Quantum Mechanics

Week 5

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Pre-Reading Note

Dear Students,

Welcome to the course on Quantum Mechanics. As part of your learning resources, I will prepare a series of educational materials and sheets designed to complement the lectures.

Please note that these materials are **abridged versions** of the content from the textbook ***"Introduction to Quantum Mechanics By David J. Griffiths"***. They have been tailored to align with the class schedule and topics, providing you with concise summaries and key points for each topic covered.

It's important to understand that these sheets are **not standalone resources**. They are intended to be used in conjunction with the class material. For a deeper understanding and a more comprehensive view of each topic, I strongly encourage you to refer to the mentioned textbook.

The book provides detailed explanations, examples, and insights that go beyond the scope of our summaries. It will be an invaluable resource for you to solidify your understanding of Quantum Mechanics.

I cannot guarantee neither correctness nor completeness of the script. Please report any mistake directly to me.

Have fun with Quantum Mechanics!

Best regards,

Mark Benazet Castells

1 Quantum Mechanics of Finite Potentials

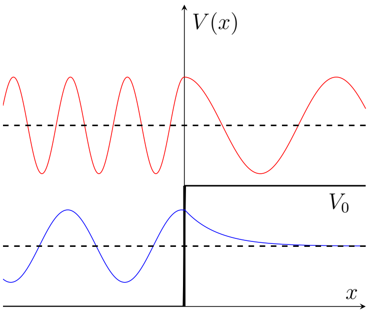
In quantum mechanics, the behavior of a particle in a potential is fundamentally dictated by the energy of the particle relative to the potential. For any potential, finite or infinite, the conditions for bound and scattering states are as follows:

$$\begin{cases} E < V(\pm\infty) & \Rightarrow \text{ bound state} \\ E > V(\pm\infty) & \Rightarrow \text{ scattering state} \end{cases}$$

- In both finite and infinite potentials, bound states occur when the particle's energy is less than the potential at infinity, $V(\pm\infty)$.
- Scattering states are observed when the particle's energy exceeds the potential at infinity.
- All transmission and reflection processes conserve the total energy of the system.

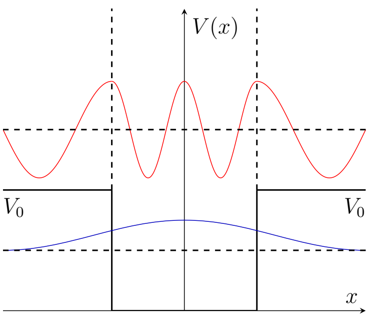
1.1 Finite Potential Step

- $E > V_0$: There is both transmission and reflection. Scattering state.
- $0 < E < V_0$: The particle is reflected, and there is some penetration into the barrier. Scattering state.
- $E < V_{min}$: There is no physical solution.



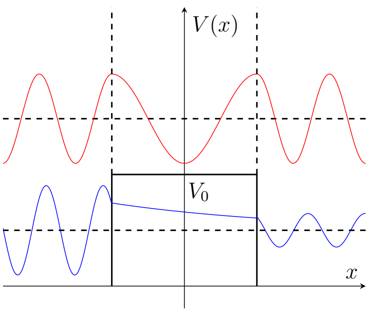
1.2 Finite Potential Well

- $E > V_0$: The particle experiences transmission and reflection. Scattering state.
- $0 < E < V_0$: There are bound states with some penetration into the barrier. Even if $V_0 \approx 0$, there is always at least one bound state.
- $E < V_{min}$: There is no physical solution.



1.3 Finite Potential Barrier

- $E > V_0$: The particle is transmitted and reflected. Scattering state.
- $0 < E < V_0$: There is transmission and reflection, with exponential decay in the barrier. Scattering state.
- $E < V_{min}$: There is no physical solution.



We can see that the wavelength of a particle's state is influenced by the potential region it occupies. This relationship is grounded in the wave-particle duality and can be mathematically expressed through the wave number k. As established in previous theory sheets, the wave number in a region with potential V_0 is given by:

$$k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}},$$

where E represents the energy of the particle, m is its mass, and $\hbar$ is the reduced Planck constant. The wavelength λ of the particle's wave function is inversely proportional to the wave number, as indicated by the relationship:

$$k = \frac{2\pi}{\lambda}.$$

1.4 Quantum Mechanical Tunneling

Quantum tunneling is a phenomenon that allows a particle to penetrate through a potential barrier that it classically should not be able to pass. The probability T of a particle being transmitted through such a barrier is given by:

$$T \approx \frac{16E(V_0 - E)}{V_0^2} \exp\left[-4\frac{\sqrt{2m(V_0 - E)}}{\hbar}a\right]$$

Quantum tunneling is a purely quantum mechanical effect with no classical counterpart.

