Quantum Mechanics II

from the context of the courses
PHY 851-852: Quantum Mechanics

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Contents

0.1 The SI System

In physics it's often important to have precisely defined units for the purposes of making very accurate measurements or simply having a coherent unit system. It's possible to derive all necessary units from five measurements of **length, mass, time, current, and temperature**. The standard SI units for these properties are listed bellow:

Type	Unit	Definition
Length	Meter(m)	Length of distance light in a vacuum travels in $\frac{1}{299792458}$ seconds
Mass	Kilogram(kg)	Defined by fixing the Planck's constant $h = 6.62607015 \times 10^{-34} kg\ m^2 s^{-1}$
Time	Second(s)	Defined by fixing the ground-state hyperfine transition frequency of the caesium-133 atom, to be $9192631770 s^{-1}$
Current	Ampere(A)	Defined by fixing the charge of an electron as $1.602176634 \times 10^{-19} A \cdot s$
Temperature	Kelvin(K)	Defined by fixing the value of the Boltzmann constant k to $1.380649 \times 10^{-23} kg \cdot m^2 s^{-2} K^{-1}$

Common prefixes are listed bellow:

Prefix	Symbol	Definition
mega	M	10^6
kilo	k	10^3
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}

Additionally, the following are defined constants:

Symbol	Definition
$\hbar$	$\hbar = \frac{h}{2\pi} \approx 1.0546 \times 10^{-34} \mathrm{kg\,m^2\,s^{-1}}$
e	Charge of an electron $e = 1.602176634 \times 10^{-19} \mathrm{C}$

0.2 Why make a second book?

I've found that in the course of study it is incredibly difficult to make a universal reference book across classes. Maybe that is something I will make in the future. Until I know the exact topics that are covered in this course and the depth at which they are covered, I will keep the two books separate to make studying for the current course simpler.

Another major difference between these two books is the notation. The first book used strictly Schrödinger notation. With the hope of standardizing notation and consistently representing quantum systems, this book will strive to use Heisenberg notation.

0.3 Stern-Gerlach Experiments

The Stern-Gerlach experiments are a great example of a system that cannot be accurately described by classical mechanics.

Definition 0.3.1. Recall from classical mechanics that **Classical Magnetic Moment** is defined using the following formula

$$\mu = \frac{q}{2m}\mathbf{L} \tag{0.3.1}$$

$$\mathbf{L} = rmv \tag{0.3.2}$$

r is radius, m is mass, v is tangential velocity, q is charge, $\mathbf{L}$ is angular momentum, and μ is magnetic moment.

Definition 0.3.3. Electron, Protons, and Neutrons all have an **intrinsic angular momentum** called **spin** denoted $\mathbf{S}$.

Definition 0.3.4. Electrons, Protons, and Neutrons also have an **intrinsic magnetic moment** defined by

$$\mu = g\frac{q}{2m}\mathbf{S} \tag{0.3.4}$$

g is the dimensionless gyroscopic ratio or g-factor which can be derived using quantum mechanics.

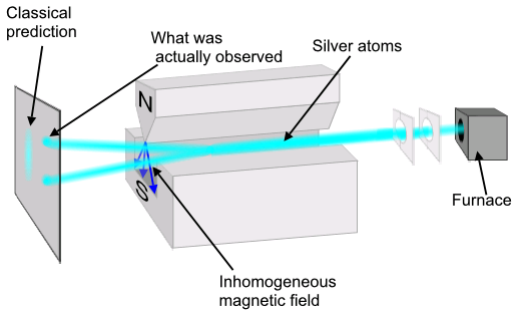


Figure 1: Diagram of the Stern-Gerlach experiment

The first Stern-Gerlach experiment seeks to measure the magnetic moment of the valence electron. A silver atom has 47 electrons and 47 protons. The magnetic moments depends on the inverse of mass, so we can neglect heavy protons and neutrons. Silver has an electron configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 4d^{10} 5s^1$, so the only electron that contributes to the magnetic moment is the valence electron $5s^1$. Knowing this we expect the magnetic moment of the silver atom to be

$$\mu = -g_e\frac{e}{2m_e}\mathbf{S} \tag{0.3.5}$$

Following the laws of electromagnetism the force in the z direction is

$$F_z = -g_e\frac{e}{2m_e}S_z\frac{\partial B_z}{\partial z} \tag{0.3.6}$$

The deflection of the beam is therefore a measurement of the spin of the valence electron of the silver atoms in the z-direction. Classically, we would expect the magnetic moment to be aligned in random directive and to observe a continuous range of deflection. Instead we observe two distinct magnetic moments. The magnitudes of these deflections are consistent with the spins of

$$S_z = \pm\frac{\hbar}{2} \tag{0.3.7}$$

This is called **quantization** of the electron's spin angular momentum component. The factor $\frac{1}{2}$ in the equation is why we refer to electrons as having **spin-1/2**.

Chapter 1

Quantum Systems

This chapter will outline our system of notation and the fundamental concepts of quantum mechanics.

1.1 Axioms of Quantum Mechanics

Axiom 1. The state of any quantum system can be represented as a ket in a complex ket space.

Axiom 2. Any measurement on a quantum system can be represented as Hermitian operator X where the eigenvalues of X represent the possible outcomes.

1.2 Ket Space

Definition 1.2.1. A **ket** denoted $|\alpha\rangle$ is an element of a ket space.

Definition 1.2.2. A **ket space** K is a set of kets equipped with addition $+$, and complex scalar multiplication such that the following properties hold for any three kets $|\alpha\rangle, |\beta\rangle, |\gamma\rangle \in K$ and complex scalar $z, y \in \mathbb{C}$.

- **Associativity** $|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$.
- **Commutativity** $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$
- **Identity** $\exists\, |\emptyset\rangle \in K$ such that $|\alpha\rangle + |\emptyset\rangle = |\alpha\rangle$.
- **Inverse** $|\alpha\rangle - |\alpha\rangle = |\emptyset\rangle$.
- **Compatibility** $z(y\,|\alpha\rangle) = (zy)\,|\alpha\rangle$.
- **Identity** $1\,|\alpha\rangle = |\alpha\rangle$.
- **Distributivity** $z(|\alpha\rangle + |\beta\rangle) = z\,|\alpha\rangle + z\,|\beta\rangle$ and $(z+y)\,|\alpha\rangle = z\,|\alpha\rangle + y\,|\beta\rangle$.

Definition 1.2.3.

Definition 1.2.4. The **inner product** of two kets denoted $\langle a|b\rangle$ is a complex number defined as the sum of the element-wise product of $|a\rangle$ and $|b\rangle$ with the following properties:

- $\langle a|b\rangle = \langle b|a\rangle^*$
- $\langle a|a\rangle \geq 0$

Definition 1.2.5. Two kets $|a\rangle$ and $|b\rangle$ are **orthogonal** iff $\langle a|b\rangle = 0$

Definition 1.2.6. The **norm** of a ket $|a\rangle$ is $\sqrt{\langle a|a\rangle}$.

Definition 1.2.7. A ket $|a\rangle$ is **normalized** iff $\langle a|a\rangle = 1$.

Corollary 1.2.8. For any ket $|a\rangle$ the ket $\frac{1}{\sqrt{\langle a|a\rangle}}\,|a\rangle$ is normalized.

1.3 Operators

Definition 1.3.1. An **operator** X acts on kets to produce a new ket.

Definition 1.3.2. A **linear operator** is an operator with the properties for any two kets $|a\rangle, |b\rangle$ and any scalar $z \in \mathbb{C}$:

- $X(|a\rangle + |b\rangle) = X|a\rangle + X|b\rangle$
- $X(z|a\rangle) = zX|a\rangle$

Corollary 1.3.3. Addition of linear operators is associative and commutative. For any linear operators A, B, C, $A + B = B + A$ and $A + (B + C) = (A + B) + C$.

Corollary 1.3.4. Multiplication of linear operators is associative but not commutative. For any linear operators A, B, C, $A(BC) = (AB)C$ and in general $AB \neq BA$.

Definition 1.3.5. The **Hermitian adjoint** of a matrix X denoted with dagger $X^\dagger$ is defined by

$$\langle\alpha| X^\dagger |\beta\rangle = (\langle\beta| X |\alpha\rangle)^* \tag{1.3.5}$$

Definition 1.3.6. An operator X is a **unitary operator** or a **symmetry operator** iff $XX^\dagger = I$.

Definition 1.3.7. An operator X is **Hermitian** iff $X = X^\dagger$.

Corollary 1.3.8. If X is a Hermitian operator, then X has real eigenvalues and eigenvectors with different eigenvalues are orthogonal.

Definition 1.3.9. The **projection operators** denoted $A_{|\alpha\rangle}$ is an operator defined for any ket $|\alpha\rangle$

$$A_{|\alpha\rangle} = |\alpha\rangle\langle\alpha| \tag{1.3.9}$$

1.4 Bases and Matrix Representation

Definition 1.4.1. The **Kronecker delta** denoted δ_{ij} for any $i, j \in \mathbb{N}$ is defined as

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{1.4.1}$$

Definition 1.4.2. The **Levi-Civita symbol** denoted ε_{ijk} for any $i, j, k \in \mathbb{N}$ is defined as

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k \text{ is } (1,2,3), \text{ or } (2,3,1), \text{ or } (3,1,2) \\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1), \text{ or } (1,3,2), \text{ or } (2,1,3) \\ 0 & \text{if } i = j, \text{ or } i = k, \text{ or } j = k \end{cases} \tag{1.4.2}$$

Definition 1.4.3. A **basis** is a set of kets $\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$ such that any ket in the ket space can be uniquely represented as a linear combination of basis kets.

Definition 1.4.4. An **orthonormal basis** is a basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$ such that $\langle e_i|e_j\rangle = \delta_{ij}$.

Corollary 1.4.5. For an orthonormal basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$ the completeness relation is the identity:

$$\sum_{i=1}^{n} |e_i\rangle\langle e_i| = I \tag{1.4.5}$$

Proposition 1.4.6. For any ket $|\alpha\rangle$ with a basis $\{|e_1\rangle, \ldots, |e_n\rangle\}$, there exists unique complex numbers $\alpha_i \in \mathbb{C}$ such that

$$|\alpha\rangle = \sum_{i=0}^{n} \alpha_i |\alpha\rangle, \qquad \langle e_i|\alpha\rangle = \alpha_i \tag{1.4.6}$$

Definition 1.4.7. We represent bras and kets as **row and column vectors** with respect to a basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$. For any ket $|\alpha\rangle = \sum_{i=0}^{n} \alpha_i |\alpha\rangle$.

$$\text{if } |\alpha\rangle = \sum_{i=0}^{n} \alpha_i |\alpha\rangle, \quad \langle\alpha| = \begin{pmatrix} \alpha_1^* \alpha_2^* \ldots \alpha_n^* \end{pmatrix}, \quad |\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} \tag{1.4.7}$$

Definition 1.4.8. We represent operators as a **matrix** with respect to a basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$.

$$X = \begin{pmatrix} \langle e_1| X |e_1\rangle & \langle e_1| X |e_2\rangle & \langle e_1| X |e_3\rangle & \ldots & \langle e_1| X |e_n\rangle \\ \langle e_2| X |e_1\rangle & \langle e_2| X |e_2\rangle & \langle e_2| X |e_3\rangle & \ldots & \langle e_2| X |e_n\rangle \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \langle e_n| X |e_1\rangle & \langle e_n| X |e_2\rangle & \langle e_n| X |e_3\rangle & \ldots & \langle e_n| X |e_n\rangle \end{pmatrix} \tag{1.4.8}$$

Corollary 1.4.9. Under these definitions standard vector and matrix multiplication are consistent.

