Introduction to Quantum Mechanics

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December 6, 2024

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Chapter 1

Quantum States

1.1 Amplitudes and Interference

Quantum mechanics is probabilistic. Let us consider fig. 1.1, where a particle has a probability $P_1(x)$ of travelling through path 1 and ending up at x, and a probablility of $P_2(x)$ of travelling through path 2 and ending up at x. Classically, the total probablility of the system ending up at x is,

$$P(x) = P_1(x) + P_2(x), \tag{1.1}$$

however, this is not the case in quantum mechanics. In quantum mechanics, probablities are determined using *amplitudes*, which, unlike probablilities, can be negative and complex. The probablility is then given by,

$$P(x) = |A(x)|^2 = A^*(x)A(x). \tag{1.2}$$

In order to get the total probablity of event occurring, we must then add the amplitudes together, or rather **superimpose** them.

Let us write the amplitudes for the two paths,

$$A_1(x) = \sqrt{P_1(x)}e^{i\phi_1} \tag{1.3}$$
$$A_2(x) = \sqrt{P_2(x)}e^{i\phi_2} \tag{1.4}$$
$$A(x) = A_1(x) + A_2(x). \tag{1.5}$$

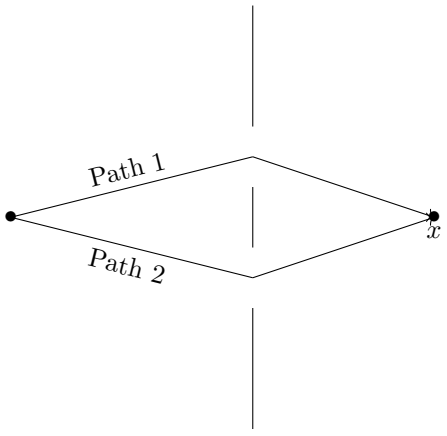

Figure 1.1: An event occurs where a ball can go through one of two paths, each with a different probability $P_1(x)$ and $P_2(x)$ of ending up at position x.

The total probability of the particle ending up at x is then,

$$\begin{aligned} P(x) &= |A(x)|^2 = |A_1(x) + A_2(x)|^2 \\ &= |\sqrt{P_1}e^{i\phi_1} + \sqrt{P_2}e^{i\phi_2}|^2 \\ &= (\sqrt{P_1}e^{i\phi_1} + \sqrt{P_2}e^{i\phi_2})(\sqrt{P_1}e^{-i\phi_1} + \sqrt{P_2}e^{-i\phi_2}) \\ &= P_1 + P_2 + \sqrt{(P_1P_2)}\left(e^{i(\phi_1-\phi_2)} + e^{i(\phi_2-\phi_1)}\right) \\ &= \underbrace{P_1 + P_2}_{\text{Classical Terms}} + \overbrace{2\cos(\theta_1-\theta_2)\sqrt{P_1P_2}}^{\text{Interference Terms}}. \end{aligned} \tag{1.6}$$

We see that the approach of adding amplitudes added *interference terms* to the latter half of eq. (1.6). If this term is +ive, we get constructive interference, and if it is −ive, we get destructive interference.

1.2 States of Quantum Systems

Wavefunctions as we have met previously are only approximation of quantum mechanics. We often talk about *information* in quantum systems, of which there are two types,

1. **What is the system?** This determines the Hamiltonian of the system.
2. **What state is the system in?** These are the dynamical properties of the system. These describe the quantum state.

We can denote a configuration of a qunatum system with using *ket* notation, such that,

$$|\text{configuration}\rangle\,. \tag{1.7}$$

For a system which can be in more than 1 configuration, its state is in a **superposition** of all possible configurations. For example, the state of flipping a coin is,

$$|\psi\rangle = A_H\,|H\rangle + A_T\,|T\rangle \tag{1.8}$$

where A_H and A_T are the amplitudes corresponding to flipping a heads or a tails.

We are able to perform a measurement to find out what state a system is in, and when we do so, we **collapse the superposition** into the state that we measured. So, lets say we measured a heads - our state would go from that in eq. (1.8), to

$$|\psi\rangle \to |H\rangle\,. \tag{1.9}$$

Further, we require the state of the system to be **normalised**, i.e.,

$$|A_1|^2 + |A_2|^2 = 1. \tag{1.10}$$

Generally, a quantum state $|\psi\rangle$ can be represented as so,

$$\boxed{|\psi\rangle = \sum_j c_j\,|j\rangle} \tag{1.11}$$

$$\boxed{\sum_j |c_j|^2 = 1, c_j \in \mathbb{C}} \tag{1.12}$$

1.2.1 Transforming a quantum state

Over time a system may evolve, and transform the quantum state. For example, turning the coin over will transform the quantum state of the coin by,

$$|\Psi\rangle \to A_H\,|T\rangle + A_T\,|H\rangle\,. \tag{1.13}$$

1.3 Quantum States as Vectors

Quantum mechanics is formulated from postulates, such as below,

Postulate 1. *The quantum state $|\psi\rangle$ of a system is represented by a normalised vector with complex elements (is a member of a Hilbert space).*

We can then simply say that the inner product of a quantum sate vector must equal 1 for it to be normalised. The inner product of a Euclidian space can be defined by the transpose of that vector. I.e, if the vector is $\mathbf{v}$ with real elements v_i,

$$\mathbf{v} \cdot \mathbf{v} = \mathbf{v}^T \mathbf{v} = \sum_i v_i^2. \tag{1.14}$$

and its *norm* $|\mathbf{v}|$ is the square root of this. However, in Hilbert space (complex vector space), the inner product is defined,

$$\langle \mathbf{v}, \mathbf{v} \rangle = \sum_i |v_i|^2. \tag{1.15}$$

We must then create a new operation which both takes the transpose of the vector and the conjugate of each element. This is known as the **Hermitian conjugate**, represented by, †. It has the followig properties,

$$B^{\dagger\dagger} = B \tag{1.16}$$

$$(AB)^\dagger = B^\dagger A^\dagger. \tag{1.17}$$

1.3.1 Dual of the quantum state

We can take the Hermitian conjugate of the quantum state, known as a *dual*. We denote it using a *Bra*,

$$\boxed{\langle \psi | = |\psi\rangle^\dagger}. \tag{1.18}$$

From this, we can clearly see that the norm of $|\psi\rangle$ is given by,

$$| \, |\psi\rangle \, | = \sqrt{\boldsymbol{\psi}^\dagger \boldsymbol{\psi}} \tag{1.19}$$

where $\boldsymbol{\psi}$ is the quantum state vector. It is obvious that the norm may also be written by a combination of the bra and the ket,

$$\boxed{\langle \psi | \psi \rangle = \boldsymbol{\psi}^\dagger \boldsymbol{\psi}}. \tag{1.20}$$