2 Dirac Notation

Dirac notation is particularly useful for describing states in complex quantum systems.

2.1 The Hilbert Space and State Vectors

Physically meaningful quantum states are represented in Hilbert Space $\boldsymbol{\mathcal{H}}$, a complex vector space equipped with an inner product. The state of a quantum system is described by a wave function $\Psi(\vec{r}, t)$, which must satisfy two key properties:

- **Square Integrability:** The probability density associated with Ψ should be integrable over the entire space.
- **Normalizability:** The integral of the probability density over all space must equal one.

These properties ensure that Ψ resides in $\mathcal{H}$.

This properties were already treated in the Theory Sheet of Week 2.

2.2 Dirac Notation: Kets and Bras

In Dirac notation:

- A *ket* $|\Psi\rangle$ represents the state vector:

$$\Psi = \sum_n c_n f_n(\vec{r}) \Rightarrow (c_1 \ c_2 \ldots c_n)^T = |\Psi\rangle \tag{1}$$

- A *bra* $\langle\Psi|$ represents the complex conjugate transpose of the ket:

$$\Psi^* = \sum_n c_n^* f_n^*(\vec{r}) \Rightarrow (c_1^* \ c_2^* \ldots c_n^*) = \langle\Psi| \tag{2}$$

2.3 Inner Product, Orthogonality, and Completeness

The inner product in $\mathcal{H}$ is defined as $\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\, dx$, which leads to two important concepts:

- **Orthonormality:** Functions f_n are orthonormal if $\langle f_m|f_n\rangle = \delta_{mn}$.
- **Completeness:** A set of functions is complete if any function $F(x)$ in $\mathcal{H}$ can be expressed as a sum of these functions.

2.4 Normalization and Expectation Values

Normalization of a state vector is given by $\langle\Psi|\Psi\rangle = 1$. The expectation value of an observable $\hat{A}$ in state Ψ is $\langle\hat{A}\rangle = \langle\Psi|\hat{A}\Psi\rangle$.

3 Hermitian Operators

Hermitian operators play a crucial role in quantum mechanics, particularly in defining observables and ensuring the physical reality of measured quantities.

3.1 Definition and Requirements

An operator $\hat{Q}$ is Hermitian if it satisfies the following condition for all functions f and g:

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$$
$$\hat{Q} = \hat{Q}^\dagger$$

This condition ensures that observables, which are represented by Hermitian operators, yield real and physically meaningful values.

3.2 Properties of Hermitian Operators

- **Orthogonality of Eigenstates:** The eigenstates $|\psi_m\rangle$ and $|\psi_n\rangle$ of a Hermitian operator $\hat{Q}$ are orthogonal if their eigenstates are non-degenerate. This is expressed as:

  $$\langle \psi_m|\psi_n\rangle = 0 \quad \text{for} \quad m \neq n.$$

  Orthogonality ensures that distinct states are independent.

- **Completeness:** The eigenstates of a Hermitian operator form a complete basis set for the Hilbert Space $\mathcal{H}$. Any state $|\phi\rangle$ in $\mathcal{H}$ can be expressed as a linear combination of these eigenstates:

  $$|\phi\rangle = \sum_n c_n |\psi_n\rangle .$$

  Completeness is fundamental for expanding states in terms of observable eigenstates.

- **Real Eigenvalues:** The eigenvalues of a Hermitian operator are always real. If $|\psi\rangle$ is an eigenstate of $\hat{Q}$ with eigenvalue λ, then:

  $$\hat{Q}|\psi\rangle = \lambda |\psi\rangle , \quad \text{where} \quad \lambda \in \mathbb{R}.$$

  This property ensures that physical observables, which are represented by Hermitian operators, yield real-valued measurements.

4 Determinate States

Determinate states in quantum mechanics are defined by the certainty in measurement outcomes of specific observables. These states are directly tied to the eigenfunctions and eigenvalues of the observables' corresponding Hermitian operators.

4.1 Eigenvalue Equation

The eigenvalue equation for a Hermitian operator $\hat{Q}$ provides a mathematical basis for determinate states:

$$\hat{Q}\Psi = q\Psi$$

where:

- Ψ is an eigenfunction of $\hat{Q}$.
- q is the corresponding eigenvalue, representing the measurable value of the observable associated with $\hat{Q}$.

