Quantum Mechanics

Week 8

Mark Benazet Castells
mbenazet@ethz.ch

FS2024

Contents

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 Angular Momentum in Quantum Mechanics

Angular momentum in quantum mechanics is a fundamental concept, revealing the rotational symmetries of quantum systems. Unlike classical angular momentum, quantum angular momentum has discrete eigenvalues and is governed by the principles of quantum mechanics.

$$\vec{L} = \vec{r} \times \vec{p} \tag{1}$$

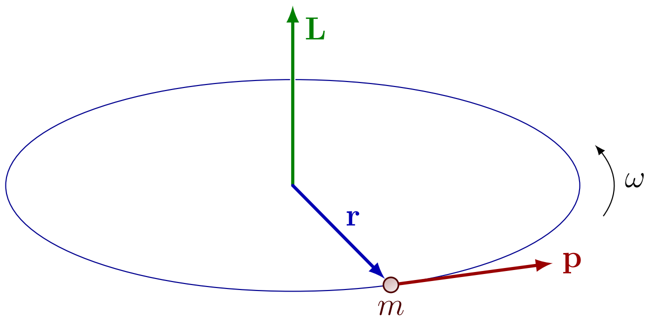

Figure 1: Angular Momentum

1.1 Quantum Angular Momentum Operators

In quantum mechanics, the angular momentum operators are denoted as $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$, corresponding to the x, y, and z axes, respectively. These operators do not commute, which means their observables cannot be simultaneously measured with infinite precision. The commutation relations are given by:

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= i\hbar\hat{L}_z, \\
[\hat{L}_y, \hat{L}_z] &= i\hbar\hat{L}_x, \\
[\hat{L}_z, \hat{L}_x] &= i\hbar\hat{L}_y.
\end{aligned}$$

1.2 Quantum Angular Momentum and Spherical Harmonics

The total angular momentum operator $L^2 = L_x^2 + L_y^2 + L_z^2$ commutes with each of the individual angular momentum components, expressed in the commutation relations $[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0$. However, the individual components L_x, L_y, and L_z do not commute with each other. This non-commutativity means that only L^2 and one component (typically L_z) can be simultaneously known with certainty. The eigenvalue equations for these operators are:

$$\begin{aligned}
L^2 f_\ell^{m_\ell} &= \hbar^2 \ell(\ell+1) f_\ell^{m_\ell} \quad &\Rightarrow \quad |\vec{L}| &= \sqrt{\ell(\ell+1)}\hbar, \\
L_z f_\ell^{m_\ell} &= \hbar m_\ell f_\ell^{m_\ell} \quad &\Rightarrow \quad L_z &= m_\ell \hbar,
\end{aligned}$$

Since $Y_\ell^{m_\ell}$ are eigenfunctions of Hermitian operators (L^2 and L_z) the $Y_\ell^{m_\ell}$ are orthogonal.

1.3 Ladder Operator

The ladder operators are invaluable tools due to their systematic capability to alter the magnetic quantum number (m) within the eigenstates of angular momentum. They consist of two operators which increase or decrease the eigenvalue of L_z by $\hbar$:

$$L_+ = L_x + iL_y \qquad L_- = L_x - iL_y$$

These operators have the following transformative properties:

$$L_+ f_\ell^{m_\ell} = \hbar\sqrt{\ell(\ell+1) - m_\ell(m_\ell+1)}\, f_\ell^{m_\ell+1} \qquad L_- f_\ell^{m_\ell} = \hbar\sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}\, f_\ell^{m_\ell-1}$$

Ladder operators are instrumental in quantum mechanics for several reasons:

- **Quantum State Transitions:** Ladder operators facilitate the study of transitions between quantum states of different angular momentum. They allow us to explore the properties of these states without solving the Schrödinger equation for each state individually.
- **Simplifying Calculations:** They greatly simplify the process of finding the eigenvalues and eigenstates of angular momentum. Instead of solving complex differential equations, ladder operators provide a straightforward algebraic method to determine these quantities.

Example

Consider an electron in a quantum state $|\psi\rangle = f_1^1 = |1,1\rangle$, an eigenstate of $\hat{L}^2$ and $\hat{L}_z$ with quantum numbers $\ell = 1$ and $m = 1$. We want to calculate the expectation values $\langle \hat{L}_x \rangle$ and $\langle \hat{L}_y \rangle$ in this state.