If eq. (1.20) does not equal 1, then the state is not normalised. If this is the case, the amplitudes must be scaled by a factor of

$$\frac{1}{\sqrt{\langle \psi | \psi \rangle}}$$

1.3.2 Quantum State Overlaps

The inner product between two different qunatum states gives their **overlap**. If we have a state $|\psi\rangle = \sum_i a_i |i\rangle$ and $|\phi\rangle = \sum_j b_j |j\rangle$, their overlap (inner product) is denoted,

$$\langle \psi | \phi \rangle = \sum_i a_i^* b_i \tag{1.21}$$

and commutes by,

$$\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^* . \tag{1.22}$$

1.3.3 Basis States

Eq. (1.21), carries the implication that, for *configuarations* of a quantum state $|i\rangle$ and $|j\rangle$, the overlap is defined,

$$\langle i|j\rangle = \delta_{ik} \tag{1.23}$$

where Kronecker-Delta (δ_{ik}) is defined,

$$\delta_{ik} = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases}. \tag{1.24}$$

If a set of configuration states are all,

1. normalised,
2. mutually orthogonal,
3. and span a complete set of mutually exclusive configurations of a quantum state,

they form an *orthonormal basis* for the quantum state of the system.

Changing of basis

If a quantum state $|\psi\rangle$ is defined in terms of a set of basis states $\{|i\rangle\}$, we can redefine the quantum state in terms of a new set basis states $\{|j\rangle\}$ by,

$$|\psi\rangle = \sum_j \langle j|\psi\rangle \, |j\rangle \, . \tag{1.25}$$

Chapter 2

Measurement

Postulate 2. *When measuring a system in a quantum state $|\psi\rangle$ using a measurement basis that includes a configuration $|\phi\rangle$, the probability amplitude of the measurement outcome of $|\phi\rangle$ is $\langle\psi|\phi\rangle$.*

When performing measurement, we must first specify the *measurement basis*. Suppose we wish to measure the probablility amplitude of the outcome $|\phi_n\rangle$ of a quantum state $|\psi\rangle$ in the basis $\{\phi_i\}$. In the case that the quantum state $|\psi\rangle$ is defined in the basis $\{\phi_i\}$, the measurement of the amplitude is trivial, and we simply read the amplitude off of the quantum state. However, if the quantum state is defined using some other basis $\{\Phi_i\}$, the probaility amplitude of measuring outcome $|\phi_n\rangle$ in the measurement basis of $\{\phi_i\}$ is,

$$A(\text{Outcome}\,|\phi_n\rangle\,,\,\text{in state}\,|\psi\rangle) = \langle\phi_n|\psi\rangle \tag{2.1}$$

as long as each element in the measurement basis $\{\phi_i\}$ is defined in terms of the basis of the quantum state $\{\Phi_i\}$.

2.1 Stern-Gerlach Experiment

The Stern-Gerlach experiment essentially confirmed quantum mechanics, and the idea that *measurement affects outcomes of future measurement*. Let us consider a particle which is equally likely to be in one of two states. We can measure these states using one of two basis, $\{|0\rangle\,,|1\rangle\}$ and $\{|+\rangle\,,|-\rangle\}$. If the particle's initial state is,

$$|\psi\rangle = |+\rangle\,, \tag{2.2}$$

then we can then make the following measurements,

Measurement 1: Using the $\{|0\rangle\,,|1\rangle\}$ basis, only particles in state $|0\rangle$ proceed to the next measurement.

Measurement 2: Using Using the $\{|+\rangle\,,|-\rangle\}$ basis, all particles proceed to the next measurement.

Measurement 3: Using the $\{|0\rangle\,,|1\rangle\}$ basis, only particles in state $|1\rangle$ proceed to the end of the experiment.

We can perform two forms this experiement: one where we omit measurement 2, and one where we perform all 3 measurements, represented by figs. 2.1 and 2.2 respectively. Let's analyse the results of each variation.

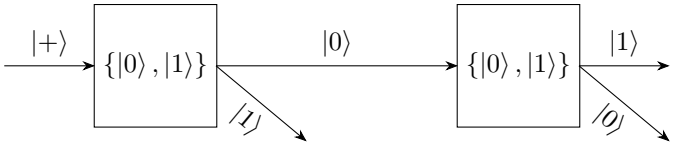

Figure 2.1: A measurement of a particle initially in a $|+\rangle$ state is measured in a $\{|0\rangle\,,|1\rangle\}$ basis, and only particles in state $|0\rangle$ can proceed. The particles are measured again in the $\{|0\rangle\,,|1\rangle\}$ basis, and only particles in state $|1\rangle$ proceed.

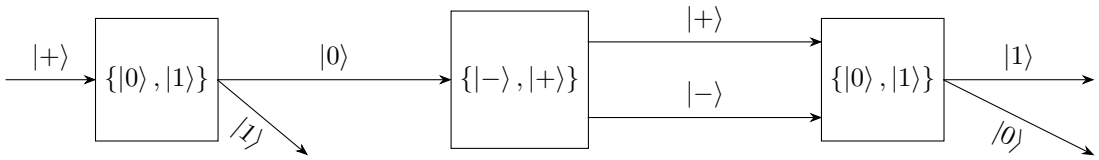

Figure 2.2: As in fig. 2.1, with an additional intermediary measurement, where the particles in a $|0\rangle$ state are measured in a $\{|+\rangle, |-\rangle\}$ basis where all particles procede.

Omitting measurement 2: We begin with all particles in a state as in eq. (2.2). During measurement 1, the particles have an equal chance to be in state $|0\rangle$ or $|1\rangle$, and since,

$$|\langle 0|+\rangle|^2 = \frac{1}{2} \tag{2.3}$$

only half of the particles proceed to measurement 3. All particles are now in state $|0\rangle$, and since,

$$\langle 0|1\rangle = 0 \tag{2.4}$$

no particles are measured in a $|1\rangle$ state, so no particles make it to the end of the experiment.