Theorem 1.4.10. Given two basis $\{|a_1\rangle, \ldots, |a_n\rangle\}$ and $\{|b_1\rangle, \ldots, |a_n\rangle\}$ there exsits a unitary operator such that for any operator X_a written in the basis $\{|a_1\rangle, \ldots, |a_n\rangle\}$ and the same operator X_b written in the basis $\{|b_1\rangle, \ldots, |b_n\rangle\}$,

$$U = \sum_{i=1}^{n} \langle b_i|a_i\rangle, \quad |b_i\rangle = U |a\rangle, X_b = U^T X_a \tag{1.4.10}$$

1.5 Eigenvalues and Eigenvectors

Definition 1.5.1. For an operator X an **eigenvector** is a ket $|\alpha\rangle$ such that $X |\alpha\rangle = \lambda |\alpha\rangle$ for some **eigenvalue** $\lambda \in \mathbb{C}$.

Definition 1.5.2. An **eigenspace** for an eigenvalue λ of an operator X is the set of eigenvectors with λ as an eigenvalue.

Definition 1.5.3. An eigenvalue is **degenerate** iff the corresponding eigenspace has more than one linearly independent eigenvector.

Definition 1.5.4. An eigenvalue is **non-degenerate** iff it is not degenerate.

1.6 Expectation Value and Uncertainty

Definition 1.6.1. The **commutator** of two operators A and B denoted $[A, B]$ is defined as

$$[A, B] = AB - BA \tag{1.6.1}$$

Definition 1.6.2. The **anticommutator** of two operators A and B denoted $\{A, B\}$ is defined as

$$\{A, B\} = AB + BA \tag{1.6.2}$$

Definition 1.6.3. Two operators A and B are **compatible operators** iff $[A, B] = 0$.

Definition 1.6.4. Two operators A and B are **incompatible operators** iff $[A, B] \neq 0$.

Corollary 1.6.5. Compatible operators have the same eigenvalues and eigenvectors.

Definition 1.6.6. The **expectation value** of a Hermitian operator X for a state $|\psi\rangle$ denoted $\langle X\rangle$ is defined as

$$\langle X\rangle = \langle\psi| X |\psi\rangle = \sum_{i=1}^{n} P(\alpha_i)\alpha_i \tag{1.6.6}$$

Definition 1.6.7. The **variance** of a Hermitian operator X for a state $|\psi\rangle$ denoted $\langle(\Delta X)^2\rangle$ is defined as

$$\langle(\Delta X)^2\rangle = \langle X^2\rangle - \langle X\rangle^2 = \langle(X - \langle X\rangle)^2\rangle \tag{1.6.7}$$

Definition 1.6.8. The **standard deviation** of a Hermitian operator X for a state $|\psi\rangle$ denoted σ_X is defined as

$$\sigma_X = \sqrt{\langle(\Delta X)^2\rangle} \tag{1.6.8}$$

Theorem 1.6.9. The **uncertainty principle** states that for any two observables A and B, the following relation holds

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4} |\langle[A, B]\rangle|^2 \tag{1.6.9}$$

1.7 Spin-1/2 System

The spin 1/2 system is the simplist finite system in quantum mechanics it consists of single particles such as an electron with two possible quantum eigenvalues.

Definition 1.7.1. The spin-1/2 system is a 2 dimensional complex ket space where the system will collapse into either spin up or spin down in the direction of measurement. The standard basis is $\{|+\rangle, |-\rangle\}$ where $|+\rangle$ is spin up along the z-axis and $|-\rangle$ is spin down along the z-axis.

$$\begin{aligned} |+\rangle_X &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, |-\rangle_X = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \\ |+\rangle_Y &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, |-\rangle_Y = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \\ |+\rangle &= \begin{pmatrix}1\\0\end{pmatrix}, |-\rangle = \begin{pmatrix}0\\1\end{pmatrix} \end{aligned} \tag{1.7.1}$$

Definition 1.7.2. The S_z, S_y, S_z operators measure the spin along the x, y or z axis. The possible eigenvalues are $\pm\frac{\hbar}{2}$.

$$\begin{aligned} S_x &= \frac{\hbar}{2}\left[(|+\rangle\langle -|) + (|-\rangle\langle +|)\right] = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \\ S_y &= \frac{\hbar}{2}\left[i(|-\rangle\langle +|) - i(|+\rangle\langle -|)\right] = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix} \\ S_z &= \frac{\hbar}{2}\left[(|+\rangle\langle +|) - (|-\rangle\langle -|)\right] = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} \end{aligned} \tag{1.7.2}$$

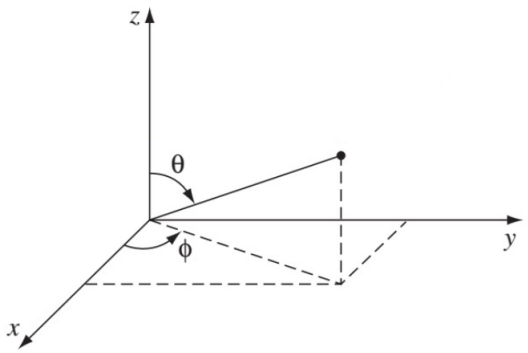
Result 1.7.3. The comutation relations for the spin operators are

$$\begin{aligned} [S_x, S_y] &= i\hbar S_z \\ [S_y, S_z] &= i\hbar S_x \\ [S_z, S_x] &= i\hbar S_y \end{aligned} \tag{1.7.3}$$

Definition 1.7.4. The **general spin operator** $S_{\hat{\mathbf{n}}}$ is defined by

$$S_{\hat{n}} = S_x \sin\theta\cos\phi + S_y \sin\theta\sin\phi + S_z\cos\theta = \begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix} \tag{1.7.4}$$

for a unit vector $\hat{\mathbf{n}}$ defined by $\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$



Corollary 1.7.5. The eigenvalues and eigenvectors for the $S_{\hat{\mathbf{n}}}$ operator are

$$\begin{aligned} |+\rangle_n &= \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi}|-\rangle \\ |-\rangle_n &= \sin\frac{\theta}{2}|+\rangle - \cos\frac{\theta}{2}e^{i\phi}|-\rangle \end{aligned} \tag{1.7.5}$$

Chapter 2

Continuous Ket Space

2.1 Continuous Inner Products

Definition 2.1.1. Continuous ket space is a ket space were observables exhibit continuous eigenvalue spectra. For a continuous operator Ξ with eigenvalues ξ and eigenvectors $|\xi\rangle$ that form a complete set,

$$\Xi |\xi\rangle = \xi |\xi\rangle \tag{2.1.1}$$

Definition 2.1.2. The **continuous inner product** in continuous space is defined using the Dirac delta function δ. The inner product of two continuous kets $|a\rangle$ and $|b\rangle$ with eigenvalues a and b of a complete continuous operator Ξ is

$$\langle a|b\rangle = \delta(a-b) \tag{2.1.2}$$

Corollary 2.1.3. Let Ξ be a continuous operator with eigenvalue ξ and eigenvectors $|\xi\rangle$ that form a complete set. For any operator A and any kets $|\alpha\rangle$ and $|\beta\rangle$, the continuous inner products are

$$|a\rangle = \int |\xi\rangle \langle\xi| \, d\xi, \quad \langle\beta|\alpha\rangle = \int \langle\beta|\xi\rangle \langle\xi|\alpha\rangle \, d\xi, \quad \langle\beta| A |\alpha\rangle = \int \langle\beta|\xi\rangle \langle\xi| A |\alpha\rangle \, d\xi \tag{2.1.3}$$

Corollary 2.1.4. The probability of measuring a complete continuous operator Ξ between a region of $a \leq \xi \leq b$ for any ket $|\alpha\rangle$ is given by the integral

$$|\langle a \leq \xi \leq b|\alpha\rangle|^2 = \int_a^b |\langle\xi|\alpha\rangle|^2 \, d\xi = \int_a^b \langle\alpha|\xi\rangle \langle\xi|\alpha\rangle \, d\xi \tag{2.1.4}$$

2.2 Multidimensional Continuous Inner Products

Definition 2.2.1. Multidimensional continuous ket space is defined as a simultaneous eigenvectors of coninuous ket spaces. The multidimensional continuous operator $\boldsymbol{\Xi}$ is defined in terms of the component continuous operators $\Xi_1, \Xi_2, \ldots, \Xi_n$ with eigenvalues $\xi_1, \xi_2, \ldots, \xi_n$ and eigenvalues $|\xi_1, \xi_2, \ldots, \xi_n\rangle$ that form a complete set.

$$\begin{gathered} |\boldsymbol{\xi}\rangle = |\xi_1, \xi_2, \ldots, \xi_n\rangle \\ \Xi_1 |\boldsymbol{\xi}\rangle = \xi_1 |\boldsymbol{\xi}\rangle \quad , \quad \Xi_2 |\boldsymbol{\xi}\rangle = \xi_2 |\boldsymbol{\xi}\rangle \quad , \quad \cdots \quad , \quad \Xi_n |\boldsymbol{\xi}\rangle = \xi_n |\boldsymbol{\xi}\rangle \end{gathered} \tag{2.2.1}$$

Definition 2.2.2. The **multidimensional continuous inner product** in multidimensional continuous is defined using the Dirac delta function δ. The inner product of two continuous kets $|\alpha\rangle$ and $|\beta\rangle$ with eigenvalues $\alpha_1, \alpha_2, \ldots, \alpha_n$ of a complete multidimensional continuous operator $\boldsymbol{\Xi}$ is

$$\langle a|b\rangle = \delta^n(\boldsymbol{\alpha} - \boldsymbol{\beta}) = \delta(\alpha_1 - \beta_1)\delta(\alpha_2 - \beta_2)\ldots\delta(\alpha_n - \beta_n) \tag{2.2.2}$$

