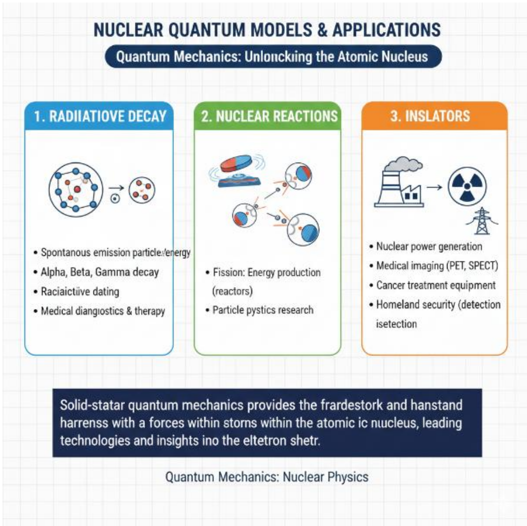
Quantum models of nuclei are essential for understanding nuclear reactions and decay.

Radioactive decay: Processes such as alpha decay, beta decay, and gamma emission are explained by nuclear models.

Nuclear reactions: Models predict outcomes of collisions between nuclei, including fusion and fission.

Applications: Nuclear models are used in energy production, medical imaging, and particle physics.

Fill in the blank: Alpha decay involves the emission of a ______ particle from the nucleus.



Caption: Box 4.4: Applications of nuclear quantum models

Pilot questions 4.4

What is the nuclear shell model, and what are magic numbers?
How does the collective model extend the shell model?
What are vibrational excitations in nuclei?
Give one example of a nuclear decay process explained by quantum models.
Name two practical applications of nuclear quantum models.

Series Summary

In this Series, we explored how quantum mechanics provides models to explain the behaviour of matter across different systems: atoms, molecules, solids, and nuclei. We began with **atomic systems**, where the Schrödinger equation describes hydrogen and approximation methods extend to multi-electron atoms, leading to insights into atomic spectra and fine structure. We then examined **molecular systems**, focusing on molecular orbital theory, vibrational and rotational spectra, and their applications in spectroscopy. Next, we studied **solid-state physics**, where free electron and band theory, Bloch's theorem, and applications in semiconductors and superconductors explain the properties of materials. Finally, we turned to **nuclear phenomena**, where the nuclear shell model, collective models, and applications in nuclear reactions and decay processes reveal the structure and behaviour of nuclei. Together, these models demonstrate the unifying power of quantum mechanics across scales.

Glossary of Terms

Schrödinger equation: Fundamental equation of quantum mechanics that determines allowed energy levels and wave functions. **Quantum numbers**: Numbers that describe the energy, shape, and orientation of atomic orbitals. **Molecular orbital theory**: A theory explaining how atomic orbitals combine to form molecular orbitals. **Hybridisation**: Mixing of atomic orbitals to form new orbitals suited for bonding. **Vibrational spectra**: Spectra arising from transitions between quantised vibrational energy levels. **Rotational spectra**: Spectra arising from transitions between quantised rotational energy levels. **Band theory**: A model explaining electron behaviour in solids, with energy bands separated by band gaps. **Bloch's theorem**: A principle describing electron wave functions in periodic crystal lattices. **Semiconductors**: Materials with small band gaps whose conductivity can be controlled. **Superconductors**: Materials that conduct electricity without resistance below a critical temperature. **Nuclear shell model**: A model describing nucleons occupying discrete energy levels in the nucleus. **Magic numbers**: Specific numbers of nucleons that lead to especially stable nuclei. **Collective model**: A nuclear model describing vibrational and rotational excitations of nuclei. **Radioactive decay**: Processes such as alpha, beta, and gamma decay explained by nuclear models.

Concept Check Questions 4

Objective Questions

The Schrödinger equation for hydrogen shows that electrons can only occupy ______ energy levels.

In multi-electron atoms, electron–electron interactions make exact solutions of the Schrödinger equation ______.

When atomic orbitals combine constructively, they form ______ orbitals.

Infrared spectroscopy is used to study ______ transitions in molecules.

The energy difference between the valence band and the conduction band is called the ______.

Bloch's theorem describes the wave function of electrons in a ______ potential.

Superconductors conduct electricity without ______ below a critical temperature.

Nuclei with closed shells at magic numbers are especially ______.

Rotational excitations occur when nuclei rotate as a whole, especially in ______ nuclei.

Alpha decay involves the emission of a ______ particle from the nucleus.