The ladder operators, which facilitate transitions between angular momentum states, are defined as:

$$\begin{aligned} \hat{L}_+ &= \hat{L}_x + i\hat{L}_y, \\ \hat{L}_- &= \hat{L}_x - i\hat{L}_y. \end{aligned}$$

Method: Expressing $\hat{L}_x$ and $\hat{L}_y$ in terms of ladder operators:

$$\begin{aligned} \langle \hat{L}_x \rangle &= \frac{1}{2}\langle \psi | (\hat{L}_+ + \hat{L}_-)\psi \rangle, \\ \langle \hat{L}_y \rangle &= \frac{1}{2i}\langle \psi | (\hat{L}_+ - \hat{L}_-)\psi \rangle. \end{aligned}$$

Calculation: Applying $\hat{L}_+$ and $\hat{L}_-$ to the state $|1,1\rangle$:

$$\begin{aligned} &\hat{L}_+|1,1\rangle = 0 \text{ (since } m \text{ cannot be greater than } \ell), \\ &\hat{L}_-|1,1\rangle = \hbar\sqrt{1(1+1) - 1(1-1)}|1,0\rangle = \sqrt{2}\hbar|1,0\rangle. \end{aligned}$$

Using the orthogonality characteristic of the eigenstates,

$$\begin{aligned} \langle \hat{L}_x \rangle &= \frac{1}{2}(0 + \langle 1,1|(\sqrt{2}\hbar|1,0\rangle) = \frac{\sqrt{2}\hbar}{2}\langle 1,1|1,0\rangle = 0, \\ \langle \hat{L}_y \rangle &= \frac{1}{2i}(0 - \langle 1,1|(\sqrt{2}\hbar|1,0\rangle) = -\frac{\sqrt{2}\hbar}{2i}\langle 1,1|1,0\rangle = 0. \end{aligned}$$

1.4 Visualization of Angular Momentum

Quantum angular momentum is a cornerstone concept in quantum mechanics, uniquely characterized by its quantized nature. Distinct from classical angular momentum, it manifests through the following quantum-specific attributes:

- The magnitude of the angular momentum vector, denoted as $|\vec{L}|$, is quantized according to the equation $|\vec{L}| = \sqrt{\ell(\ell+1)}\hbar$, where ℓ is the orbital quantum number.
- The z-axis projection of the angular momentum, represented as $|L_z|$, is quantized as well, given by $|L_z| = m_\ell \hbar$ with m_ℓ being the magnetic quantum number.

Due to the inherent uncertainty principles in quantum mechanics, while the magnitudes of $|\vec{L}|$ and $|L_z|$ are precisely known, the exact orientations of L_x and L_y remain undefined due to their non-commutative properties. For $\ell > 0$, either L_x or L_y may be zero, but the inequality $\ell(\ell+1) > m_\ell^2$ guarantees the positivity of the total angular momentum L^2, inclusive of $L_x^2 + L_y^2$.

This unique nature of quantum angular momentum is depicted through the following illustration:

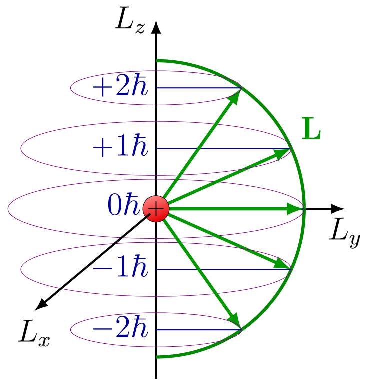

Figure 2: Quantum Angular Momentum

The illustration uses an inverted cone to represent the angular momentum vector in a quantum system. This cone is placed such that its base aligns with $m_\ell \hbar$, visually interpreting the fact that the exact direction of $\vec{L}$ within the x-y plane is uncertain, yet its magnitude and z-component are well-defined.

2 Spin

Spin is an intrinsic property of elementary particles, composite particles (like hadrons), and atomic nuclei. Unlike orbital angular momentum, which is derived from the spatial movement of particles, spin is an inherent characteristic of particles, similar in nature to properties like charge or mass. This quantum mechanical attribute has no direct equivalent in classical physics.

Spin in quantum mechanics can be thought of as a "rotation" property, but it is important to note that this does not involve a particle physically spinning around an axis. Elementary particles such as electrons are point-like, without a defined structure or volume, making the classical idea of rotation inapplicable. This uniqueness of spin underlines its purely quantum mechanical nature.

The quantum mechanical operators for spin are defined analogously to those for angular momentum. They follow eigenvalue equations, which describe the quantized nature of spin. These equations are:

$$\begin{aligned} S^2 f_s^{m_s} &= \hbar^2 s(s+1) f_s^{m_s} && \Rightarrow && |\vec{S}| = \sqrt{s(s+1)}\hbar, \\ S_z f_s^{m_s} &= \hbar m_s f_s^{m_s} && \Rightarrow && S_z = m_s \hbar. \end{aligned}$$

In these equations, S^2 is the square of the spin operator, representing the total spin angular momentum, while S_z is the z-component of the spin.