Corollary 2.2.3. Let $\boldsymbol{\Xi}$ be a multidimensional with eigenvalues $\xi_1, \xi_2, \ldots, \xi_n$ and eigenvalues $|\xi_1\rangle, |\xi_2\rangle, \ldots, |\xi_n\rangle$ that form a complete set. For any operator A and any kets α and $|\beta\rangle$, the multidimensional continuous inner products are

$$|\alpha\rangle = \int |\boldsymbol{\xi}\rangle \langle\boldsymbol{\xi}|\alpha\rangle \, d^n\boldsymbol{\xi}, \quad \langle\beta|\alpha\rangle = \int \langle\beta|\boldsymbol{\xi}\rangle \langle\boldsymbol{\xi}|\alpha\rangle \, d^n\boldsymbol{\xi}, \quad \langle\beta| A |\alpha\rangle = \int \langle\beta|\boldsymbol{\xi}\rangle \langle\boldsymbol{\xi}| A |\alpha\rangle \, d^n\boldsymbol{\xi} \tag{2.2.3}$$

2.3 Position and Momentum Operators

Definition 2.3.1. The **position operator** X (also written x) with eigenvalues x and eigenvectors $|x\rangle$ that form a complete set.

$$X\,|x\rangle = x\,|x\rangle \tag{2.3.1}$$

Definition 2.3.2. The **position space wavefunction** of a ket $|\psi\rangle$ denoted $\psi(x)$ is the inner product

$$\psi(x) = \langle x|\psi\rangle \tag{2.3.2}$$

Definition 2.3.3. The **translation operator** U is a unitary operator that translates the eigenvalues $|x\rangle$ of X to the eigenvalue $|x + \Delta x\rangle$.

$$U(\Delta x)\,|x\rangle = |x + \Delta x\rangle \tag{2.3.3}$$

Proposition 2.3.4. The infinitesimal translation $U(dx)$ is generated by a Hermitian operator K.

$$U(dx) = I - iKdx, \quad [X, K] = i \tag{2.3.4}$$

Definition 2.3.5. The **momentum operator** p is defined in terms of the generator of translation.

$$P = \hbar K \tag{2.3.5}$$

Definition 2.3.6. The **momentum space wavefunction** of a ket $|\psi\rangle$ denoted $\tilde{\psi}(x)$ is the inner product

$$\tilde{\psi}(p) = \langle p|\psi\rangle \tag{2.3.6}$$

Theorem 2.3.7. The **canonical commutation relation** states that the commutator between X and P is

$$[X, P] = i\hbar \tag{2.3.7}$$

Corollary 2.3.8. The **Heisenburg uncertainty relation** is the uncertainty principle applied to X and P

$$< (\Delta X)^2 >< (\Delta P)^2 >= \sigma_X \sigma_P \geq \frac{\hbar}{2} \tag{2.3.8}$$

Theorem 2.3.9. The finite translation operator can be written in terms of the momentum operator

$$U(\Delta x) = \lim_{N\to\infty} \left(I - \frac{iP}{\hbar}\frac{\Delta x}{N}\right)^N = e^{-iP\Delta x/\hbar} \tag{2.3.9}$$

Theorem 2.3.10. P in the position basis and X in the momentum basis are derivatives.

$$\begin{gathered}
\langle x|\,P\,|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle \\
\langle \phi|\,P\,|\psi\rangle = \int \langle\psi|x\rangle\,(-i\hbar)\frac{\partial}{\partial x}\langle x|\psi\rangle\,dx = \int \phi^*(x)(-i\hbar)\frac{\partial}{\partial x}\psi(x)dx \\
\langle p|\,X\,|\psi\rangle = i\hbar\frac{\partial}{\partial p}\langle p|\psi\rangle \\
\langle \phi|\,X\,|\psi\rangle = \int \langle\psi|p\rangle\,i\hbar\frac{\partial}{\partial p}\langle p|\psi\rangle\,dp = \int \phi^*(p)i\hbar\frac{\partial}{\partial p}\psi(p)dp
\end{gathered} \tag{2.3.10}$$

Theorem 2.3.11. The inner product $\langle x|p\rangle$ can be written as an exponential.

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{2.3.11}$$

Corollary 2.3.12. The position space wavefunction and momentum space wavefunction are related to each other by the Fourier transform.

$$\begin{aligned}
\psi(x) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\tilde{\psi}(p)dp \\
\tilde{\psi}(x) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\psi(x)dx
\end{aligned} \tag{2.3.12}$$

2.4 Multidimensional Position and Momentum Operators

Definition 2.4.1. The **multidimensional position operator X** (also written $\mathbf{x}$) is defined in terms of the component position operators $X_1, X_2, \ldots, X_n$ with eigenvalues $x_1, x_2, \ldots, x_n$ and eigenvectors $|x_1, x_2, \ldots, x_n\rangle$ that form a complete set.

$$\begin{gathered} |\mathbf{x}\rangle = |x_1, x_2, \ldots, x_n\rangle \\ X_1 |\mathbf{x}\rangle = x_1 |\mathbf{x}\rangle \quad , \quad X_2 |\mathbf{x}\rangle = x_2 |\mathbf{x}\rangle \quad , \quad \ldots \quad , \quad X_n |\mathbf{x}\rangle = x_n |\mathbf{x}\rangle \end{gathered} \tag{2.4.1}$$

In 3d space, the X_1, X_2, X_3 operators are commonly written X, Y, Z (also written x, y, z).

Definition 2.4.2. The **multidimensional translation operator** $U(\mathbf{\Delta x})$ for a vector $\mathbf{\Delta x} = (\Delta x_1, \Delta x_2, \ldots, \Delta x_n)$ is a unitary operator that translates the eigenvalues $|\mathbf{x}\rangle$ of $\mathbf{X}$ to the eigenvalue $|\mathbf{x} + \mathbf{\Delta x}\rangle$.

$$U(\mathbf{\Delta x}) |\mathbf{x}\rangle = |\mathbf{x} + \mathbf{\Delta x}\rangle = |x_1 + \Delta x_1, x_2 + \Delta x_2, \ldots, x_n + \Delta x_n\rangle \tag{2.4.2}$$

Proposition 2.4.3. The infinitesimal multidimensional translation $\mathbf{U(dx)}$ is generated by a multidimensional operator $\mathbf{K}$ with Hermitian component operators $K_1, K_2, \ldots, K_n$.

$$\mathbf{U(dx)} = I - i\mathbf{K} \cdot \mathbf{dx} = I - iK_1 dx_1 - iK_2 dx_2 - \cdots - iK_n dx_n \tag{2.4.3}$$

Definition 2.4.4. The **multidimensional momentum operator P** (also written $\mathbf{p}$) is defined in terms of the component momentum operators $P_1, P_2, \ldots, P_n$ which are defined in terms of the generators of translation.

$$\begin{gathered} \mathbf{P} = \hbar \mathbf{K} \\ P_1 = \hbar K_1 \quad , \quad P_2 = \hbar K_2 \quad , \quad \ldots \quad , \quad P_n = \hbar K_n \end{gathered} \tag{2.4.4}$$

In 3d space, the P_1, P_2, P_3 operators are commonly written P_z, P_y, P_z also written (p_x, p_y, p_z).

Proposition 2.4.5. The commutation relations between components of $\mathbf{X}$ and $\mathbf{P}$ are

$$[X_i, X_j] = 0 \quad , \quad [P_i, P_j] = 0 \quad , \quad [X_i, P_j] = i\hbar\delta_{ij} \tag{2.4.5}$$

Theorem 2.4.6. The multidimensional finite translation operator can be written in terms of the momentum operator

$$\mathbf{U(\Delta x)} = \lim_{N\to\infty} \left(I - \frac{i\mathbf{P}}{\hbar} \cdot \frac{\mathbf{\Delta x}}{N} \right)^N = e^{-i\mathbf{P}\cdot\mathbf{\Delta x}/\hbar} = e^{-i(P_1\Delta x_1 + P_2 \Delta x_2 + \cdots + \Delta x_n)/\hbar} \tag{2.4.6}$$

Theorem 2.4.7. $\mathbf{P}$ in the position basis and $\mathbf{X}$ in the momentum basis are gradients.

$$\begin{gathered} \langle \mathbf{x}| \mathbf{P} |\psi\rangle = -i\hbar \nabla_{\mathbf{x}} \langle \mathbf{x}|\psi\rangle \\ \langle \varphi| \mathbf{P} |\psi\rangle = \int \langle \psi|\mathbf{x}\rangle (-i\hbar) \nabla_{\mathbf{x}} \langle \mathbf{x}|\psi\rangle \, d^n\mathbf{x} = \int \phi^*(\mathbf{x})(-i\hbar)\nabla_{\mathbf{x}}\psi(\mathbf{x}) d^n\mathbf{x} \\ \langle \mathbf{p}| \mathbf{X} |\psi\rangle = i\hbar \nabla_{\mathbf{p}} \langle \mathbf{p}|\psi\rangle \\ \langle \varphi| \mathbf{X} |\psi\rangle = \int \langle \psi|\mathbf{p}\rangle \, i\hbar \nabla_{\mathbf{p}} \langle \mathbf{p}|\psi\rangle \, d^n\mathbf{p} = \int \phi^*(\mathbf{p}) i\hbar \nabla_{\mathbf{p}} \psi(\mathbf{p}) d^n\mathbf{p} \end{gathered} \tag{2.4.7}$$

Theorem 2.4.8. The inner product $\langle \mathbf{x}|\mathbf{p}\rangle$ can be written as an exponential.

$$\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \tag{2.4.8}$$

Corollary 2.4.9. The position space wavefunction and momentum space wavefunction are related to each other by the Fourier transform.

$$\begin{aligned} \psi(\mathbf{x}) &= \int \frac{1}{\sqrt{2\pi\hbar}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \tilde{\psi}(\mathbf{p}) d^n\mathbf{p} \\ \tilde{\psi}(\mathbf{p}) &= \int \frac{1}{\sqrt{2\pi\hbar}} e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} \psi(\mathbf{x}) d^n\mathbf{x} \end{aligned} \tag{2.4.9}$$

Chapter 3

Time Evolution

3.1 Schrödinger's Equation

Definition 3.1.1. The **time evolution operator** $U(t)$ is the continuous unitary operator that describes how a system evolves with time t.

$$\begin{gathered} |\psi\rangle(t) = U(t)|\psi\rangle \\ U^\dagger(t)U(t) = I \\ \lim_{t_1 \to t_0} U(t_1) - U(t_0) = 0 \end{gathered} \tag{3.1.1}$$

Definition 3.1.2. The **generator of time evolution** is the Hermitian operator Ω that generates U for an infinitesimal dt

$$U(dt) = I - i\Omega dt \tag{3.1.2}$$

Definition 3.1.3. The **hamiltonian** H is defined in terms of the generator of time evolution

$$H = \hbar\Omega \tag{3.1.3}$$

Result 3.1.4. Schrödinger's equation in terms of $U(t)$ is

$$i\hbar\frac{\partial}{\partial t}U(t) = HU(t) \tag{3.1.4}$$

3.2 Time Independent Schrödinger's equation

Result 3.2.1. The **time independent Schrödinger's equation** for a time independent H is

$$\begin{gathered} H|E_i\rangle = E_i|E_i\rangle \\ U(t) = e^{-iHt/\hbar} \end{gathered} \tag{3.2.1}$$

Result 3.2.2. The **time independent solution** to any quantum system $|\psi\rangle$ with a time independent Hamiltonian where $|\psi\rangle = \sum_i c_i|E_i\rangle$ is

$$U(t)|\psi\rangle = \sum_i c_i e^{-iE_i t/\hbar}|E_i\rangle \tag{3.2.2}$$

Definition 3.2.3. A **stationary state** is a eigenstate of the Hamiltonian.