Short-Answer Questions

What are the three quantum numbers that describe hydrogen orbitals?

Why are approximation methods necessary for multi-electron atoms?

What is hybridisation, and why is it important in molecular bonding?

How does Raman spectroscopy differ from infrared spectroscopy?

State Bloch's theorem in simple terms.

What property makes superconductors unique?

What are vibrational excitations in nuclei?

Give one example of a nuclear decay process explained by quantum models.

Long-Answer Questions

Analyse how the Schrödinger equation and approximation methods together explain atomic systems beyond hydrogen.

Discuss the role of molecular orbital theory and spectroscopy in understanding molecular behaviour.

Evaluate the importance of band theory and Bloch's theorem in explaining solid-state phenomena.

Assess how the nuclear shell model and collective models complement each other in explaining nuclear structure and excitations.

Integrate knowledge of atomic, molecular, solid-state, and nuclear quantum models to explain how quantum mechanics unifies our understanding of matter.

Answers to Pilot Questions 4

Part 4.1 Quantum Models of Atomic Systems

The hydrogen atom is simple and solvable, making it an ideal starting point.

Principal (n), angular momentum (l), and magnetic (m).

Electron–electron interactions make exact solutions impossible.

Hartree–Fock and perturbation theory.

Relativistic effects and spin interactions.

Part 4.2 Quantum Models of Molecular Systems

Molecular orbital theory describes bonding and anti-bonding orbitals.
Hybridisation mixes orbitals to form new bonding orbitals.
Infrared spectroscopy.
Rotational transitions.
Raman detects changes in polarizability, while infrared detects dipole moment changes.

Part 4.3 Quantum Models in Solid-State Physics

Electrical conductivity and heat capacity.
Band gap.
Electron wave functions in periodic potentials.
Semiconductors have small band gaps; insulators have large ones.
Zero resistance below critical temperature.

Part 4.4 Quantum Models of Nuclear Phenomena

Shell model; magic numbers are stable nucleon counts.
It adds vibrational and rotational behaviours.
Oscillations around equilibrium shape.
Alpha decay.
Nuclear energy, medicine, and particle physics.

References and Attributions 4

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COURSE CODE: PHY 402
COURSE TITLE: Quantum Mechanics II
COURSE UNIT: 3 UNITS

Here are five comprehensive series titles that fully cover the scope of the attached PHY 402 course:

Series 1: Perturbation Methods in Quantum Mechanics

Series 2: Quantum Scattering Theory and Elastic Potential Scattering

Series 3: Symmetries and Selection Rules in Quantum Mechanics

Series 4: Quantum Models of Atomic, Molecular, Solid-State, and Nuclear Phenomena

Series 5: Relativistic Wave Equations and Quantum Motion in Electromagnetic Fields

Here is a proposed outline:

Series 5: Relativistic Quantum Equations and Motion in Fields

Part 5.1: Foundations of Relativistic Quantum Mechanics

5.1.1 Limitations of non-relativistic Schrödinger equation
5.1.2 Introduction to relativistic wave equations
5.1.3 Physical significance of relativistic corrections

Part 5.2: Klein–Gordon Equation

5.2.1 Derivation from relativistic energy–momentum relation
5.2.2 Properties and solutions
5.2.3 Applications to spin-0 particles

Part 5.3: Dirac Equation

5.3.1 Motivation and derivation
5.3.2 Spin and the role of gamma matrices
5.3.3 Predictions: antimatter and fine structure corrections

Part 5.4: Quantum Motion in Electromagnetic Fields

5.4.1 Minimal coupling and gauge invariance
5.4.2 Landau levels and charged particle motion
5.4.3 Applications in quantum Hall effect and condensed matter physics

Introduction

Relativistic effects become essential when dealing with particles moving close to the speed of light or interacting strongly with electromagnetic fields. The non-relativistic Schrödinger equation, while powerful, cannot fully capture these phenomena. To address this, physicists developed **relativistic wave equations**, such as the Klein–Gordon and Dirac equations, which extend quantum mechanics to include special relativity. These equations not only explain the behaviour of high-energy particles but also predict new phenomena, such as antimatter.

The aim of this Series is to introduce you to the foundations of relativistic quantum mechanics and to show how particles behave when subjected to electromagnetic fields. You will learn the limitations of the non-relativistic Schrödinger equation, the derivation and applications of the Klein–Gordon equation for spin-0 particles, and the Dirac equation for spin-½ particles. Finally, you will explore how quantum motion in electromagnetic fields leads to phenomena such as Landau levels and the quantum Hall effect.