Spin is fundamentally quantized and is described by two quantum numbers: the spin quantum number (s) and the magnetic spin quantum number (m_s). The spin quantum number s determines the magnitude of the spin and can assume half-integer or integer values, such as $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. Particles with half-integer spins ($\frac{1}{2}, \frac{3}{2}, \ldots$) are fermions, such as electrons, while those with integer spins ($0, 1, 2, \ldots$) are bosons, like photons.

2.1 Quantum Mechanical Treatment of Spin

In quantum mechanics, spin is treated as an angular momentum vector, described by operators analogous to those for orbital angular momentum. However, spin operators do not correspond to any physical motion in space; they are abstract mathematical constructs that obey the angular momentum commutation relations.

For an electron with a spin quantum number $s = \frac{1}{2}$, the spin angular momentum operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ represent the components of the spin vector along the x, y, and z axes, respectively. These operators satisfy the same commutation relations as the orbital angular momentum operators:

$$\begin{aligned} [\hat{S}_x, \hat{S}_y] &= i\hbar \hat{S}_z, \\ [\hat{S}_y, \hat{S}_z] &= i\hbar \hat{S}_x, \\ [\hat{S}_z, \hat{S}_x] &= i\hbar \hat{S}_y. \end{aligned}$$

Moreover, the total spin angular momentum squared operator, $\hat{S}^2$, commutes with each of the spin component operators similar to the quantum angular momentum.

2.2 Visualization of Spin

Quantum spin angular momentum is an intrinsic and fundamental property of particles in quantum mechanics, distinguished by its quantized characteristics. Unlike classical angular momentum, quantum spin exhibits these unique quantum-specific attributes:

- The magnitude of the spin vector, denoted as $|\vec{S}|$, is quantized and described by the equation $|\vec{S}| = \sqrt{s(s+1)}\hbar$, where s is the spin quantum number.
- The z-axis projection of the spin, represented as $|S_z|$, is also quantized and given by $|S_z| = m_s\hbar$, where m_s is the magnetic spin quantum number.

Due to the inherent uncertainty principles in quantum mechanics, while the magnitudes of $|\vec{S}|$ and $|S_z|$ are precisely quantified, the exact orientations of the S_x and S_y components remain indeterminate. This arises from the non-commutative nature of the spin components. However, for $s > 0$, neither S_x nor S_y can be zero, as the condition $s(s+1) > m_s^2$ is always satisfied, ensuring that the spin vector $\vec{S}$ always has a component in the x-y plane.

This unique aspect of quantum spin angular momentum is depicted in the accompanying illustration:

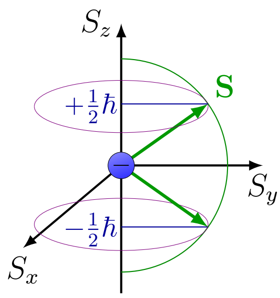

Figure 3: Quantum Spin Angular Momentum

The illustration uses a geometric structure, resembling an inverted cone, to represent the spin angular momentum vector in a quantum system. This structure's base aligns with $m_s\hbar$, illustrating that while the exact direction of $\vec{S}$ within the x-y plane is uncertain, its magnitude and z-component are quantized and well-defined.

Remark: This illustration is particularly designed for an electron with a spin quantum number of $s = \frac{1}{2}$.

We can clearly see the similarity with the angular momentum talked in the last section.

2.3 Spin and Dirac Notation

Dirac notation, also known as bra-ket notation, offers a compact and intuitive framework for handling quantum states, especially useful in the context of spin angular momentum.

Representation of Spin States: For particles with a spin quantum number $s = \frac{1}{2}$ (like electrons), the spin states can be represented in two dimensions ($m_s = \pm\frac{1}{2}$), corresponding to the two possible orientations of spin along a given axis (commonly the z-axis). These states are:

$$\begin{aligned} \text{Spin-up state:} \quad & \left|\frac{1}{2}, \frac{1}{2}\right\rangle \equiv \left|\uparrow\right\rangle = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right), \\ \text{Spin-down state:} \quad & \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \equiv \left|\downarrow\right\rangle = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right). \end{aligned}$$

Here, $\left|\uparrow\right\rangle$ and $\left|\downarrow\right\rangle$ are the basis vectors for the spin-1/2 system, representing the spin aligned and anti-aligned with the z-axis, respectively.