Result 3.2.4. The **expectation values of energy** for a time independent Hamiltonian does not depend on time and the expectation value of any operator A for a stationary state $|E_i\rangle$ does not depend on time.

$$\begin{aligned} \langle H(t)\rangle &= \langle\psi|U^\dagger(t)HU(t)|\psi\rangle = \langle\psi|H|\psi\rangle = \langle H\rangle \\ \langle A(t)\rangle &= \langle E_i|U^\dagger(t)AU(t)|E_i\rangle = \langle E_i|A|E_i\rangle = \langle A\rangle \end{aligned} \tag{3.2.4}$$

Result 3.2.5. The **general time dependence of expectation value** of any operator A for any quantum system $|\psi\rangle$ with a time independent Hamiltonian where $|\psi\rangle = \sum_i c_i|E_i\rangle$ for energy eigenstates $|E_i\rangle$ is

$$\langle A\rangle(t) = \sum_{ij} c_i^* c_j e^{-i(E_j - E_i)t/\hbar}\langle E_i|A|E_j\rangle \tag{3.2.5}$$

3.3 Spin-1/2 System in a Magnetic Field

Definition 3.3.1. The **Hamiltonian for a spin-1/2 system with a magnetic field pointing in the Z-direction** is

$$H = -\mu \cdot \mathbf{B} = g_e \frac{e}{2m_e} \mathbf{S} \cdot B \approx \frac{-eB}{mc} S_z \tag{3.3.1}$$

Definition 3.3.2. The **cyclotron frequency** denoted ω is the frequency of oscillation of the spin-1/2 system in a magnetic field defined by

$$\omega = \frac{|e|B}{mc} \tag{3.3.2}$$

Result 3.3.3. The time dependence of the spin-1/2 system is given by

$$U(t) |\psi\rangle = c_+ e^{-i\omega t/2} |+\rangle + c_- e^{i\omega t/2} |-\rangle \tag{3.3.3}$$

3.4 Time Dependent Operators

Definition 3.4.1. The time dependence of an operator A is defined in terms of the time translation operator $U(t)$ by

$$A(t) = U^\dagger(t) A U(t) \tag{3.4.1}$$

Result 3.4.2. The **heisenberg equations of motion** describe how operators evolve with time

$$\begin{aligned} \frac{\partial U(t)}{\partial t} &= \frac{1}{i\hbar} HU \\ \frac{\partial U(t)}{\partial t} &= \frac{1}{-i\hbar} U^\dagger H \\ \frac{\partial A(t)}{\partial t} &= \frac{1}{i\hbar} [A(t), H] \end{aligned} \tag{3.4.2}$$

Result 3.4.3. For eigenvalues $|a_i(t)\rangle$ of a time dependent operator $A(t)$,

$$\begin{aligned} |a_i(t)\rangle &= U^\dagger(t) |a_i(0)\rangle \\ i\hbar \frac{\partial}{\partial t} |a_i(t)\rangle &= -H |a_i(t)\rangle \end{aligned} \tag{3.4.3}$$

Proposition 3.4.4. For any function F the following commutation relations hold.

$$\begin{aligned} [X, F(P)] &= i\hbar \frac{\partial}{\partial P} F(P) \\ [P, F(X)] &= -i\hbar \frac{\partial}{\partial X} F(X) \end{aligned} \tag{3.4.4}$$

Theorem 3.4.5. Ehrenfest's Theorem states that the free particle Hamiltonian follows the laws of classical mechanics.

$$\begin{aligned} H &= \frac{\mathbf{P}^2}{2m} + V(\mathbf{X}) \\ \frac{dX_i}{dt} &= \frac{P_u}{m} \\ \frac{d^2 X_i}{dt^2} &= \frac{1}{m} \frac{dp_i}{dt} \\ m \frac{d^2 \mathbf{X}}{dt^2} &= -\nabla V(\mathbf{X}) \\ m \frac{\partial^2 \langle \mathbf{x} \rangle}{\partial t^2} &= \frac{\partial \langle \mathbf{p} \rangle}{\partial t} = -\langle \nabla V(\mathbf{x}) \rangle \end{aligned} \tag{3.4.5}$$

Proposition 3.4.6. The position uncertainty relation states that $\sigma_x(t) \geq \frac{\hbar t}{2\sigma_x(0) m}$

Theorem 3.4.7. The **virial theorem** state that for a

3.5 Simple Harmonic Oscillator

Definition 3.5.1. The **simple harmonic oscillator** is a quantum system defined by the following Hamiltonian.

$$H = \frac{P^2}{2m} + \frac{1}{2}kX^2 \tag{3.5.1}$$

Result 3.5.2. The Schrödinger equation for the harmonic oscillator is

$$\begin{gathered} H\left|\psi\right\rangle = E\left|\psi\right\rangle \\ \left(\frac{P^2}{2m} + \frac{1}{2}kX^2\right)\left|\psi\right\rangle = E\left|\psi\right\rangle \end{gathered} \tag{3.5.2}$$

Result 3.5.3. The position and momentum space Schrödinger equation for the harmonic oscillator is

$$\begin{gathered} \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kX^2\right)\psi(x) = E\psi(x) \\ \left(\frac{P^2}{2m} - \frac{\hbar^2 k}{2}\frac{d^2}{dp^2}\right)\tilde{\psi}(p) = E\tilde{\psi}(p) \end{gathered} \tag{3.5.3}$$

Definition 3.5.4. The **angular frequency for the harmonic oscillator** is the frequency $\omega = \sqrt{\frac{k}{m}}$.

3.5.5 Raising and Lowering Operators

Definition 3.5.6. The **lowering operator** or the **annihilation operator** a is defined

$$a = \sqrt{\frac{m\omega}{2\hbar}}X + \frac{iP}{\sqrt{2m\hbar\omega}} \tag{3.5.6}$$

Definition 3.5.7. The **raising operator** or the **creation operator** $a^\dagger$ is defined

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}X - \frac{iP}{\sqrt{2m\hbar\omega}} \tag{3.5.7}$$

Result 3.5.8. The harmonic oscillator Hamiltonian can be written in terms of the raising and lowering operators.

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \tag{3.5.8}$$

Definition 3.5.9. The **quantization operator** N is defined by

$$\begin{gathered} N = a^\dagger a \\ N\left|n\right\rangle = n\left|n\right\rangle \end{gathered} \tag{3.5.9}$$

Proposition 3.5.10. The following commutation relations hold for the harmonic oscillator

$$\begin{gathered} [a, a^\dagger] = 1 \\ [N, a] = [a^\dagger a, a] = [a^\dagger, a]a = -a \\ [N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger[a, a^\dagger] = a^\dagger \end{gathered} \tag{3.5.10}$$

Result 3.5.11. For eigenstates $|n\rangle$ of H the raising and lowering operators have the following properties

$$\begin{gathered} \left|n\right\rangle = \frac{1}{\sqrt{n}}(a^\dagger)^n\left|0\right\rangle \\ a^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle \\ a\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \\ \left\langle n\right|N\left|n\right\rangle = \left\langle n\right|a^\dagger a\left|n\right\rangle = \left|a\left|n\right\rangle\right|^2 >= 0 \end{gathered} \tag{3.5.11}$$

Result 3.5.12. The **harmonic oscillator energy eigenvalues and eigenstates** are

$$\begin{aligned} E_n &= \left(n + \frac{1}{2}\right)\hbar\omega \\ x_0 &= \sqrt{\frac{\hbar}{m\omega}} \\ \langle x|0\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-x^2/2x_0^2} \\ \langle x|n\rangle &= \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}x_0}\right)^n \left(x - x_0^2\frac{d}{dx}\right)^n \langle x|0\rangle \end{aligned} \tag{3.5.12}$$

Result 3.5.13. The operators X and P can be written in terms of the raising and lowering operators

$$\begin{aligned} X &= \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \\ P &= i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a) \end{aligned} \tag{3.5.13}$$

Result 3.5.14. For two eigenstates $|n\rangle$ and $|n'\rangle$ of the harmonic oscillator,

$$\begin{aligned} \langle n'|\, X\, |n\rangle &= \sqrt{\frac{\hbar}{2mw}}(\delta_{n',n-1}\sqrt{n} + \delta_{n',n+1}\sqrt{n+1}) \\ \langle n'|\, P\, |n\rangle &= i\sqrt{\frac{m\hbar\omega}{2}}(-\delta_{n',n-1}\sqrt{n} + \delta_{n',n+1}\sqrt{n+1}) \end{aligned} \tag{3.5.14}$$

3.5.15 Hermite polynomials

Definition 3.5.16. The **Hermite polynomials** are the series of polynomials defined by

$$H_n(x) = (-1)^n e^{x^2}\frac{\partial^n}{dx^n}e^{-x^2} \tag{3.5.16}$$

Corollary 3.5.17. The Hermite polynomials can also be derived recursively.

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{3.5.17}$$

$$H_n(x) = \sum_{j=0}^{n} c_j x^n, \quad c_{j+2} = \frac{2(j-n)}{(j+2)(j+1)}c_j \tag{3.5.18}$$

Result 3.5.19. The eigenfunctions of the simple harmonic oscillator can be written in terms of Hermite polynomials.

$$\langle x|n\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}}e^{-x^2/2}H_n(x) \tag{3.5.19}$$

3.5.20 Time Dependent Simple Harmonic Oscillator

Result 3.5.21. The **time dependent raising and lowering operators** for the harmonic oscillator are

$$\begin{aligned} a(t) &= a(0)e^{-i\omega t} \\ a^\dagger(t) &= a^\dagger(0)e^{i\omega t} \end{aligned} \tag{3.5.21}$$

Result 3.5.22. The **time dependent position and momentum operators** for the harmonic oscillator are

$$\begin{aligned} X(t) &= X(0)\cos\omega t + \frac{P(0)}{m\omega}\sin\omega t \\ P(0) &= -m\omega X(0)\sin\omega t + P(0)\cos\omega t \end{aligned} \tag{3.5.22}$$

3.6 Finite Square Well

Definition 3.6.1. The **finite square well** is a quantum system for a potential well of width $2a$ and depth V_0 defined with the following Hamiltonian.

$$H = \frac{P^2}{2m} + V$$
$$V(x) = \begin{cases} 0 & x \leq -a \\ -V_0 & -a < x < a \\ 0 & a \leq x \end{cases} \tag{3.6.1}$$

Theorem 3.6.2. For a particle with a potential $V(x) = V(-x)$, the energy eigenstates are either even $\psi(x) = \psi(-x)$ or odd $\psi(x) = -\psi(-x)$.