We shall begin this Series by studying the **foundations of relativistic quantum mechanics**, where we highlight the need for relativistic corrections and introduce the concept of relativistic wave equations. Next, we will examine the **Klein–Gordon equation**, its derivation from the relativistic energy–momentum relation, and its applications to spin-0 particles. Following this, we will focus on the **Dirac equation**, which incorporates spin and predicts antimatter, as well as fine structure corrections. Finally, we will conclude with **quantum motion in electromagnetic fields**, exploring minimal coupling, gauge invariance, Landau levels, and applications in condensed matter physics.

Series Learning Outcomes

Series 5: Relativistic Quantum Equations and Motion in Fields

By the end of this Series, you should be able to:

SLO 5.1 explain the limitations of the non-relativistic Schrödinger equation and the need for relativistic quantum mechanics,

SLO 5.2 derive the Klein–Gordon equation from the relativistic energy–momentum relation and discuss its properties and applications to spin-0 particles,

SLO 5.3 analyse the Dirac equation, including its derivation, the role of gamma matrices, and its predictions such as spin and antimatter,

SLO 5.4 apply the principles of minimal coupling and gauge invariance to describe quantum motion in electromagnetic fields,

SLO 5.5 evaluate phenomena such as Landau levels and the quantum Hall effect as applications of quantum motion in fields,

SLO 5.6 integrate knowledge of relativistic wave equations and electromagnetic field interactions to interpret experimental results in high-energy and condensed matter physics.

5.1 Foundations of Relativistic Quantum Mechanics

Quantum mechanics, as originally formulated, is based on the **Schrödinger equation**, which successfully explains atomic and molecular systems at low energies. However, when particles move close to the speed of light, or when high-energy processes are involved, the Schrödinger equation becomes inadequate because it does not incorporate the principles of **special relativity**. This is where **relativistic quantum mechanics** comes in, extending the framework to account for relativistic effects.

5.1.1 Limitations of non-relativistic Schrödinger equation

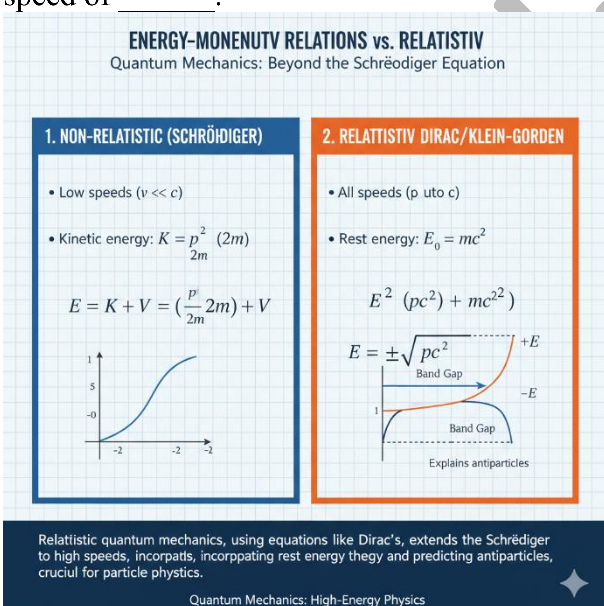
The Schrödinger equation assumes that particle velocities are much smaller than the speed of light. At relativistic speeds, this assumption breaks down.

It does not account for relativistic energy–momentum relations.

It cannot explain phenomena such as particle creation and annihilation.

It fails to predict the existence of antimatter.

Fill in the blank: The Schrödinger equation becomes inadequate when particles move close to the speed of ______.



Caption: Limitations of the Schrödinger equation at relativistic speeds.

5.1.2 Introduction to relativistic wave equations

To overcome these limitations, physicists developed **relativistic wave equations**. These equations combine quantum mechanics with special relativity to describe particles at high energies.

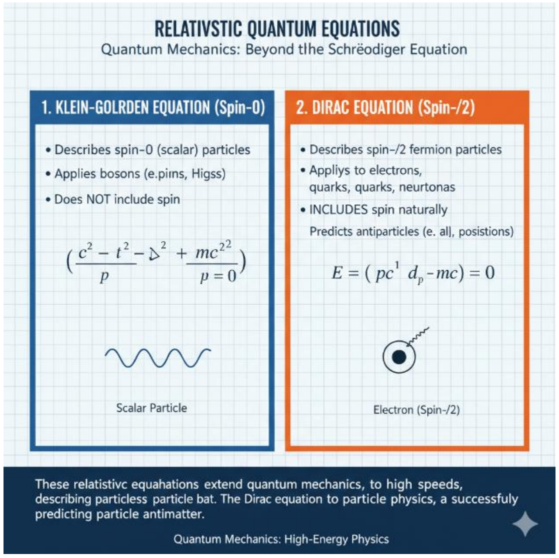
Klein–Gordon equation: Describes spin-0 particles such as mesons.