General Spin State: A general spin state $|\chi\rangle$ of a spin-1/2 particle is a linear combination of the spin-up and spin-down states:

$$|\chi\rangle = a\left|\uparrow\right\rangle + b\left|\downarrow\right\rangle,$$

where a and b are complex coefficients. These coefficients, also known as probability amplitudes, determine the likelihood of finding the particle in the respective spin states upon measurement.

Normalization of Spin States: The normalization condition is crucial in quantum mechanics, as it ensures that the total probability associated with the quantum state is unity. For a normalized spin state $|\chi\rangle$, this condition is expressed as:

$$\langle\chi|\chi\rangle = a^*a + b^*b = 1,$$

where a^* and b^* are the complex conjugates of a and b, respectively.

Probabilities and Observables: The probability of measuring a particular spin state, such as spin-up or spin-down along the z-axis, is given by the absolute square of the corresponding coefficient in the state's linear combination. For instance, the probability of measuring the state $\left|\uparrow\right\rangle$ in the general state $|\chi\rangle$ is $|a|^2$, while that of $\left|\downarrow\right\rangle$ is $|b|^2$.

Expectation Values: The expectation value of an observable in a given state is calculated using the corresponding operator. For example, the expectation value of the spin component along the z-axis in state $|\chi\rangle$ is given by:

$$\langle\hat{S}_z\rangle_\chi = \langle\chi|\,\hat{S}_z\,|\chi\rangle.$$

This value represents the average outcome of many measurements of the spin component along the z-axis on a large ensemble of identically prepared systems in state $|\chi\rangle$.

2.4 Spin as Matrices

In quantum mechanics, the concept of spin is elegantly encapsulated using matrix representations. This approach allows for a deeper understanding of spin operators and their effects on quantum states, particularly in the context of spin-$\frac{1}{2}$ particles like electrons.

Hermitian Operators for Spin $s = \frac{1}{2}$: The spin operators in quantum mechanics are associated with the spin angular momentum of particles. For a particle with spin $s = \frac{1}{2}$, these operators are represented as 2×2 Hermitian matrices. The square of the spin operator, $\hat{S}^2$, and its components along the x, y, and z axes ($\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$) are given by:

$$\begin{aligned}
\hat{S}^2 &\rightarrow \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\
\hat{S}_z &\rightarrow \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\
\hat{S}_x &\rightarrow \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
\hat{S}_y &\rightarrow \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.
\end{aligned}$$

These matrices correspond to the observables of spin in each respective direction. They are crucial for understanding the behavior of spin in various quantum states and interactions.

Raising and Lowering Operators: The raising ($\hat{S}_+$) and lowering ($\hat{S}_-$) operators play a vital role in quantum mechanics, particularly in changing the spin state of a quantum system. These operators are used to increase or decrease the magnetic spin quantum number (m_s) by one unit. The matrices representing these operators for spin-$\frac{1}{2}$ particles are:

$$\begin{aligned}
\hat{S}_+ &\rightarrow \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\
\hat{S}_- &\rightarrow \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.
\end{aligned}$$

The action of $\hat{S}_+$ on a spin-down state ($|\downarrow\rangle$) converts it to a spin-up state ($|\uparrow\rangle$), while $\hat{S}_-$ does the opposite. These operators are instrumental in understanding transitions between spin states and are a cornerstone in the study of quantum systems with angular momentum.

3 Wave Function, Spin, and Indistinguishable Fermions

As we proceed into the coming weeks, let's outline some fundamental concepts that will form the basis of our discussions:

Incorporating Spin into the Wave Function: Spin is an intrinsic quantum property, integral to the overall wave function of a particle. It is combined with the spatial part of the wave function to fully describe a quantum state. Mathematically, this is represented as:

$$\psi_{\text{overall}}(x, s) = \psi_{\text{spatial}}(x) \cdot \chi_{\text{spin}}(s),$$

where $\psi_{\text{spatial}}(x)$ is the spatial wave function and $\chi_{\text{spin}}(s)$ is the spin state of the particle.

Indistinguishable Fermions and Wave Function Symmetry: Fermions, such as electrons, are indistinguishable in quantum mechanics, requiring their overall wave function to be antisymmetric under particle exchange. This principle, derived from the Pauli exclusion rule, implies that swapping any two fermions reverses the wave function's sign:

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_i, \vec{r}_j, \ldots) = -\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_j, \vec{r}_i, \ldots).$$

This antisymmetry shapes the unique characteristics of multi-fermion systems.