Result 3.6.3. The **finite square well energy eigenvalues** for even and odd energies must satisfy the following equations
Allowed Even Energies satisfy this equation:

$$\sqrt{\frac{2mE}{\hbar^2}} \tan\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \tag{3.6.3}$$

Allowed Odd Energies satisfy this equation:

$$-\sqrt{\frac{2mE}{\hbar^2}} \cot\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \tag{3.6.4}$$

Result 3.6.5. The **finite square well energy eigenstates** must also be split up by even and odd solution. And since the number of energies varies they must also be normalized for each case.
Even Energy Eigenstates are given by

$$\varphi_E(x) = \begin{cases} Ae^{\sqrt{\frac{2m}{\hbar^2}(V_0-E)}x} & x \leq -a \\ B\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) & -a < x < a \\ Ae^{-\sqrt{\frac{2m}{\hbar^2}(V_0-E)}x} & a \leq x \end{cases} \tag{3.6.5}$$

Odd Energy Eigenstates are given by

$$\varphi_E(x) = \begin{cases} Ae^{\sqrt{\frac{2m}{\hbar^2}(V_0-E)}x} & x \leq -a \\ C\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) & -a < x < a \\ -Ae^{-\sqrt{\frac{2m}{\hbar^2}(V_0-E)}x} & a \leq x \end{cases} \tag{3.6.6}$$

3.7 Delta Function Potential

Definition 3.7.1. The **delta function potential** is a quantum system for a delta function potential well defined with the following Hamiltonian.

$$\begin{aligned} H &= \frac{P^2}{2m} + V \\ V(x) &= \frac{-\hbar\lambda}{2ma}\delta(x) \end{aligned} \tag{3.7.1}$$

Result 3.7.2. The Schrödinger equation for the delta function potential is

$$\begin{aligned} H\left|\psi\right\rangle &= E\left|\psi\right\rangle \\ \left(\frac{P^2}{2m} - \frac{\hbar\lambda}{2ma}\delta(x)\right)\left|\psi\right\rangle &= E\left|\psi\right\rangle \end{aligned} \tag{3.7.2}$$

Result 3.7.3. The solutions to the Schrödinger equation for the delta function potential are of the form

$$\psi(x) = \begin{cases} Ae^{kx} & x \leq 0 \\ Ae^{-kx} & 0 \leq x \end{cases}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{3.7.3}$$

Result 3.7.4. By integrating a small neighborhood of zero on both sides of the Schrödinger equation for small $\varepsilon > 0$ it can be shown that there is only one bound state.

$$\int_{-\varepsilon}^{\varepsilon}\left(\frac{P^2}{2m} - \frac{\hbar\lambda}{2ma}\delta(x)\right)\left|\psi\right\rangle dx = \int_{-\varepsilon}^{\varepsilon} E\left|\psi\right\rangle dx \tag{3.7.4}$$

$$\frac{\partial\psi}{\partial x}(\epsilon) - \frac{\partial\psi}{\partial x}(\epsilon) = \frac{-\lambda}{a}\psi(0) \tag{3.7.5}$$

$$k = \frac{\lambda}{2a} \tag{3.7.6}$$

$$E = \frac{-\hbar^2k^2}{2m} = \frac{-\hbar^2\lambda^2}{8ma^2} \tag{3.7.7}$$

Chapter 4

Flux and Continuity

4.1 Probability Density

Definition 4.1.1. The **probability density** denoted $\rho(\mathbf{x}, t)$ is defined by

$$\rho(\mathbf{x}, t) = |\langle \mathbf{x}| U(t) |\psi\rangle|^2 \tag{4.1.1}$$

Definition 4.1.2. The **probability current density** or **probability flux** denoted $\vec{J}$ is defined by

$$\mathbf{J}(\mathbf{x}, t) = \frac{\hbar}{2mi} (\psi^* \nabla\psi - \psi \nabla\psi^*) \tag{4.1.2}$$

Theorem 4.1.3. The **continuity equation** states that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0 \tag{4.1.3}$$

Corollary 4.1.4. Gauss's law follows from the continuity equation

$$\frac{\partial}{\partial t} \int_V \rho(\mathbf{x}, t) \partial^3 \mathbf{x} = -\int_V \nabla \cdot \mathbf{J} \partial^3 \mathbf{x} = -\oint_A \mathbf{J} \cdot \partial \mathbf{A} \tag{4.1.4}$$

4.2 Scattering of a Potential Step

Definition 4.2.1. The **potential step** is the quantum system of a potential step defined by the following Hamiltonian.

$$H = \frac{P^2}{2m} + V, \quad V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & 0 \leq x \end{cases} \tag{4.2.1}$$

Result 4.2.2. The solution to scattering of a potential step is split into two regions I and II.

$$\Psi_I = \underbrace{e^{ikx}}_{\substack{\text{Incoming} \\ \text{Wave}}} + \underbrace{Re^{-ikx}}_{\substack{\text{Reflected} \\ \text{Wave}}}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{4.2.2}$$

$$\Psi_{II} = \underbrace{Te^{iqx}}_{\substack{\text{Transmitted} \\ \text{Wave}}}, \quad q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \tag{4.2.2}$$

Result 4.2.3. The magnitudes of the wavefunctions of the scattering of a potential step are

$$T = \frac{2k}{k + q} \tag{4.2.3}$$

$$R = \frac{k - q}{k + q} \tag{4.2.4}$$

Result 4.2.5. The probability current density in regions I and II of the scattering of a potential step is

$$J_I = \frac{\hbar k}{m}\left(1 - |R|^2\right) = J_A + J_R \tag{4.2.5}$$

$$J_{II} = \frac{\hbar q}{m}|T|^2 = J_T \tag{4.2.6}$$

$$J_A = \frac{\hbar k}{m} \tag{4.2.7}$$

$$J_R = -\frac{\hbar k}{m}|R|^2 = \frac{-\hbar k}{m}\left(\frac{k-q}{k+q}\right)^2 \tag{4.2.8}$$

$$J_T = \frac{\hbar q}{m}|T|^2 = \frac{\hbar q}{m}\left(\frac{2k}{k+q}\right)^2 \tag{4.2.9}$$

4.3 Resonance in a Finite Square Well

Result 4.3.1. The solution to scattering in a finite square well is split into regions I for $x < -a$, II for $-a < x < a$, and III for $a < x$.

$$\Psi_I(x) = e^{ikx} + Re^{ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{4.3.1}$$

$$\Psi_{II}(x) = Ae^{iqx} + Be^{-iqx}, \quad q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \tag{4.3.2}$$

$$\Psi_{III}(x) = Te^{ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{4.3.3}$$

Result 4.3.4. The magnitudes of the wavefunctions of the scattering of a potential step are

$$R = \frac{e^{-2ika}(q^2-k^2)\sin(2qa)}{2kq\cos(2qa) - i(q^2+k^2)\sin(2qa)} \tag{4.3.4}$$

$$T = \frac{e^{-2ika}(q^2-k^2)\sin(2qa)}{2kq\cos(2qa) - i(q^2+k^2)\sin(2qa)} \tag{4.3.5}$$

Result 4.3.6. The probability current density in regions I and II of the scattering of a potential step is

$$J_I = \frac{\hbar k}{m}\left(1 - |R|^2\right) = J_A + J_R \tag{4.3.6}$$

$$J_{II} = \frac{\hbar k}{m}|T|^2 = J_T \tag{4.3.7}$$

$$J_A = \frac{\hbar k}{m} \tag{4.3.8}$$

$$J_R = -\frac{\hbar k}{m}|R|^2 = \frac{-\hbar k}{m}\left|\frac{e^{-2ika}(q^2-k^2)\sin(2qa)}{2kq\cos(2qa) - i(q^2+k^2)\sin(2qa)}\right|^2 \tag{4.3.9}$$

$$J_T = \frac{\hbar k}{m}|T|^2 = \frac{\hbar k}{m}\left|\frac{e^{-2ika}(q^2-k^2)\sin(2qa)}{2kq\cos(2qa) - i(q^2+k^2)\sin(2qa)}\right|^2 \tag{4.3.10}$$

Theorem 4.3.11. The Ramsaur-Townzend effect states for the finite square well that at the resonance condition $\sin(2qa) = 0$, the entire incoming wave will be transmitted and there will be no reflection $T = 1, R = 0$.

Chapter 5

Quantum Electrodynamics

5.1 Classical Electrodynamics

Definition 5.1.1. The **electromagnetic scalar potential** $\Phi(\mathbf{x}, t)$ and vector potential $\mathbf{A}(\mathbf{x}, t)$ are defined in terms of the electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ by

$$\mathbf{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A} \tag{5.1.1}$$

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{5.1.2}$$

Definition 5.1.3. The **classical Lagrangian** $L(\mathbf{x}, \mathbf{v})$ describes the potential energy of a particle with position $\mathbf{x}$, velocity $\mathbf{v}$, charge e and mass m.

$$L(\mathbf{x}, \mathbf{v}) = \frac{m\mathbf{v}^2}{2} - e\Phi + \frac{e}{c}\mathbf{A} \cdot \mathbf{v} \tag{5.1.3}$$

Theorem 5.1.4. The **gauge invariance** state that Φ and $\mathbf{A}$ are not uniquely determined by $\mathbf{E}$ and $\mathbf{B}$. For any function $f(\mathbf{x}, t)$

Definition 5.1.5. The **canonical momentum** is momentum that takes the electromagnetic vector potential $\mathbf{A}$ in account.

$$\mathbf{p} = m\mathbf{v} + \frac{e}{c}\mathbf{A} \tag{5.1.5}$$

Definition 5.1.6. The **Euler-Lagrange Equation** describes how the classical fields change with time.

$$m\frac{d\mathbf{v}}{dt} = e\mathbf{E} + \frac{e}{c}\mathbf{v} \times \mathbf{B} \tag{5.1.6}$$

Definition 5.1.7. The **classical electrodynamics Hamiltonian** is defined as

$$H(\mathbf{p}, \mathbf{x}) = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\Phi \tag{5.1.7}$$

Theorem 5.1.8. The Gauge Invariance Theorem states that the electromagnetic scalar and vector potentials are not unique. For an arbitrary function $f(\mathbf{x}, \mathbf{t})$, the scalar Φ' and vector $\mathbf{A}'$ potentials have the same E and B fields.

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla f \tag{5.1.8}$$

$$\Phi \to \Phi' = \Phi - \frac{1}{c}\frac{\partial}{\partial t}f \tag{5.1.9}$$

Corollary 5.1.10. The canonical momentum is Gauge dependent.