Dirac equation: Describes spin-½ particles such as electrons and predicts antimatter.

These equations ensure consistency with the relativistic energy–momentum relation:

E2=p2c2+m2c4

Fill in the blank: The Klein–Gordon equation is used to describe particles with spin ______.



Caption: Box 5.1: Key relativistic wave equations

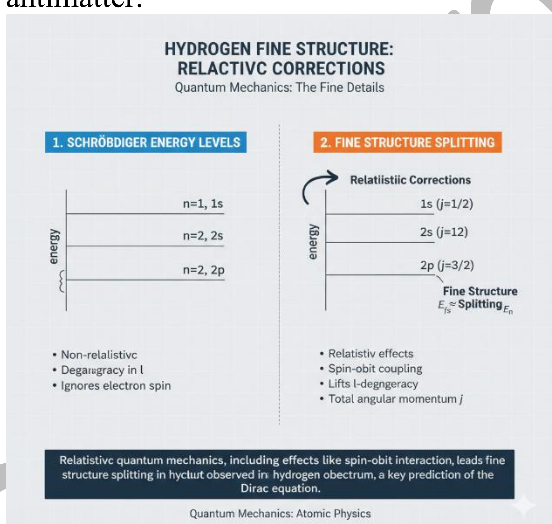
5.1.3 Physical significance of relativistic corrections

Relativistic corrections are not just mathematical refinements; they have observable consequences.

- They explain fine structure in atomic spectra.
- They predict the existence of antimatter, confirmed by the discovery of the positron.
- They account for spin and magnetic interactions in particles.

These corrections are essential for high-energy physics, particle physics, and condensed matter systems where relativistic effects become significant.

Fill in the blank: The discovery of the ______ confirmed the Dirac equation's prediction of antimatter.



Caption: Relativistic corrections explain fine structure in atomic spectra.

Pilot questions 5.1

- Why does the Schrödinger equation fail at relativistic speeds?
- What is the relativistic energy–momentum relation?
- Which relativistic wave equation describes spin-0 particles?
- Which relativistic wave equation predicts antimatter?
- What experimental discovery confirmed the Dirac equation's prediction?

5.2 Klein–Gordon Equation

The **Klein–Gordon equation** is the simplest relativistic wave equation. It was developed to describe spin-0 particles, such as mesons, and is derived directly from the relativistic energy–momentum relation. Although it preceded the Dirac equation, it remains an important tool in quantum field theory and high-energy physics.

5.2.1 Derivation from relativistic energy–momentum relation

The relativistic energy–momentum relation is given by:

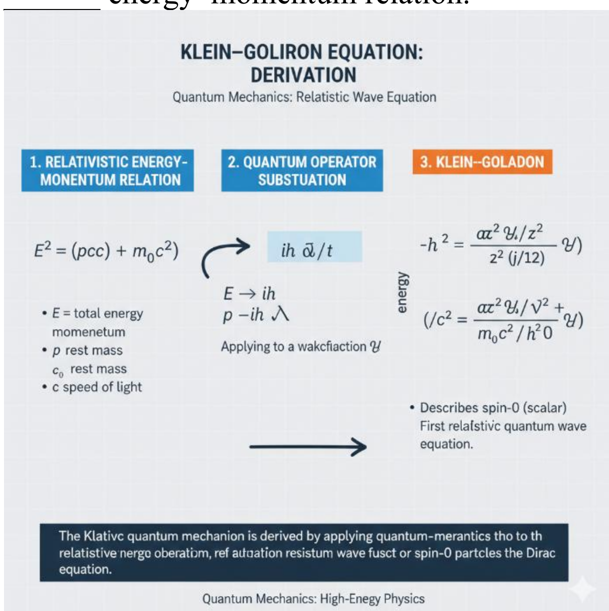
$$E^2=p^2c^2+m^2c^4$$

By substituting the quantum operators for energy ($E\to i\hbar\frac{\partial}{\partial t}$) and momentum ($p\to -i\hbar\nabla$), we obtain the **Klein–Gordon equation**:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla^2+\frac{m^2c^2}{\hbar^2}\right)\psi=0$$

This equation is second-order in both time and space, unlike the Schrödinger equation, which is first-order in time.