Performing all measurements: We have the same scenario as in the first experiment. After passing through the measurement 1, only particles in state $|0\rangle$ proceed to measurement 2. When we measure the particles in basis $\{|-\rangle, |+\rangle\}$, their state will *collapse* to either state. Since $|-\rangle$ and $|+\rangle$ are both equally likely, the wave function of half of the particles will go to,

$$|\psi\rangle \to |+\rangle \tag{2.5}$$

and the other half,

$$|\psi\rangle \to |-\rangle . \tag{2.6}$$

At measurement 3, the probability of a particle in a $|-\rangle$ state to collapse to a $|1\rangle$ state is a half, etc. So, only half of the particles which entered the measurement 3 filter proceed to the end of the experiment. And thus, a quarter of the particles which entered the experiment proceed to the end!

Significance of the Stern-Gerlach experiment

As we have seen, the addition of an intermediate changes the final outcome of an experiment. We have shown that *measurement alone has an observable effect on a quantum system.*

2.2 Operators

A linear operator maps a set of inputs $\mathbb{A}$ to outputs of the same set, i.e.,

$$\hat{L} \text{ maps } \mathbb{A} \to \mathbb{A}. \tag{2.7}$$

Linear operators are written in terms of the outerproducts of a given orthonormal basis, where the outer product is $|\psi\rangle\langle\psi|$. To transform an operator to a basis $\{j\}$, we write,

$$\hat{L} = \sum_j \sum_{j'} |j\rangle\langle j|\hat{L}|j'\rangle\langle j'| . \tag{2.8}$$

The identity operator $\hat{I}$ leaves a state unchanged. The identity operator for a given basis $\{j\}$ is,

$$\hat{I} = \sum_J |j\rangle\langle j| . \tag{2.9}$$

We are able to represent linear operators in a matrix form. This becomes clear when we write,

$$\hat{L} = \sum_{j,k} c_{jk} |j\rangle\langle k| \tag{2.10}$$

so that we can write the elements of the matrix form of $\hat{L}$ as,

$$L_{jk} = c_{jk}. \tag{2.11}$$

2.2.1 Functions of linear operators

We borrow rules from matrices when applying functions to operators, i.e.,

$$\hat{L}^n = \hat{L}\hat{L}\underbrace{\cdots}_{\substack{n \\ \text{times}}}\hat{L} \tag{2.12}$$

where $\hat{L}$ is applied n times. We can also define more exotic operations such as,

$$e^{\hat{L}} = \sum_{k=0}^{\infty} \frac{1}{k!}\hat{L}^k \tag{2.13}$$

if a function has a given power series expansion. We note that linear operators are non-commutative,

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}. \tag{2.14}$$

2.2.2 Eigenstates of linear operators

Every operator has given **eigenstates** $|v\rangle$ and **eigenvalues** λ which satisfy,

$$\hat{L}\,|v\rangle = \lambda\,|v\rangle \tag{2.15}$$

We can define a hermitian operator $\hat{H}$ which has all the properties of a Hermitian matrix. This operator is diagonal under the basis ascribed by its eigenstates, such that,

$$\hat{H} = \sum_j \lambda_j\,|v_j\rangle\,\langle v_j|\,. \tag{2.16}$$

If we have a function f which can be expanded by a power series, then,

$$f(\hat{H}) = \sum_j f(\lambda_j)\,|v_j\rangle\,\langle v_j| \tag{2.17}$$

2.3 Observables and Measurement

The choice of basis will change which **observables** we are able to measure. Every observable $\mathcal{A}$ has an associated linear operator $\hat{A}$ which returns its expectation value, such that,

$$\langle\mathcal{A}\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle\,. \tag{2.18}$$

We define $\hat{A}$,

$$\hat{A} = \sum_j A_j\,|a_j\rangle\,\langle a_j| \tag{2.19}$$

where $\{a_j\}$ is a set of configuration states each with a given value A_j, which in turn define the observable $\mathcal{A}$. We can write the configuration of the observable more compactly if we treat each term of the operator as its own linear operator. We define a **projector** to be,

$$\boxed{\hat{A}_j = |a_j\rangle\,\langle a_j|} \tag{2.20}$$

then the operator is,

$$\boxed{\hat{A} = \sum_j a_j\hat{A}_j}. \tag{2.21}$$

We further require that *linear operators of observables are all Hermitian.*

With the above stated, we can now write postulate 2 more formally.

Postulate 2. *A measurement $\mathcal{M}$ of a quantum system is a set of Hermitian linear operators $\left\{\hat{M}_j\right\}$ with non-negative eigenvalues that satisfy,*

$$\sum_j \hat{M}_j = \hat{I} \tag{2.22}$$

and the probability of an outcome j when in state $|\psi\rangle$ is,

$$\boxed{P(|j\rangle) = \langle\psi_j|\psi_j\rangle}. \tag{2.23}$$

2.4 Commutators

We define the *commutater* of a linear operator as,

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{2.24}$$

whose output is a linear operator. If this operator is null, i.e., if $\hat{A}\hat{B} = \hat{B}\hat{A}$, we say that the operators $\hat{A}$ and $\hat{B}$ commute.

Theorem. *If two operators $\hat{A}$ and $\hat{B}$ have a complete set of eigenstates and commute, then there exists a set of simultaneous eigenstates for both operators.*

Proof. Assuming $\hat{A}$ has no degenerate eigenvalues. Let $|v\rangle$ be the eigenstates of $\hat{A}$ and λ the eigenvalues. We have,

$$\hat{B}\hat{A}\,|v\rangle = \hat{B}\lambda\,|v\rangle = \lambda\hat{B}\,|v\rangle\,. \tag{2.25}$$

Since $\hat{A}$ and $\hat{B}$ commute, we have,

$$\hat{B}\hat{A}\,|v\rangle = \hat{A}\hat{B}\,|v\rangle\,, \tag{2.26}$$

and putting all this together,

$$\hat{A}\left(\hat{B}\,|v\rangle\right) = \lambda(\hat{B}\,|v\rangle). \tag{2.27}$$

We have that $\hat{B}\,|v\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue λ. Since $\hat{A}$ is not degenerate, then $\hat{B}\,|v\rangle \propto |v\rangle$, i.e., $|v\rangle$ is an eigenvalue of $\hat{B}$. Thus, if $\hat{A}$ is non-degenerate, then the *eigenstates of $\hat{A}$ are also eigenstaets of $\hat{B}$.* □

2.4.1 Compatibility of Measurement

If an two operators corresponding to two different observables commute, i.e., $\mathcal{A}$ and $\mathcal{B}$ to $\hat{A}$ and $\hat{B}$, then we say that the measurements of those observables are *compatible*, and we can measure them both simulatenously. This is because the operators of the observables correspond to the same eigenbasis.