5.2 Quantum Electrodynamics

Definition 5.2.1. The **quantum electrodynamics Hamiltonian** is defined as

$$H(\mathbf{P},\mathbf{X}) = \frac{1}{2m}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}(\mathbf{X})\right)^2 + e\Phi(\mathbf{X}) \tag{5.2.1}$$

s

Result 5.2.2. From the quantum electrodynamics Hamiltonian we can derive the following equations of motion

$$\frac{d\mathbf{x}}{dt} = \frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) \tag{5.2.2}$$

$$\frac{d^2\mathbf{x}}{dt^2} = e\mathbf{E} + \frac{e}{2c}\left(\frac{d\mathbf{x}}{dt}\times\mathbf{B} - \mathbf{B}\times\frac{d\mathbf{x}}{dt}\right) \tag{5.2.3}$$

Theorem 5.2.4. The continuity equation for quantum electrodynamics states that

$$\mathbf{J}(\mathbf{x},t) = \frac{\hbar}{2mi}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) - \frac{e}{mc}\mathbf{A}p(\mathbf{x},t) \tag{5.2.4}$$

5.3 Aharanov-Bohn Effect

Definition 5.3.1. The **double slit Aharanov-Bohn experiment** is a simple example of the Aharanov-Bohn effect for a double slit experiment with a solenoid.

$$\Psi(\mathbf{X},t) = \Psi_1(\mathbf{X},t) + \Psi_2(\mathbf{X},t) \tag{5.3.1}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}\right)\Psi + V\Psi \tag{5.3.2}$$

Result 5.3.3. Each of the two paths sees a phase shift as a result of the electromagnetic vector potential along the path

$$\Psi_i'(\mathbf{X},t) = e^{ig(\mathbf{X})}\Psi_i(\mathbf{X},t), \quad g(\mathbf{X}) = \int_{\mathbf{x_0}}^{\mathbf{X}}\mathbf{A}(\mathbf{X})\cdot d\mathbf{x}' \tag{5.3.3}$$

$$\left|\Psi'(x)\right|^2 = \left|\Psi_1\right|^2 + \left|\Psi_2\right|^2 + 2\,\mathrm{Re}(\Psi_1\Psi_2^* e^{i\delta}) \tag{5.3.4}$$

$$\delta = \frac{e}{\hbar c}\left[\int_{\mathbf{x_0}}^{\mathbf{x_f}}\mathbf{A}\cdot d\mathbf{x}' - \int_{\mathbf{x_0}}^{\mathbf{x_f}}\mathbf{A}\cdot d\mathbf{x}'\right] = \frac{e\Phi_B}{\hbar c}, \qquad \Phi_B = \text{the total flux} \tag{5.3.5}$$

Chapter 6

Angular Momentum

6.1 Rotations and Angular Momentum

Definition 6.1.1. A **rotation** $R(\mathbf{n}, \varphi)$ is a transformation of coordinates in a space that rotates coordinates about an axis $\mathbf{n}$ by angle φ.

Corollary 6.1.2. A rotation is unitary and has a determinant of 1.

$$R^\dagger R = I, \quad \det R = 1 \tag{6.1.2}$$

Definition 6.1.3. The **3D rotation matrices** are

$$R(\mathbf{x}, \varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix}, \quad R(\mathbf{y}, \varphi) = \begin{pmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{pmatrix}, \quad R(\mathbf{z}, \varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6.1.3}$$

Definition 6.1.4. The **rotation operator** $D(\mathbf{n}, \varphi)$ is a unitary operator that rotates the eigenvalues $|\mathbf{x}\rangle$ of $\mathbf{X}$ to the eigenvalue rotated by $R(\mathbf{n}, \varphi)$.

$$D(\mathbf{n}, \varphi) |\mathbf{x}\rangle = |R(\mathbf{n}, \varphi)\mathbf{x}\rangle \tag{6.1.4}$$

Definition 6.1.5. The **angular momentum operators** J_x, J_y, J_z, and $\mathbf{J}$ are defined in terms of the generator of rotation.

$$D(\mathbf{x}, d\varphi) = I - \frac{i}{\hbar} d\varphi J_x, \quad D(R(\mathbf{y}, d\varphi)) = I - \frac{i}{\hbar} d\varphi J_y, \quad D(R(\mathbf{z}, d\varphi)) = I - \frac{i}{\hbar} d\varphi J_z, \tag{6.1.5}$$

$$D(\mathbf{n}, d\varphi) = I - \frac{i}{\hbar} d\varphi \mathbf{n} \cdot \mathbf{J} \tag{6.1.6}$$

Result 6.1.7. For finite rotations the rotation operator can be written as an exponential of angular momentum.

$$D(\mathbf{n}, \varphi) = \lim_{N \to \infty} \left(I - \frac{i\varphi}{\hbar N} \mathbf{n} \cdot \mathbf{J} \right)^N = e^{-i\varphi \mathbf{n} \cdot \mathbf{J}/\hbar} \tag{6.1.7}$$

Proposition 6.1.8. The rotation operator preserves the properties of the rotation group.

$$[R(\mathbf{x}, \alpha), R(\mathbf{y}, \beta)] = R(\mathbf{z}, \alpha\beta) - I, \qquad [D(\mathbf{x}, \alpha), D(\mathbf{y}, \beta)] = D(\mathbf{z}, \alpha\beta) - I \tag{6.1.8}$$

Theorem 6.1.9. The fundamental angular momentum commutation relation states that

$$[J_i, J_j] = i\hbar \varepsilon_{i,j,k} J_k \tag{6.1.9}$$

Proposition 6.1.10. If $D^\dagger(R) J_i D(R) = R_{i,j} J_j$, then the expectation value of angular momentum rotates as a 3D vector $\langle D(R)\mathbf{J} \rangle = R\langle \mathbf{J} \rangle$.

6.2 General Angular Momentum

Definition 6.2.1. General Angular Momentum is an operator denoted $\hat{\mathbf{J}}$ with eigenvalues $|j, m_j\rangle$ for $j = 0, 1, 2, \ldots$ and $m_j = -j, -j+1, \ldots, 0, \ldots, j-1, j$ that is used to generalize the properties of angular momentum.

Proposition 6.2.2. $|j, m_j\rangle$ are simultaneous eigenstates of $\hat{J}^2$ and $\hat{J}_z$.

$$[\hat{J}^2, \hat{J}_z] = 0, \quad [\hat{J}^2, \hat{J}_x] = 0, \quad [\hat{J}^2, \hat{J}_y] = 0 \tag{6.2.2}$$

Proposition 6.2.3. The operators $\hat{J}^2$ and $\hat{J}_z$ have the following eigenvalues

$$\hat{J}^2 |j, m_j\rangle = \hbar^2 j(j+1) |j, m_j\rangle \tag{6.2.3}$$

$$\hat{J}_z |j, m_j\rangle = \hbar m_j |j, m_j\rangle \tag{6.2.4}$$

Proposition 6.2.5. The angular momentum components do not commute.

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x, \quad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y \tag{6.2.5}$$

Definition 6.2.6. The **angular momentum latter operators** are the operators $\hat{J}_+$ and $\hat{J}_-$ defined

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \tag{6.2.6}$$

$$\hat{J}_- = \hat{J}_x - i\hat{J}_y \tag{6.2.7}$$

Proposition 6.2.8. The latter operators are Hermitian conjugates.

$$\hat{J}_+^\dagger = \hat{J}_- \tag{6.2.8}$$

Proposition 6.2.9. The latter operators commute with $\hat{J}^2$

$$[\hat{J}^2, \hat{J}_\pm] = 0 \tag{6.2.9}$$

Proposition 6.2.10. The latter operators do not commute with each other

$$[\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_z \tag{6.2.10}$$

Proposition 6.2.11. The latter operators do not commute with $\hat{J}_z$

$$[\hat{J}_z, \hat{J}_+] = \hbar \hat{J}_+ \tag{6.2.11}$$

$$[\hat{J}_z, \hat{J}_-] = \hbar \hat{J}_- \tag{6.2.12}$$

Proposition 6.2.13. The angular momentum latter operators can be used to raise and lower eigenstates.

$$\hat{J}_+ |j, m_j\rangle = \hbar \sqrt{j(j+1) - m_j(m_j+1)} \, |j, m_j + 1\rangle \tag{6.2.13}$$

$$\hat{J}_- |j, m_j\rangle = \hbar \sqrt{j(j+1) - m_j(m_j-1)} \, |j, m_j - 1\rangle \tag{6.2.14}$$

$$\hat{J}_+ |j, j\rangle = 0 \tag{6.2.15}$$

$$\hat{J}_- |j, -j\rangle = 0 \tag{6.2.16}$$

6.3 Coupling of Angular Momentum

For a system consisting of two angular momentum operators we can find a basis consisting of eigenstates of the combined angular momentum.

Definition 6.3.1. The **total angular momentum** for two angular momentum operators $\mathbf{J}_1$ and $\mathbf{J}_2$ is the operator

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \tag{6.3.1}$$

Definition 6.3.2. An **uncoupled basis** is a basis of a system of angular momentum that consists of eigenstates of the original separate momentum operators. For two angular momentum operators $\mathbf{J}_1$ and $\mathbf{J}_2$ the uncoupled basis is written $|j_1, j_2, m_1, m_2\rangle$ in terms of the quantum numbers j_1, m_1, j_2, and m_2.

Definition 6.3.3. An **coupled basis** is a basis of a system of angular momentum that consists of eigenstates of the total angular momentum written $|J, M\rangle$ in terms of to total quantum numbers J and M.

Proposition 6.3.4. The min and max value of J are determined by the values of j_1 and j_2

$$J^{max} = j_1 + j_2 \tag{6.3.4}$$

$$J^{min} = |j_1 - j_2| \tag{6.3.4}$$

$$M = m_1 + m_2 \tag{6.3.4}$$

Definition 6.3.5. The **Clebsch-Gordan Coefficients** are the terms $C^{j_1,j_2,J}_{m_1,m_2,M}$ that can be used to write the coupled basis in terms of the uncoupled basis.

$$C^{j_1,j_2,J}_{m_1,m_2,M} = \langle j_1, j_2, m_1, m_2 | J, M\rangle \tag{6.3.5}$$

$$|J, M\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C^{j_1,j_2,J}_{m_1,m_2,M} \, |j_1, j_1, m_1, m_2\rangle \tag{6.3.6}$$

$$|j_1, j_2, m_1, m_2\rangle = \sum_{J=|j_1-j_2|}^{j_1+j_2} C^{j_1,j_2,J}_{m_1,m_2,M} \, |J, M\rangle \tag{6.3.7}$$

Proposition 6.3.8. The Clebsch-Gordan Coefficients are always real and $C^{j_1,j_2,J}_{m_1,m_2,M} = 0$ for all $m_1 + m_2 \neq M$.