Fill in the blank: The Klein–Gordon equation is derived by substituting quantum operators into the ______ energy–momentum relation.



Caption: Derivation of Klein–Gordon equation from relativistic principles.

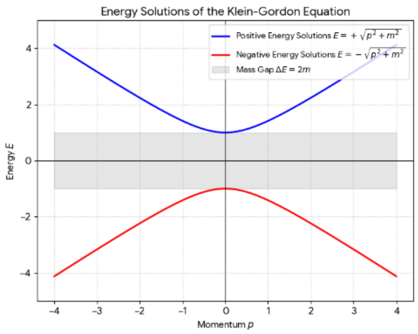
5.2.2 Properties and solutions

The Klein–Gordon equation has several important properties:

- It is consistent with special relativity.
- It describes particles with **spin-0**.
- Its solutions include both positive and negative energy states.

The presence of negative energy solutions initially caused confusion, but later these were reinterpreted as representing antiparticles.

Fill in the blank: Negative energy solutions of the Klein–Gordon equation were later reinterpreted as representing ______.



Caption: Positive and negative energy solutions of the Klein–Gordon equation.

5.2.3 Applications to spin-0 particles

The Klein–Gordon equation is particularly useful for describing **spin-0 particles**, which have no intrinsic angular momentum.

- Examples include mesons such as pions and kaons.
- It is widely used in quantum field theory to model scalar fields.
- It provides a foundation for more advanced theories, including quantum electrodynamics (QED).

Fill in the blank: The Klein–Gordon equation is used to describe particles such as ______, which are spin-0 mesons.

Caption: Box 5.2: Applications of Klein–Gordon equation

Pilot questions 5.2

- From which relation is the Klein–Gordon equation derived?
- What type of particles does the Klein–Gordon equation describe?
- Why did negative energy solutions initially cause confusion?
- How were negative energy solutions later reinterpreted?
- Give one example of a spin-0 particle described by the Klein–Gordon equation.

5.3 Dirac Equation

The **Dirac equation** is one of the most important achievements in theoretical physics. It extends quantum mechanics to include both relativity and spin, providing a complete description of spin-½ particles such as electrons. Unlike the Klein–Gordon equation, which applies to spin-0 particles, the Dirac equation successfully explains fine structure in atomic spectra and predicts the existence of antimatter.

5.3.1 Motivation and derivation

The Klein–Gordon equation, while relativistically consistent, is second-order in time and does not naturally incorporate spin. To address this, Paul Dirac sought a wave equation that was:

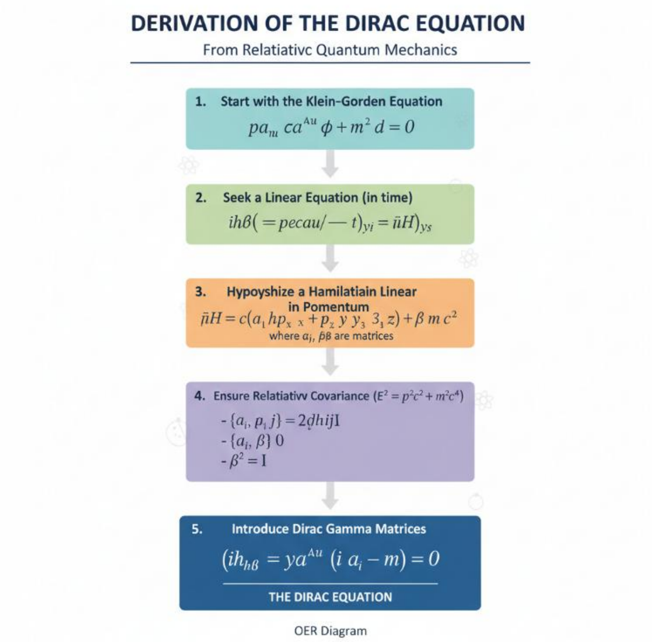
- First-order in both time and space.
- Consistent with the relativistic energy–momentum relation.
- Capable of describing spin-½ particles.

Dirac introduced **matrices** into the equation, leading to a linear form:

(iℏγμ∂μ−mc)ψ=0

Here, γμ are the **gamma matrices**, which ensure the equation is Lorentz invariant.