If two operators are non-commutative, then their measurements are *incompatible*. The amount of information we can know about two given incompatible observables is encapsulated by the uncertainty principle. If we define the standard deviation on an observable as,

$$\begin{aligned}\Delta\mathcal{A} &= \left\langle \mathcal{A}^2 \right\rangle - \langle \mathcal{A} \rangle^2 \\ &= \langle\psi|\,\hat{A}^2\,|\psi\rangle - \left(\langle\psi|\,\hat{A}\,|\psi\rangle\right)\end{aligned} \tag{2.28}$$

then the uncertainty principle states,

$$\Delta\mathcal{A}\Delta\mathcal{B} \geq \frac{1}{2}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right| \tag{2.29}$$

Chapter 3

Spin and Real Uses of Quantum Mechanics

All particles have an intrinsic angular momentum (that differs from orbital angular momentum). Every quantum particle has an associated *spin quantum number* which can take non-negative, half integer values (i.e., 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, etc.) We divide particles into 2 different classes,

- **Fermions**: Half integer spin values.
- **Bosons**: Integer spin values.

The spin of a particle corresponds to an axis. The *spin itself* isn't an observable, but *spin along an axis* is. We can define the spin operator on a given axis for any normalised vector $\mathbf{n}$ as,

$$\hat{S}_n = n_x \hat{S}_x + n_y \hat{S}_y + n_z \hat{S}_z \tag{3.1}$$

which we can write in the vector form,

$$\hat{\mathbf{S}} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix} \tag{3.2}$$

where

$$\hat{S}_{\mathbf{n}} = \hat{\mathbf{S}} \cdot \mathbf{n}. \tag{3.3}$$

The spin quantum number s restricts the value of spin a particle can have along any given axis. The spin S of a particle must satisfy,

$$S \leq \hbar s. \tag{3.4}$$

Furthermore, a particle has *quantised* spin values spaced by $\hbar$. I.e., a spin-1 particle can have spin values,

$$S = -\hbar, 0, \hbar \tag{3.5}$$

while a spin-$\frac{1}{2}$ particle can have spin values,

$$S = -\frac{1}{2}\hbar, \frac{1}{2}\hbar. \tag{3.6}$$

3.1 Spin Operators

We will state properties of spin operators without proof.

Spin canonical commutation relations state that for any principle axis $\{j, k, l\}$, the spin operators satisfy,

$$\left[\hat{S}_j, \hat{S}_k\right] = i\hbar\epsilon_{ijk}\hat{S}_l \tag{3.7}$$

which implies that spin measurements along different axis are incompatible.

3.1.1 Spin-$\frac{1}{2}$ Particles

Pauli Operators

If we work in a basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ corresponding to spin states $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ respectively, and using a cartesian axis, we have,

$$\hat{\mathbf{S}} = \frac{\hbar}{2}\begin{pmatrix} |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \\ -i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow| \\ |\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow| \end{pmatrix}. \tag{3.8}$$

We often use *Pauli operators* $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ which take the form as in eq. (3.8) without the $\frac{\hbar}{2}$ factor,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.9}$$

Ladder Operators

These transform spin states by increasing or decreasing the spin along a given axis by 1 unit. We often specify them for the z-axis.

Let $|m_s\rangle$ be the eigenstate of $\hat{S}_z$ corresponding to the eigenvalue $\hbar m_s$ such that,

$$\hat{S}_z|m_s\rangle = \hbar m_s|m_s\rangle. \tag{3.10}$$

Then, the spin ladder operators $\hat{S}_+$ and $\hat{S}_-$ for a spin-s particle are as follows,

$$\hat{S}_+|m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s+1)}\,|m_s+1\rangle, \tag{3.11}$$

$$\hat{S}_-|m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s-1)}\,|m_s-1\rangle. \tag{3.12}$$

NOTE: Ladder operators are not Hermitian $\implies$ do not correspond to observables. However, it can be shown,

$$\hat{S}_+^\dagger = \hat{S}_-. \tag{3.13}$$

Furthermore, for any spin-s,

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y. \tag{3.14}$$

Spin Eigenstates

The magnitude of the spin operator is defined,

$$|\hat{\mathbf{S}}|^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2. \tag{3.15}$$

Given the relation by eq. (3.14), combined with eq. (3.12) and eq. (3.14), we can show,

$$\hat{S}^2|m\rangle = \hbar^2 s(s+1)|m\rangle. \tag{3.16}$$

Since this is true for all eigenstaets of $\hat{S}_z$, *every state* of the system is an eigenstate of $\hat{S}^2$ with eigenvalues $\hbar^2 s(s+1)$. Thus,

$$\hat{S}^2 = \hbar s(s+1)\hat{I}. \tag{3.17}$$

3.2 Quantum Hamiltonians

In quantum mechanics, a system's energy is quantised. If the energy of the system is directly measured, the value we find must be consistent with the set described by the *energy spectrum* of the system. We specify this energy spectrum by the Hamiltonian $\hat{H}$. The energy spectrum $\{E_i\}$ corresponds to the associated energy eigenstates $\{|E_i\rangle\}$. The eigenvalue equation for these eigenstates takes the form,

$$\hat{H}|E_i\rangle = E_i|E_i\rangle \tag{3.18}$$

which is also known as the *Time-Independent Schrodinger Equation.*

The smallest energy of a system is known as the *ground state* with a corresponding *ground state energy.* All other energy eigenstates are known as *excited states.*

3.2.1 Time evolution of a quantum system

We can use the Hamiltonian to describe the time evolution of a quantum system. By the *Time Dependent Schrodinger Equation*,

$$\boxed{i\hbar\frac{\mathrm{d}\left|\psi\right\rangle}{\mathrm{d}t} = \hat{H}\left|\psi\right\rangle}. \tag{3.19}$$

If we have a quantum state $|\psi\rangle = |\psi(t)\rangle$, and given we know an initial state $|\psi(t_0)\rangle$, we can obtain the quantum state at any time t by solving eq. (3.19). The general solution is given by,

$$\left|\psi(t)\right\rangle = \exp\left(-\frac{i\hat{H}(t-t_0)}{\hbar}\right)\left|\psi(t_0)\right\rangle. \tag{3.20}$$

The solution for the state is much simpler if we work in the energy eigenbasis. If we work in an energy eigenbasis $\{|E_i\rangle\}$ in an energy spectrum $\{E_i\}$, and the initial state is defined,

$$\left|\psi(0)\right\rangle = \sum_i c_i\left|E_i\right\rangle \tag{3.21}$$

the general solution for the state at time t is,

$$\left|\psi(t)\right\rangle = \sum_i c_i \exp\left(-\frac{iE_it}{\hbar}\right)\left|E_i\right\rangle. \tag{3.22}$$

From this we can write postulate 3,

Postulate 3. *The time evolution of a closed quantum state is governed by the time dependent Schrodinger equation.*

$$i\hbar\frac{\mathrm{d}\left|\psi\right\rangle}{\mathrm{d}t} = \hat{H}\left|\psi\right\rangle \tag{3.23}$$

with solution,

$$\left|\psi(t)\right\rangle - \exp\left(-\frac{i\hat{H}t}{\hbar}\right)\left|\psi(0)\right\rangle \tag{3.24}$$

where $\hat{H}$ is a hermitian operator known as the Hamiltonain.