Theorem 6.3.9. Procedure for Finding an Uncoupled Basis

1. The highest element on the ladder is $|J^{max}, J^{max}\rangle = |j_1, j_2, j_1, j_2\rangle$
2. Apply $\hat{J}_- = \hat{J}_{1-} + \hat{J}_{2-}$ to find $\left|J^{max}, \hat{J}^{max} - 1\right\rangle$.
3. Use orthogonality to find $\left|\hat{J}^{max} - 1, \hat{J}^{max} - 1\right\rangle$.

Chapter 7

Hydrogen-Like Systems

7.1 Radial Solution

7.2 Angular Solution

Definition 7.2.1. The **angular momentum operator L** is for the hydrogen atom is defined in terms of position and momentum

$$\mathbf{L} = \mathbf{x} \times \mathbf{p} \tag{7.2.1}$$

7.2.2 Runge-Lenz Vector

Definition 7.2.3. The **Lenz vector operator M** is defined as

$$\mathbf{M} = \frac{1}{2m}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{Ze^2}{r}\mathbf{x} \tag{7.2.3}$$

Proposition 7.2.4. The eigenvalues of $\mathbf{M}^2$ correspond with the quantum numbers m found in the angular solution.

7.3 3D Harmonic Oscillator

Chapter 8

Symmetry

8.1 Symmetry Operators

Definition 8.1.1. An **infinitesimally generated operator** is a symmetry operator that differs infinitesimally from the identity operator. For some Hermitian operator G, a symmetry operator O can be written as

$$O = I - \frac{1\varepsilon}{\hbar} G \tag{8.1.1}$$

Proposition 8.1.2. If the Hamiltonian H is invariant under an infinitesimally generated operator O, that is $O^\dagger HO = H$, then the generating Hermitian operator G commutes with H, that is $[G, H] = 0$ and $\frac{\partial G}{\partial t} = 0$.

Proposition 8.1.3. If G is the generating Hermitian operator of an infinitesimally generated operator O that invariant acts on H, then if $|g\rangle$ is an eigenstate of G, $U(t)\,|g\rangle$ is also an

8.2 Parity

Definition 8.2.1. The **parity operator** is a Hermitian symmetry operator denoted Π defined by

$$\Pi^\dagger \mathbf{X} \Pi = -\mathbf{X}, \quad \Pi\,|\mathbf{x}\rangle = |-\mathbf{x}\rangle\,, \quad \Pi\,|\mathbf{p}\rangle = |-\mathbf{p}\rangle \tag{8.2.1}$$

Definition 8.2.2. A **polar vector** is a vector operator $\mathbf{V}$ that is inverted under parity $\Pi^\dagger \mathbf{V} \Pi = -\mathbf{V}$.

Definition 8.2.3. A **pseudo vector** is a vector operator $\mathbf{V}$ that is invarient under parity $\Pi^\dagger \mathbf{V} \Pi = \mathbf{V}$.

Definition 8.2.4. A **polar scalar** is a scalar operator S that is invarient under parity $\Pi^\dagger S \Pi = S$.

Definition 8.2.5. A **pseudo scalar** is a scalar operator S that is inverted under parity $\Pi^\dagger S \Pi = -S$.

Result 8.2.6. Angular momentum and general angular momentum are pseudo vectors.

$$\Pi^\dagger \mathbf{L} \Pi = \mathbf{L}, \quad \Pi^\dagger \mathbf{J} \Pi = \mathbf{J} \tag{8.2.6}$$

Proposition 8.2.7. The parity operator acts on wave functions by inverting the input eigenket.

$$\Pi\Psi(\mathbf{x}) = \langle \mathbf{x}|\,\Pi\,|\Psi\rangle = \langle \mathbf{x}|\,\Pi^\dagger\,|\Psi\rangle = \langle -\mathbf{x}|\Psi\rangle = \Psi(-\mathbf{x}) \tag{8.2.7}$$

Definition 8.2.8. A wave function $\Psi(\mathbf{x})$ has **even parity** iff $\Psi(-\mathbf{x}) = \Psi(\mathbf{x})$.

Definition 8.2.9. A wave function $\Psi(\mathbf{x})$ has **odd parity** iff $\Psi(-\mathbf{x}) = -\Psi(\mathbf{x})$.

Theorem 8.2.10. A spherical harmonic Y_ℓ^m has even parity iff ℓ is even and odd parity iff ℓ is odd.

Theorem 8.2.11. If $[H, \Pi] = 0$, then non-degenerate energy eigenstates $|\Psi_n\rangle$ are also eigenstates of Π.

Theorem 8.2.12. Let $|\alpha\rangle$ and $|\beta\rangle$ be parity eigenstates with corresponding eigenvalues $\varepsilon_\alpha = \pm 1$ and $\varepsilon_\beta = \pm 1$. For an operator Ω such that $\Pi^\dagger \Omega \Pi = \varepsilon_\Omega \Omega$ for $\varepsilon_\Omega = \pm 1$,

$$\langle \alpha|\,\Omega\,|\beta\rangle = 0 \quad \text{if } \varepsilon_\alpha \varepsilon_\Omega \varepsilon_\beta \neq 1 \tag{8.2.12}$$

8.3 Time Reversal

Definition 8.3.1. The **conjugation operator** K defined in terms of a basis $\{|\phi_n\rangle\}$ is a non-linear operator that acts on a ket by taking to complex conjugate of the coefficients of the representation of the ket in term of the basis $\{|\phi_n\rangle\}$. That is for any ket $|\psi\rangle = \psi_1 |\phi_1\rangle + \cdots + \psi_n |\phi_n\rangle$,

$$K |\psi\rangle = \psi_1^* |\phi_1\rangle + \cdots + \psi_n^* |\phi_n\rangle \tag{8.3.1}$$

Definition 8.3.2. An **anti-unitary operator** is a non-linear operator that can be written as a product of a unitary operator U and the conjugation operator K.

Definition 8.3.3. The **time reversal operator** Θ is defined by an anti-unitary operator such that

$$e^{-iHt/\hbar}\Theta = \Theta e^{iHt/\hbar} \tag{8.3.3}$$

$$\Theta^{-1}(-iH)\Theta = iH \tag{8.3.4}$$

Theorem 8.3.5. Wigner's Theorem states that for any operator that maintains the normalization of kets is either unitary or anti-unitary.

Proposition 8.3.6. For an anti-unitary operator O, and any two kets $|\alpha\rangle, |\beta\rangle$,

$$\langle\alpha| O^{-1}O |\beta\rangle = \langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle \tag{8.3.6}$$

$$O(c_1 |\alpha\rangle + c_2 |\beta\rangle) = c_1^* O |\alpha\rangle + c_2^* |\beta\rangle \tag{8.3.7}$$

Theorem 8.3.8. If a H is invariant under time-reversal symmetry then,

$$\Theta^{-1}(-iH)\Theta = iH, \quad [H, \Theta] = 0 \tag{8.3.8}$$

Definition 8.3.9. An operator under time reversal is defined as

$$\langle\beta| A |\alpha\rangle = \langle\alpha| \Theta^{-1}\Theta A^\dagger \Theta^{-1}\Theta |\beta\rangle \tag{8.3.9}$$

Definition 8.3.10. An operator A is **even under time reversal** iff $\Theta A \Theta^{-1} = A$.

Definition 8.3.11. An operator A is **odd under time reversal** iff $\Theta A \Theta^{-1} = -A$.

Result 8.3.12. For the time reversal operator Θ, eigenstates $|\mathbf{x}\rangle, |\mathbf{p}\rangle$ of the position operator $\mathbf{X}$ and of the momentum operator $\mathbf{P}$, $\mathbf{J}$ is the generalized angular momentum operator.

$$\Theta \mathbf{X} \Theta^{-1} = \mathbf{X}, \quad \Theta \mathbf{P} \Theta^{-1} = -\mathbf{P}, \quad \Theta \mathbf{J} \Theta^{-1} = -\mathbf{J} \tag{8.3.12}$$

$$\Theta |\mathbf{x}\rangle = e^{i\delta} |\mathbf{x}\rangle, \quad \text{for some } \delta \in \mathbb{R} \tag{8.3.13}$$

$$\Theta\psi(\mathbf{x}, t) = \Theta^*(\mathbf{x}, -t) \tag{8.3.14}$$

$$\Theta Y_\ell^m(\theta, \phi) = \Theta^*(\mathbf{x}, -t) = (-1)^m Y_\ell^m(\theta, \phi) \tag{8.3.15}$$

Result 8.3.16. The electric dipole momentum violates time reversal symmetry.

Chapter 9

Time-Independent Approximation Methods

Definition 9.0.1. A Hamiltonian is **exactly solved** if an exact representation of the energy eigenvalues and energy eigenvectors can be found.

Definition 9.0.2. A **perturbation** is a system consisting of a small change from a exactly solved system $\hat{H}_0$. $\hat{H}'$ is the small change that is applied. The solution of a perturbation is found with an infinite series.

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{9.0.2}$$

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \dots \tag{9.0.3}$$

$$|n\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle + \left|n^{(3)}\right\rangle + \dots \tag{9.0.4}$$

9.1 Non-degenerate Time-Independent Perturbation Theory

Result 9.1.1. First Order Perturbation Eigenvalues - The first order correction for the levels of a perturbation are given by

$$E_n^{(1)} = \left\langle n^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle \tag{9.1.1}$$

Result 9.1.2. First Order Perturbation Eigenstates - The first order correction for the eigenstates of a perturbation is given by

$$\left|n^{(1)}\right\rangle = \sum_{m\neq n} \frac{\left\langle m^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}} \left|m^{(0)}\right\rangle \tag{9.1.2}$$

Result 9.1.3. Second Order Perturbation Eigenvalues - The second order correction for the eigenstates of a perturbation is given by

$$E_n^{(2)} = \sum_{m\neq n} \frac{\left|\left\langle m^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \tag{9.1.3}$$

Result 9.1.4. Second Order Perturbation Eigenstates - The second order correction for the eigenstates of a perturbation is given by

$$\left|n^{(2)}\right\rangle = \sum_{m\neq n}\sum_{k\neq n} \frac{\left\langle m^{(0)}\right| \hat{H}' \left|k^{(0)}\right\rangle \left\langle k^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_k^{(0)}\right)} \left|m^{(0)}\right\rangle \tag{9.1.4}$$

$$- \sum_{m\neq n} \frac{\left\langle m^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle \left\langle n^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle}{\left(E_n^{(0)} - E_m^{(0)}\right)^2} \left|m^{(0)}\right\rangle - \frac{1}{2} \sum_{m\neq n} \frac{\left|\left\langle m^{(0)}\right| \hat{H}' \left|n^{(0)}\right\rangle\right|^2}{\left(E_n^{(0)} - E_m^{(0)}\right)^2} \left|n^{(0)}\right\rangle \tag{9.1.4}$$

Proposition 9.1.5. The first order correction to the energy eigenvalue of the ground state always exact or an overestimate.

Proposition 9.1.6. The second order correction to the energy eigenvalue of the ground state is always negative.