Fill in the blank: The Dirac equation is first-order in both ______ and space.



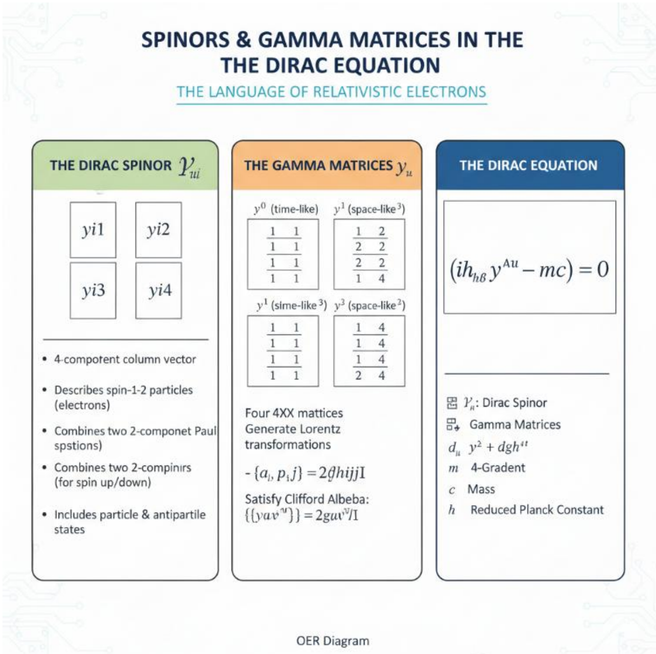
Caption: Derivation of Dirac equation incorporating gamma matrices.

5.3.2 Spin and the role of gamma matrices

The Dirac equation naturally incorporates **spin**, a fundamental property of particles that has no classical analogue.

- Spin-½ particles, such as electrons, are described by four-component wave functions called **spinors**.
- The gamma matrices encode the relativistic behaviour of these spinors.
- This framework explains magnetic interactions and fine structure in atomic spectra.

Fill in the blank: The Dirac equation describes spin-½ particles using four-component wave functions called ______.



Caption: Spinors and gamma matrices in the Dirac equation.

5.3.3 Predictions: antimatter and fine structure corrections

One of the most remarkable outcomes of the Dirac equation is its prediction of **antimatter**.

Negative energy solutions were reinterpreted as antiparticles, leading to the discovery of the positron.

The equation explains fine structure in hydrogen spectra, accounting for relativistic and spin effects.

It also provides the foundation for quantum electrodynamics (QED), the most precise theory in physics.

Fill in the blank: The discovery of the ______ confirmed the Dirac equation's prediction of antimatter.

Caption: Box 5.3: Predictions of the Dirac equation

Pilot questions 5.3

Why did Dirac seek a wave equation that was first-order in time?

What role do gamma matrices play in the Dirac equation?

What type of particles are described by the Dirac equation?

What experimental discovery confirmed the Dirac equation’s prediction of antimatter?

How does the Dirac equation explain fine structure in atomic spectra?

5.4 Quantum Motion in Electromagnetic Fields

Electromagnetic fields play a central role in quantum mechanics, influencing the behaviour of charged particles and giving rise to fascinating phenomena. By combining relativistic wave equations with electromagnetic interactions, we can understand how particles move in fields and how these motions lead to observable effects in condensed matter and high-energy physics.

5.4.1 Minimal coupling and gauge invariance

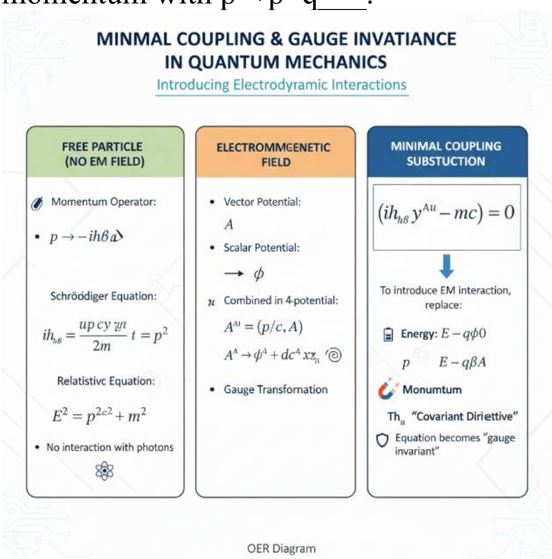
The interaction of charged particles with electromagnetic fields is introduced through the principle of **minimal coupling**.