3.2.2 Time evolution of expectation values

The time evolution of quantum expectation is known as *Ehrenfest's theorem.* We first consider the hermitian conjugate of eq. (3.19),

$$-i\hbar\frac{\mathrm{d}\left\langle\psi\right|}{\mathrm{d}t} = \left\langle\psi\right|\hat{H}. \tag{3.25}$$

We have that the expectation value of an observable $\mathcal{A}$ is given by,

$$\left\langle\mathcal{A}\right\rangle = \left\langle\psi\right|\hat{A}\left|\psi\right\rangle. \tag{3.26}$$

Taking the time derivative,

$$\frac{\mathrm{d}\left\langle\mathcal{A}\right\rangle}{\mathrm{d}t} = \frac{\mathrm{d}\left\langle\psi\right|}{\mathrm{d}t}\hat{A}\left|\psi\right\rangle + \left\langle\psi\right|\hat{A}\frac{\mathrm{d}\left|\psi\right\rangle}{\mathrm{d}t} + \underbrace{\left\langle\psi\right|\frac{\mathrm{d}\hat{A}}{\mathrm{d}t}\left|\psi\right\rangle}_{0,\ \text{Operators are static}}. \tag{3.27}$$

By using eqs. (3.19) and (3.25), we can write eq. (3.27) by,

$$\frac{\mathrm{d}\left\langle\mathcal{A}\right\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\left\langle\psi\right|\left[\hat{H},\hat{A}\right]\left|\psi\right\rangle. \tag{3.28}$$

We then have that if $\hat{H}$ and $\hat{A}$ commute, i.e., $\left[\hat{H},\hat{A}\right]$, *the expectation of the observable is static.*

3.3 Composite Systems

We divide a system into component subsystems, and assign each of these their own configuration space. We denote the two states of the subsystems $|\psi\rangle$ and $|\phi\rangle$, then the combined state representing the system, $|\Psi\rangle$, is given by,

$$|\Psi\rangle = |\psi\rangle \otimes |\phi\rangle \tag{3.29}$$

where $\otimes$ is the *tensor product*.

If $|\psi\rangle$ is in a basis $\{|e_i\rangle\}$ and $|\phi\rangle$ is in a basis $\{|e_j\rangle\}$, then the basis of the combined state is $\{|e_i \otimes e_j\rangle\}$ over all possible configurations of i and j. This is easily extended for n subsystems.

We can extend the tensor product to operators. If we have two operators $\hat{A}_1$ and $\hat{A}_2$ which act on two different subsystems, we can write the operator acting on the total subsystem,

$$\hat{A} = \hat{A}_1 \otimes \hat{A}_2. \tag{3.30}$$

If we have an operator acting on only a single subsystem, we can find the total operator by performing the tensor product with the identity operator of the other subsystem,

$$\hat{A} = \hat{A}_1 \otimes \hat{I}_2. \tag{3.31}$$

This leads to the fourth postulate,

Postulate 4. *The state space of a composite physical system is the tensor product $\otimes$ of the component physical systems.*

3.3.1 Tensor product mathematics

We can more clearly see how to compute tensor products by considering vector and matrix representations. Suppose two vectors,

$$\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \qquad\qquad \mathbf{w} = \begin{pmatrix} w_1 & \dots & w_m \end{pmatrix} \tag{3.32}$$

their tensor product is computed by,

$$\mathbf{v} \otimes \mathbf{w} = \begin{pmatrix} v_1\mathbf{w} \\ \vdots \\ v_n\mathbf{w} \end{pmatrix} = \begin{pmatrix} v_1 w_1 & \dots & v_1 w_m \\ \vdots & \ddots & \\ v_n w_1 & & v_n w_m \end{pmatrix}. \tag{3.33}$$

Similarly for two matrices,

$$A = \begin{pmatrix} a_{11} & \dots & a_{1j} \\ \vdots & \ddots & \\ a_{i1} & & a_{ij} \end{pmatrix} \qquad\qquad B = \begin{pmatrix} b_{11} & \dots & a_{1l} \\ \vdots & \ddots & \\ b_{kl} & & a_{kl} \end{pmatrix} \tag{3.34}$$

we have,

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1j}B \\ \vdots & \ddots & \\ a_{i1}B & & a_{ij}B \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & \dots & a_{1j}b_{1l} \\ \vdots & \ddots & \\ a_{i1}b_{k1} & & a_{ij}b_{kl} \end{pmatrix}. \tag{3.35}$$

NOTE: We do not require our vectors or matrices to be the same size in order to perform the tensor product on them.

3.4 Entanglement

There are composite states in quantum mechanics which cannot be written as a product of states of each individual system, i.e., that can only be written as a superposition of basis states. These states are known as *entangled*, and the converse case is known as *seperable*.

We can perform measurements on single systems when in a composite system, however we must update the system afterwards. We do this by using projector of the outcome. Suppose $|\Phi\rangle$, written in a basis $\{|e_i\rangle \otimes |e_j\rangle\}$ is our composite system. The probability of an outcome $|e_1\rangle$ on state 1, we must find the expectation value of $|e_1\rangle\langle e_1| \otimes \hat{I}$ where $\hat{I}$ corresponds to the first system. The probability is then,

$$P(|e_1\rangle) = \langle\Psi|e_1\rangle\langle e_1| \otimes \hat{I}\,|\Psi\rangle\,. \tag{3.36}$$

Post-measurement, we use the projector to update the composite state, such that,

$$|\Psi\rangle \to |e_1\rangle\langle e_1| \otimes \hat{I}\,|\Psi\rangle\,. \tag{3.37}$$

NOTE: The state must be renormalised post-update.