9.2 Degenerate Time-Independent Perturbation theory

Perturbation theory does not work for degenerate energies. To resolve this issue we will find a new energy eigenbasis of $\hat{H}_0$ such that

$$\left\langle m^{(0)} \hat{H}' \left| n^{(0)} \right\rangle \right| = 0 \tag{9.2.0}$$

For any two degenerate states m and n. The perturbation Hamiltonian $\hat{H}'$ may split the degeneracy. However, since $\hat{H}'$ is not generally diagonalizable we will consider $\hat{H}'$ in the subspace of each degenerate energy.

Definition 9.2.1. A **conservation law** is an operator $\hat{A}$ such that $[\hat{H}_0, \hat{A}] = [\hat{H}', \hat{A}] = 0$.

Theorem 9.2.2. Degenerate Perturbation Subspace Theorem - If a conservation law exists then perturbation theory can be used by finding an energy eigenbasis of $\hat{H}_0$ such that $\left\langle m^{(0)} \hat{H}' \left| n^{(0)} \right\rangle \right| = 0$ for any two degenerate states m and n. To find such an eigenbasis, apply the following for each degeneracy:

1. Consider the subspace of degenerate eigenstates $|n\rangle$.
2. Find the matrix of $\hat{H}'$ in in this subspace.
3. Diagonalize the matrix to find a new basis $|n'\rangle$.
4. The new basis elements are simultaneous eigenstates of $\hat{H}'$ and $\hat{H}_0$.
5. Repeat this process for each degeneracy.

9.3 The Stark Effect

Definition 9.3.1. The **Stark effect** is a perturbation of the hydrogen atom by a constant electric field defined

$$H' = -eEZ \tag{9.3.1}$$

Result 9.3.2. Applying non-degenerate perturbation theory to the ground state results in the following first non-zero stark effect shift.

$$E^{(2)}_{100} = e^2 E^2 \sum_{n=2}^{\infty} \frac{\left|\langle n10| Z |100\rangle\right|^2}{E_1 - E_n} \tag{9.3.2}$$

Result 9.3.3. The stark effect induces an electric dipole moment d_z in the ground state of the hydrogen atom

$$d_z = -\frac{2}{E^2} E^{(2)}_{100}, \quad d_z < \frac{16 a_0^3}{3} \tag{9.3.3}$$

9.4 The Zeeman Effect

Definition 9.4.1. The **Zeeman effect** is a perturbation of the hydrogen atom by a constant magnetic field defined

$$H' = \frac{-eB}{2mc} \left(L_z + 2S_z\right) \tag{9.4.1}$$

Definition 9.4.2. The **Bohr magneton** is the magnetic moment of an electron defined

$$\mu_B = \frac{e\hbar}{2m_e} \tag{9.4.2}$$

9.4.3 Week Field Limit

Definition 9.4.4. The **week field limit Zeeman effect** is the approximation that assumes the magnetic field is much weaker than contribution from spin orbit coupling that is $\Delta E_z << \Delta E_{LS}$.

Result 9.4.5. The first order Zeeman effect correction for the weak field limit where $j = \ell \pm 1/2$ is

$$E^{(1)}_{B(n\ell jm)} = \mu_B B m \left(1 + \frac{\langle n\ell jm| S_z |n\ell jm\rangle}{m\hbar}\right) = \mu_B B m \left(1 \pm \frac{1}{2\ell + 1}\right) \tag{9.4.5}$$

9.4.6 Strong Field Limit

Definition 9.4.7. The **strong field limit Zeeman effect** is the approximation that assumes the magnetic field is much stronger than contribution from spin orbit coupling that is $\Delta E_z >> \Delta E_{LS}$.

Result 9.4.8. The first order Zeeman effect correction for the strong field limit where is

$$E^{(1)}_{B(n\ell m_\ell m_S)} = \mu_B B(m_\ell + 2m_S) \tag{9.4.8}$$

9.5 Fine Structure

Definition 9.5.1. The **fine structure** is a perturbation of the hydrogen atom by relativistic corrections defined

$$H'_K = -\frac{1}{8}\frac{P^4}{m^3c^2} \tag{9.5.1}$$

Result 9.5.2. Angular momentum commutes with the fine structure correction.

$$[L^2, H'_K] = 0 \tag{9.5.2}$$

Result 9.5.3. The first order fine structure correction is

$$E^{(1)}_K = E^{(0)}_n \alpha^2 \left[-\frac{3}{4n^2} + \frac{1}{n(\ell + 1/2)}\right] \tag{9.5.3}$$

9.6 Spin Orbit Coupling

Definition 9.6.1. the **spin orbit coupling** is a perturbation of the hydrogen atom that approximates the effects of the interaction between the spin of the electron and the angular momentum of orbitals defined

$$H'_{LS} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r} = \frac{1}{2m^2c^2}\frac{e^2}{4^3} \tag{9.6.1}$$

Result 9.6.2. The first order spin orbit coupling correction is

$$E^{(1)}_{LS} = -E^{(0)}_n \alpha^2 \left(\frac{-1}{2n(\ell + 1/2)}\right) \begin{bmatrix} \frac{1}{\ell+1} \\ \frac{-1}{\ell} \end{bmatrix} \tag{9.6.2}$$

Result 9.6.3. The fine structure and spin orbit coupling correction for $\ell \neq 0$ and $j = \ell \pm \frac{1}{2}$ is

$$E^{(1)}_{n\ell j} = E^{(0)}_n \alpha^2 \left[\frac{1}{n(j + 1/2)} - \frac{3}{4n^2}\right] \tag{9.6.3}$$

9.6.4 The Darwin Term

Definition 9.6.5. The **Darwin term** is the correct perturbation for spin orbit coupling when $\ell = 0$ defined

$$H'_D = \frac{\pi\hbar^3 c\alpha}{2m^2c^2}\delta^{(3)}(\mathbf{r}) \tag{9.6.5}$$

Result 9.6.6. For $\ell = 0$ the first order spin orbit correction must include the Darwin term.

9.7 Hyperfine Structure

Definition 9.7.1. The **hyperfine structure** is a perturbation of the hydrogen atom that approximates the effects of the interaction between the spin of the electron and the spin of the nucleus defined

$$H'_{HF} = \frac{8\pi}{3}\left(\frac{eg_e}{2m_e c}\right)\left(\frac{eg_p}{2m_p c}\right)\mathbf{S}_e \cdot \mathbf{S}_p \delta^{(3)}(\mathbf{R}) \tag{9.7.1}$$

Result 9.7.2. The expected value of the product of electron spin and proton spin depends on the coupled spin and the coupled basis for S_e and S_p is

$$|S=0 m_s=0\rangle = \frac{1}{\sqrt{2}}(|+\rangle_e |-\rangle_p + |-\rangle_e |+\rangle_e) \tag{9.7.2}$$

$$|S=1 m_s=1\rangle = |+\rangle_e |+\rangle_p \tag{9.7.3}$$

$$|S=1 m_s=0\rangle = \frac{1}{\sqrt{2}}(|+\rangle_e |-\rangle_p - |-\rangle_e |+\rangle_p) \tag{9.7.4}$$

$$|S=1 m_s=-1\rangle = |-\rangle_e |-\rangle_p \tag{9.7.5}$$

$$\langle \mathbf{S}_e \cdot \mathbf{S}_p \rangle = \frac{\hbar^2}{2}\left[S(S+1) - \frac{3}{2}\right] \tag{9.7.6}$$

Result 9.7.7. The first order hyperfine structure correction for the ground state of hydrogen is

$$E^{(1)}_{HF} = -E^{(1)}_1 \alpha^2 \left(\frac{m_e}{m_p}\right)\left(\frac{2}{3} g_e g_p\right)\left[S(S+1) - \frac{3}{2}\right] \tag{9.7.7}$$

9.8 Variational Theory

Theorem 9.8.1. For any $|\psi\rangle$ with Hamiltonian H, $\langle\psi| H |\psi\rangle \geq E_0$

Result 9.8.2. For a perturbed system with unperturbed ground state $|0\rangle$ the ground state energy predicted by variational theory $E[\psi]$ differs from the real ground state by a factor proportional to $|\varepsilon|^2$.

$$\psi = a|0\rangle + \varepsilon |f\rangle, \quad \langle\psi|\psi\rangle = \langle f|f\rangle = \langle 0|0\rangle = 1, \quad \langle 0|f\rangle = 0 \tag{9.8.2}$$

$$E[\psi] - E_0 = |\varepsilon|^2 (E_0 + \langle f| H |f\rangle) \tag{9.8.3}$$

Chapter 10

Time-Dependent Approximation Methods

10.1 Time-Dependent Perturbation Theory

Definition 10.1.1. The **interaction picture** is a set of notation for quantum mechanics where only the perturbed component of the states depends on time and only the unperturbed component of the operators depends on time.

$$|\psi(t)\rangle_I = e^{iH_0 t/\hbar} |\psi(t)\rangle_S , \quad O_I(t) = e^{iH_0 t/\hbar} O_S e^{-iH_0 t/\hbar} \tag{10.1.1}$$

Definition 10.1.2. A **time-dependent perturbation** is a system consisting of a time-dependent small change from a exactly solved system $\hat{H}_0$. $\hat{H}'(t)$ is the small change that is applied. The solution of a time-dependent perturbation of an initial eigenstate $|k\rangle$ is found in the interaction picture as time dependent coefficients of the unperturbed eigenstates $|n\rangle$.

$$\hat{H} = \hat{H}_0 + \hat{H}'(t) \tag{10.1.2}$$

$$|\psi(t)\rangle_I = \sum_n c_n(t) |n\rangle \tag{10.1.3}$$

$$c_n(t) = c_n^{(0)}(t) + c_n^{(1)}(t) + \dots \tag{10.1.4}$$

$$c_n^{(0)}(t) = \delta_{nk} \tag{10.1.5}$$

$$c_n^{(1)}(t) = \frac{-i}{\hbar} \int_0^t e^{i\omega_{nk}t'} H'_{nk}(t') dt' \tag{10.1.6}$$

$$c_n^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \int_0^t \int_0^{t'} \sum_m e^{i\omega_{nm}t'} H'_{nm}(t') e^{i\omega_{mk}t''} H'_{mk}(t'') dt'' dt' \tag{10.1.7}$$

Proposition 10.1.8. The real component of the second order coefficient to remain in the ground state is related to the first order probability to change states.

$$2\mathrm{Re}(c_0^{(2)}) = -|c_1^{(1)}|^2 = -P^{(1)}(0 \to 1) \tag{10.1.8}$$

10.2 Constant Perturbation

Definition 10.2.1. The **constant perturbation** is a perturbation of the harmonic oscillator defined with the perturbation for $V_0 \in \mathbb{C}$,

$$H'(t) = \begin{cases} 0 & t < 0 \\ V & t \geq 0 \end{cases} \tag{10.2.1}$$