In quantum mechanics, momentum is replaced by p→p−qA, where q is the charge and A is the vector potential.

This ensures that the equations remain consistent with **gauge invariance**, meaning the physics does not change under transformations of the potentials.

Gauge invariance is a cornerstone of modern quantum field theory.

Fill in the blank: Minimal coupling introduces electromagnetic interactions by replacing momentum with p→p−q___.



Caption: Minimal coupling introduces electromagnetic interactions in quantum equations.

5.4.2 Landau levels and charged particle motion

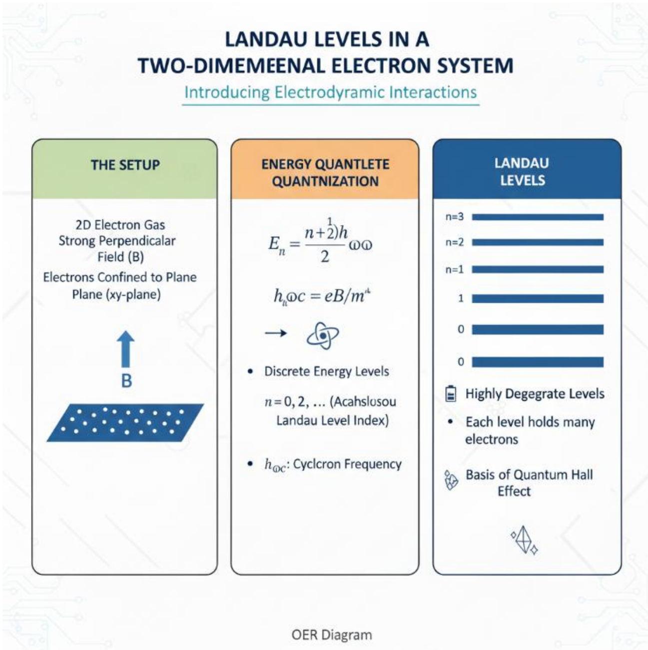
When a charged particle moves in a magnetic field, its motion becomes quantised into discrete energy levels called **Landau levels**.

These levels arise from the cyclotron motion of electrons in a magnetic field.

They explain phenomena such as the quantum Hall effect.

Landau quantisation is crucial in condensed matter physics, especially in two-dimensional electron systems.

Fill in the blank: The quantised energy levels of electrons in a magnetic field are called ______ levels.



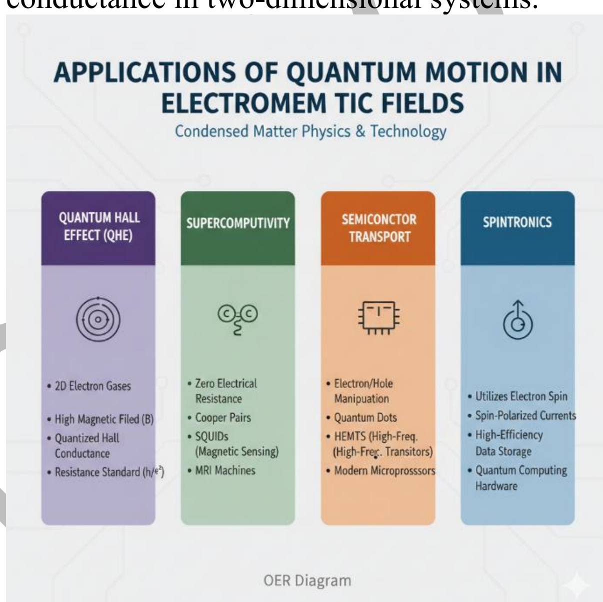
Caption: Landau levels describe quantised motion of electrons in magnetic fields.

5.4.3 Applications in quantum Hall effect and condensed matter physics

The study of quantum motion in electromagnetic fields has led to remarkable discoveries.

- **Quantum Hall effect**: Occurs when electrons in two-dimensional systems form quantised Hall conductance due to Landau levels.
- **Condensed matter applications**: Understanding superconductivity, magnetoresistance, and electron transport in semiconductors.
- These phenomena are not only of theoretical interest but also form the basis of modern electronic technologies.

Fill in the blank: The quantum Hall effect arises from the formation of quantised ______ conductance in two-dimensional systems.



Caption: Box 5.4: Applications of quantum motion in fields

Pilot questions 5.4

What principle introduces electromagnetic interactions into quantum mechanics?
What does gauge invariance ensure in quantum equations?
What are Landau levels, and how do they arise?
What phenomenon is explained by Landau quantisation in two-dimensional systems?
Name two applications of quantum motion in electromagnetic fields.