Chapter 4

Higher Dimensional Systems

4.1 Positions and Wavefunctions

Let us consider a particle present in a region in the spacial x-axis between $-w$ and w. Let us consider splitting the x-axis between these points evenly into N regions. The width Δx of each region is given by,

$$\Delta x = \frac{2W}{N}. \tag{4.1}$$

Let us denote the basis state corresponding to each region as $|n\Delta x\rangle$, where $-N/2 \leq n \leq N/2 - 1$. The state of the particle is given by,

$$|\psi\rangle = \sum_{n=-N/2}^{N/2-1} a_{n\Delta x} \, |n\Delta x\rangle \, . \tag{4.2}$$

We have that, for small Δx, $a_{n\Delta x} \sim a_{(n+1)\Delta x}$. We then have that the probality of finding a particle in a given region,

$$P(n\Delta x) = |a_{n\Delta x}|^2 \tag{4.3}$$

scaled with Δx. We may wish to consider the probaility density, rather than the probaility, to describe our system,

$$p(n\Delta x) = \frac{|n\Delta x\rangle}{\Delta x}. \tag{4.4}$$

Let us re-define the un-normalised state,

$$|x_{n\Delta x}\rangle = \frac{|n\Delta x\rangle}{\sqrt{\Delta x}}. \tag{4.5}$$

We then have,

$$\begin{aligned} \langle n\Delta x | n'\Delta x\rangle &= \delta_{nn'} \\ \implies \langle x_{n\Delta x} | x_{n'\Delta x}\rangle &= \underbrace{\frac{\delta_{nn'}}{\Delta x}}_{\text{Dirac Delta}} \, . \end{aligned} \tag{4.6}$$

Let us then further define,

$$\psi_{n\Delta x} = \frac{a_n \Delta x}{\sqrt{\Delta x}}. \tag{4.7}$$

From eq. (4.2),

$$\langle x_{n\Delta x} | \psi\rangle = \frac{\langle n\Delta x | \psi\rangle}{\sqrt{\Delta x}} = \frac{a_n \Delta x}{\sqrt{\Delta x}} = \psi_{n\Delta x}. \tag{4.8}$$

From eq. (4.4), we have that,

$$p(n\Delta x) = |\psi_{n\Delta x}|^2 \, , \tag{4.9}$$

which, in the continuous limit becomes,

$$|\psi\rangle \approx \int \mathrm{d}x \, \psi(x) \, |x\rangle \, . \tag{4.10}$$

The overlap of two points on the x-axis is given by the dirac-delta function,

$$\langle x|x'\rangle = \delta(x - x'). \tag{4.11}$$

Taking the overlap of eq. (4.10) with $|x\rangle$ yields,

$$\boxed{\begin{aligned}\langle x|\psi\rangle &= \int \mathrm{d}x' \, \langle x|x'\rangle \, \psi(x') \\ &= \int \mathrm{d}x' \, \delta(x - x')\psi(x') = \psi(x).\end{aligned}} \tag{4.12}$$

The function $\psi(x)$ is an amplitude density known as the wavefunction. Using it, we are able to obtain the probability of finding the particle between two points,

$$\boxed{P(x_0 \leq x \leq x_1) = \int_{x_0}^{x_1} \mathrm{d}x \, |\psi(x)|^2 = \int_{x_0}^{x_1} \mathrm{d}x \, |\langle x|\psi\rangle|^2 .} \tag{4.13}$$

Let us state some properties of the wavefunction,

1. We require the wavefunction to be normalised, such that,

$$|\, \langle x|\psi\rangle \,|^2 = 1 \tag{4.14}$$

   or alternatively,

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x) \, \mathrm{d}x = 1. \tag{4.15}$$

2. For a wavefunction to be normalisable, it must satisfy the normalisation condition,

$$\lim_{x \to \pm x} (\psi(x)) = 0 \tag{4.16}$$

3. If ψ_1 and ψ_2 are both allowed, normalisable wavefunctions of a system, then,

$$\psi_3 = \alpha\psi_1 + \beta\psi_2 \tag{4.17}$$

   is also an allowed, normalisable wavefunction of the system.

4.2 Continuous Operators

Continuous operators are often differential operators. Below are some common continous operators,

1D Position Operator	3D Position Operator	1D Momentum Operator	3D Momentum Operator
$\hat{x} = x$	$\hat{x} = \mathbf{x}$	$\hat{p}_{1D} = -i\hbar\dfrac{\partial}{\partial x}$	$\hat{p}_{3D} = -i\hbar\boldsymbol{\nabla}$

it is opssible to construct other operators from these 4 basic operators, such as the Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{4.18}$$

which we can use to construct the continuous Schrodinger wave equation,

$$\hat{H}\psi(x) = E\psi(x) \tag{4.19}$$

4.2.1 Commutation relations

The following are the canonical commutation relations,

$$[\hat{x}, \hat{x}] = 0 \qquad\qquad [\hat{p}, \hat{p}] = 07 \, [\hat{x}, \hat{p}] = i\hbar. \tag{4.20}$$

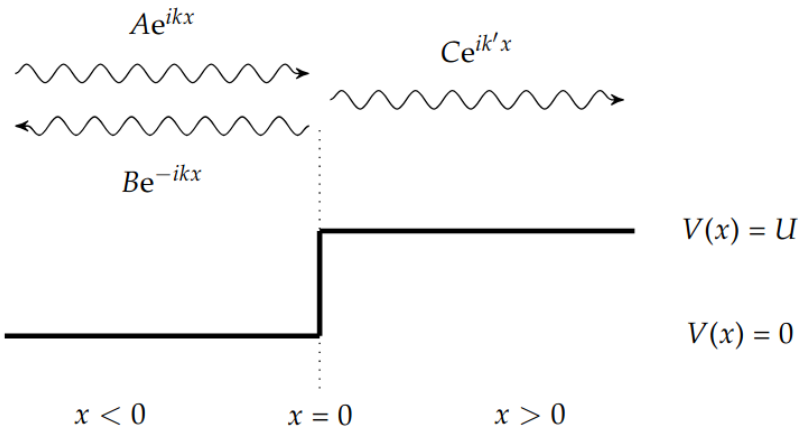

Figure 4.1

4.2.2 Hermitian Properties

Continous operators are also hermitina, i.e., $\hat{A}^\dagger = \hat{A}$. For a discrete system,

$$\left\langle \psi \middle| \hat{A}\phi \right\rangle = \left\langle \psi \hat{A}^\dagger \middle| \phi \right\rangle = \left\langle \hat{A}\psi \middle| \phi \right\rangle \tag{4.21}$$

and similarly for a continuous one,

$$\int_{-\infty}^{\infty} \psi^* \hat{A}\phi \, \mathrm{d}x = \int_{-\infty}^{\infty} (\hat{A}^\dagger \psi)^* \phi \, \mathrm{d}x = \int_{-\infty}^{\infty} (\hat{A}\psi)^* \phi \, \mathrm{d}x \,. \tag{4.22}$$