4.2 Characteristics of Determinate States

- **Consistency in Measurement:** For a quantum system in state Ψ_q, the observable Q corresponding to $\hat{Q}$ will always yield the eigenvalue q:
- **Operator Spectrum:** The spectrum of $\hat{Q}$ encompasses all its eigenvalues, denoting the set of possible measurement outcomes for Q:

  $$\text{Spectrum}(\hat{Q}) = \{q_1, q_2, \ldots, q_n\}.$$

- **Degeneracy:** Degeneracy occurs when multiple distinct eigenfunctions Ψ_i and Ψ_j correspond to the same eigenvalue q:

  $$\hat{Q}\Psi_i = q\Psi_i \text{ and } \hat{Q}\Psi_j = q\Psi_j \text{ for } i \neq j.$$

  It indicates the presence of different quantum states yielding the same measurement value.

4.3 Categories of Eigenfunctions of Hermitian Operators

Eigenfunctions of Hermitian operators can be classified into two main categories based on the nature of their spectra: discrete and continuous.

4.3.1 Discrete Spectrum

In the discrete spectrum, eigenvalues are distinct and separated:

- **Hilbert Space:** Eigenfunctions associated with a discrete spectrum lie within the Hilbert Space. These functions represent physically realizable states and form a complete set.
- **Real Eigenvalues:** The eigenvalues in a discrete spectrum are real, corresponding to observable physical quantities.
- **Orthogonality:** Eigenfunctions corresponding to distinct eigenvalues are orthogonal to each other.

4.3.2 Continuous Spectrum

The continuous spectrum is characterized by eigenvalues that cover an entire range:

- **Non-Normalizability:** Eigenfunctions in a continuous spectrum are not normalizable because their inner product may not exist and do not represent possible physical states within Hilbert Space.
- **Dirac-Orthonormality:** Despite not being normalizable, these eigenfunctions with real eigenvalues are Dirac-orthonormalizable and form a complete set (sum transitions to integral).

Specific Cases

Eigenfunctions can be defined for position and momentum operators, although they do not reside in Hilbert Space:

- **Position Operator Eigenstates:** Defined as $f_{\hat{x}} = \delta(x - q)$, where q is the eigenvalue of $\hat{x}$. Despite being complete, $\delta(x - q)$ is not square-integrable and thus not in Hilbert Space.
- **Momentum Operator Eigenstates:** Given by $f_{\hat{p}} = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{iqx}{\hbar}\right)$, where q is the eigenvalue of $\hat{p}$. These also do not exist in Hilbert Space but are complete.

5 Generalized Statistical Interpretation

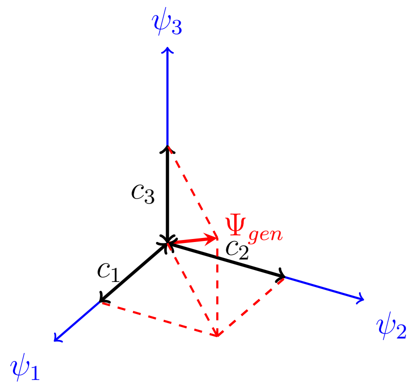
The generalized statistical interpretation in quantum mechanics provides a framework for understanding the outcomes of measurements on quantum systems. It explains how observable quantities are determined and the probabilistic nature of these measurements.

5.1 Measurement Outcomes and Probabilities

When measuring an observable $Q(x,p)$ on a particle in state Ψ, the outcome will be one of the eigenvalues of Q. The probability of obtaining a particular eigenvalue q_n associated with the eigenfunction $f_n(x)$ is given by:

$$|c_n|^2, \quad \text{where} \quad c_n = \langle f_n|\Psi\rangle .$$

Here, c_n represents the coefficient in the expansion of Ψ in terms of the eigenfunctions of Q.



Where

$$|\Psi_{gen}\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_{\psi_n}$$

5.2 Wave Function Collapse

Upon the measurement of an observable and the realization of a particular outcome, the wave function Ψ undergoes a phenomenon known as *collapse*. This means that immediately after the measurement, the wave function of the system is no longer Ψ but rather the eigenfunction f_n corresponding to the measured eigenvalue q_n. This collapse reflects the transition from a superposition of possibilities to a definite state.

Example: In a system described by a wave function Ψ that is a superposition of eigenfunctions $f_1, f_2, \ldots, f_n$, the measurement of an observable will lead to the system being found in one of these eigenstates, with probabilities given by $|c_1|^2, |c_2|^2, \ldots, |c_n|^2$ respectively.