Series Summary

In this Series, we examined how quantum mechanics is extended to include relativistic effects and electromagnetic interactions. We began with the **foundations of relativistic quantum mechanics**, highlighting the limitations of the non-relativistic Schrödinger equation and the need for relativistic corrections. We then studied the **Klein–Gordon equation**, derived from the relativistic energy–momentum relation, which describes spin-0 particles and scalar fields. Next, we explored the **Dirac equation**, which incorporates spin, predicts antimatter, and explains fine structure in atomic spectra. Finally, we analysed **quantum motion in electromagnetic fields**, focusing on minimal coupling, gauge invariance, Landau levels, and applications such as the quantum Hall effect. Together, these topics demonstrate how relativistic quantum equations unify high-energy physics and condensed matter phenomena.

Glossary of Terms

Relativistic quantum mechanics: Extension of quantum mechanics that incorporates special relativity. **Schrödinger equation**: Fundamental non-relativistic wave equation in quantum mechanics. **Klein–Gordon equation**: Relativistic wave equation describing spin-0 particles. **Dirac equation**: Relativistic wave equation describing spin-½ particles, predicting antimatter. **Gamma matrices**: Mathematical matrices used in the Dirac equation to ensure Lorentz invariance. **Spinors**: Four-component wave functions describing spin-½ particles. **Antimatter**: Matter composed of antiparticles, such as positrons, predicted by the Dirac equation. **Minimal coupling**: Principle introducing electromagnetic interactions into quantum mechanics by modifying momentum. **Gauge invariance**: Property ensuring physical laws remain unchanged under transformations of potentials. **Landau levels**: Quantised energy levels of electrons in a magnetic field. **Quantum Hall effect**: Phenomenon where Hall conductance becomes quantised due to Landau levels.

Concept Check Questions 5

Objective Questions

The Schrödinger equation becomes inadequate when particles move close to the speed of ______.
The Klein–Gordon equation is derived from the relativistic ______ relation.
The Klein–Gordon equation describes particles with spin ______.
The Dirac equation is first-order in both time and ______.
The Dirac equation describes spin-½ particles using four-component wave functions called ______.
The discovery of the ______ confirmed the Dirac equation's prediction of antimatter.
Minimal coupling introduces electromagnetic interactions by replacing momentum with $p \to p - q$___.
The quantised energy levels of electrons in a magnetic field are called ______ levels.
The quantum Hall effect arises from the formation of quantised ______ conductance.

Short-Answer Questions

Why does the Schrödinger equation fail at relativistic speeds?
What type of particles are described by the Klein–Gordon equation?
What role do gamma matrices play in the Dirac equation?
How were negative energy solutions of relativistic equations reinterpreted?
What principle ensures that physics remains unchanged under transformations of potentials?
What phenomenon is explained by Landau quantisation in two-dimensional systems?

Long-Answer Questions

Analyse how the Klein–Gordon equation extends quantum mechanics to spin-0 particles.
Discuss the derivation and significance of the Dirac equation in predicting antimatter.
Evaluate the importance of minimal coupling and gauge invariance in quantum motion in fields.
Assess how Landau levels and the quantum Hall effect demonstrate quantisation in condensed matter systems.
Integrate knowledge of relativistic wave equations and electromagnetic interactions to explain their role in modern physics.

Answers to Pilot Questions 5

Part 5.1 Foundations of Relativistic Quantum Mechanics

It fails because it does not incorporate relativistic energy–momentum relations.
E2=p2c2+m2c4.
Klein–Gordon equation describes spin-0 particles.
Dirac equation predicts antimatter.
The positron confirmed the Dirac prediction.

Part 5.2 Klein–Gordon Equation

Derived from relativistic energy–momentum relation.
Spin-0 particles.
Negative energy solutions seemed unphysical.
Later reinterpreted as antiparticles.
Example: pions.

Part 5.3 Dirac Equation

To ensure consistency with relativity and time evolution.
Gamma matrices ensure Lorentz invariance.
Spin-½ particles.
Discovery of the positron.
It explains fine structure in hydrogen spectra.

Part 5.4 Quantum Motion in Electromagnetic Fields

Minimal coupling.
Gauge invariance ensures consistency.
Landau levels are quantised energy states in magnetic fields.
Quantum Hall effect.
Applications include superconductivity and semiconductor transport.

References and Attributions 5

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