4.3 Equation of a free particle

If we consider a free particle, i.e., without any potential acting on it, we can write the energy eigen-value equation using the Hamiltonian (eq. (4.18)),

$$-\frac{\hbar^2}{2m}\frac{\partial \psi(x)}{\partial x} = E\psi x. \tag{4.23}$$

If we write E as,

$$E = \frac{k^2\hbar^2}{2m} = \frac{p^2}{2m} \tag{4.24}$$

where k is the wavenumber of our wavefunction. We then obtain a wavefunction for a free particle by a standard solution to the wave equation,

$$\psi(x) = e^{ikx} = e^{\frac{ip}{\hbar}x}. \tag{4.25}$$

NOTE: This wavefunction is different as it is not normalisable. however it is still allowed to exist.

4.3.1 Scattering of free particles

Let us now consider a particle beam travelling in space under a potential,

$$V(x) = \begin{cases} 0 & x < 0 \\ U & x \geq 0 \end{cases} \tag{4.26}$$

with an intial wavefunction,

$$\psi(x) = Ae^{ikx} \tag{4.27}$$

where it will encounter a potential step at $x = 0$, as in fig 4.1 We will have a reflected solution for $x < 0$, and a solution where the wave travels past the potential step. We can sum up this wave equation as,

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Xe^{ik'x} & x \geq 0 \end{cases}. \tag{4.28}$$

We have a different wavenumber in the region $x \geq 0$ which is related to the potential. We can define this as,

$$E - U = \frac{\hbar^2 k'^2}{2m} \qquad \sqrt{k' = \frac{2m(E-U)}{\hbar^2}}. \tag{4.29}$$

For conservation of energy, we require boundary conditions which state,

$$\psi(0) \text{ is continuous} \tag{4.30}$$

$$\left.\frac{\partial \psi(x)}{\partial x}\right|_0 \text{ is continuous.} \tag{4.31}$$

Applying eq. (4.30),

$$A + B = C \tag{4.32}$$

and applying eq. (4.31),

$$ik(A - B) = ik'C. \tag{4.33}$$

We then have the relations,

$$B = \frac{k - k'}{k + k'}A \qquad C = \frac{2k}{k + k'}A. \tag{4.34}$$

It is tempting to use eq. (4.34) in order to describe the probability of the particle beam becoming reflected off the potential step. However, given that this is a particle beam, we must instead consider the particle flux in order to calculate probabilities. These fluxes are equivalent to the *probability current*,

$$\boxed{j = -\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)}. \tag{4.35}$$

We can then define the Reflection and Transmission ratios by,

$$\boxed{\mathcal{R} = \frac{j_{\text{ref}}}{j_{\text{inc}}} = \frac{(k-k')^2}{(k+k')^2}} \qquad \boxed{\mathcal{T} = \frac{j_{\text{trans}}}{j_{\text{inc}}} = \frac{4kk'}{(k+k')^2}} \tag{4.36}$$

which further satisfy $\mathcal{R} + \mathcal{T} = 1$.

4.4 Bound Particles

4.4.1 Infinite Potential Well

Consider the potential,

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{Otherwise} \end{cases}. \tag{4.37}$$

The Schrodinger equation in this case is identical to that of the free particle,

$$-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}|\psi\rangle = E|\psi\rangle \tag{4.38}$$

but subject to the boundary conditions,

$$\psi(x) = 0 \text{ for } x \leq 0, x \geq 0. \tag{4.39}$$

Considering the general solution to the wave equation,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{4.40}$$

and applying the boundary condition at $x = 0$, we find $A = -B$, and,

$$\psi(x) = A(e^{ikx} - e^{-ikx}) = 2Ai \sin kx. \tag{4.41}$$

Applying the boundary condition at $x = L$, we find that the wavenumber is quantised, so that we have integer number of wavelengths,

$$k = \frac{n\pi}{L} \quad n \in \mathbb{Z}^+. \tag{4.42}$$

We are then able to normalise the wavefunction to,

$$\psi(x) = \sqrt{\frac{2}{L}} \sin(kx). \tag{4.43}$$

We can then find the quantised energy Eigenstates,

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{4.44}$$

which correspond to the normal modes of the wavefunction.

4.4.2 Potential Barriers

For a potential step, we have that there is a probability that the particle will be found within the potential barrier, such that $\psi(x) \propto e^{-\eta x}$. However, the particle current in the region inside the barrier is 0.

4.4.3 Finite Potential Wells

For a finite potential well, when the particle is at an energy $0 < E < -U$, we find that the general wavefunction is given by odd and even wavefunctions,

$$\psi(x)_{\text{odd}} = \begin{cases} Ae^{\eta x} & x < -a \\ \cos kx & |x| < a \\ Be^{-\eta x} & x > a \end{cases}, \qquad \psi(x)_{\text{even}} = \begin{cases} Ae^{\eta x} & x < -a \\ \sin kx & |x| < a \\ -Be^{-\eta x} & x > a \end{cases}. \tag{4.45}$$

we have that,

$$k^2 = \frac{2m(E-U)}{\hbar^2} \qquad \nu^2 = -\frac{2mE}{\hbar^2}. \tag{4.46}$$

which we can relate by,

$$\boxed{k^2 + \eta^2 \frac{2mU}{\hbar^2}}. \tag{4.47}$$

By considering the continuity boundary conditions, we find that,

$$\boxed{k \tan(ka) = \eta}. \tag{4.48}$$

We require both eq. (4.47) and eq. (4.48) to be solutions. However, no analytical soluton exists. We must then use a graphical solution, as in figure 4.2. The amount of points of interesection represent the number of solutions for the potential well, which indicate the number of eigenstates.

4.5 Expectation Values

Recall the procedure for findng the expectation value of an observable for a discrete system,

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle. \tag{4.49}$$

We can extend this to a continuous system,

$$\boxed{\langle \hat{x} \rangle = \int_{-\infty} \psi^* \hat{x} \psi \, \mathrm{d}x}. \tag{4.50}$$

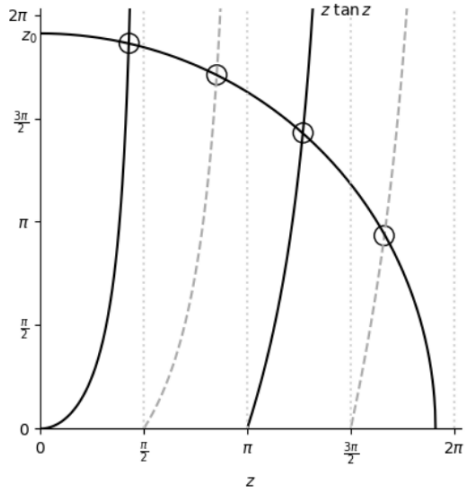

Figure 4.2: Dashes lines represent odd solutions.

4.5.1 Expectation Position of an Infinite Potential Well

Let us state the position expectation value for position (computation is trivial),

$$\frac{L}{2} = \langle \hat{x} \rangle \,. \tag{4.51}$$

Let us note that the expectation value is independent of the wavenumber, implying that the expectation value for a particle is the same for all energy states.

4.6 Time Evolution

If we have an intial wavefunction $\psi(x) \equiv \psi(x, t = 0)$, with energy eigenfucntions $\{\psi_n(x)\}$, we can rewrite the time independent wavefunction as a sum of weighted eigenfunctions,

$$\psi(x) = \sum_n c_n \phi_n(x) \tag{4.52}$$

where the coefficient c_n is determined by,

$$c_n = \langle \phi_n | \psi \rangle = \int_{-\infty}^{\infty} \phi_n^* \psi \, \mathrm{d}x \,. \tag{4.53}$$

We can describe the time evolution of the wavefunction by first considering the time evolution of the energy eigenfunctions, which is given trivially by the time-dependent Schoridinger equation, as in the discrete case,

$$\phi_n(x, t) = \phi_n(x) e^{-\frac{iE_n t}{\hbar}} \tag{4.54}$$

and thus, the time evolution of the wavefunction as a whole is given by,

$$\psi(x, t) = \sum_n c_n \phi_n(x, 0) e^{-\frac{iE_n t}{\hbar}} \,. \tag{4.55}$$

4.6.1 Time evolution of expectation values

We can simply calculate the time evolved expectation value by considering the inner produce of the time evolved wavefunction,

$$\langle \hat{x} \rangle (t) = \langle \psi(t) | \, \hat{x} \, | \psi(t) \rangle \,. \tag{4.56}$$

4.7 Simple Harmonic Oscillator

The potentials which we have studied are often not as simple. We often wish to study arbitrary potentials $V(x)$, however the Hamiltonian concerning arbitrary potentials are very difficult to solve. We often employ approximations of continuous potentials, particularly about stationary points x_0,

$$V(x-x_0) = V(x_0) + (x-x_0)\cancelto{0}{\frac{\mathrm{d}V}{\mathrm{d}x}\bigg|_{x_0}} + \frac{1}{2}(x-x_0)^2\,\frac{\mathrm{d}V}{\mathrm{d}x}\bigg|_{x_0} + \cdots \tag{4.57}$$

We can neglect the offset of our expansion, which leads to the first term of the expansion to be the quadratic term, which results in the approximation being a *harmonic oscillator*.

We can write the hamiltonina of the harmonic oscillator,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{4.58}$$

This Hamiltonian is very difficult to solve by itself. We can instead reformulate it in terms of the lowering and raising operators, defined by,

$$\hat{a}_+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right) \qquad \text{Raising} \tag{4.59}$$

$$\hat{a}_+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right) \qquad \text{Lowering} \tag{4.60}$$

Let us notice that $\hat{a}_+$ is the Hermitian conjuage of $\hat{a}_-$ and vice versa. Using these definitions, we can rewrite the position and momentum operators,

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}\,(\hat{a}_+ + \hat{a}_-)} \qquad\qquad \hat{p} = \sqrt{\frac{\hbar m\omega}{2}\,(\hat{a}_+ - \hat{a}_-)} \tag{4.61}$$

Let us analyse the behaviour of $\hat{a}_+\hat{a}_-$,

$$\begin{aligned}\hat{a}_+\hat{a}_- &= \frac{m\omega}{2\hbar}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)\\ &= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{i}{m\omega}\underbrace{[\hat{x}\hat{p} - \hat{p}\hat{x}]}_{[\hat{x},\hat{p}]=i\hbar} + \frac{\hat{p}^2}{m^2\omega^2}\right).\end{aligned} \tag{4.62}$$

Thus, we can write the Hamiltonian,

$$\hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right). \tag{4.63}$$

Let us now consider the behavour of the lowering and raising operators. We must impose the ladder termination condition on the lowering operator, which states that when acting on a ground state $|0\rangle$,

$$\boxed{\hat{a}_-\,|0\rangle = 0}. \tag{4.64}$$

The lowering and raising operators general have a behaviour,

$$\hat{a}_\pm\,|n\rangle \to |n \pm 1\rangle\,. \tag{4.65}$$

Let us keep in mind that $\langle n|n\rangle = 1$, so we require the lowering and raising operators to preserve normalisation. We then require,

$$\begin{gathered}\langle n-1|n-1\rangle = \langle n|\,\hat{a}_+\hat{a}_-\,|n\rangle = 1\\ \langle n|\,n\,|n\rangle = n\,\langle n|n\rangle = 1\end{gathered} \tag{4.66}$$

thus the normalisation conditions are,

$$\hat{a}_- |n\rangle = \sqrt{n}\,|n-1\rangle \tag{4.67}$$
$$\hat{a}_+ |n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{4.68}$$

We can define a Hermitian operator $\hat{N}$,

$$\hat{a}_+\hat{a}_- = \hat{N} \tag{4.69}$$

which behaves,

$$\hat{N}\,|n\rangle = n\,|n\rangle \tag{4.70}$$

i.e., it tells you the energy level of the observed state.

4.7.1 Energy Eigenstates of the Simple Harmonic Oscillator

Analysing the Hamiltonian more closely, if we attempt to act on an nth energy eigenstate,

$$\begin{aligned}\hat{H}\,|n\rangle &= \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)|n\rangle \\ &= \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle\end{aligned} \tag{4.71}$$

therefore, the energy of the nth eigenstate is given by,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad n \in \mathbb{Z}^+. \tag{4.72}$$

Let us now analyse the eigenfunctions of the harmonic oscillator. We have that,

$$\hat{a}_-\phi_0(x) = 0 \tag{4.73}$$

where $\phi_0(x)$ indicates the ground state of the energy eigenfunction. We then have,

$$\begin{aligned}\frac{\partial}{\partial x}\phi_0(x) &= -\frac{m\omega}{\hbar}x\phi_0(x) \\ \implies \phi_0(x) &= Ae^{-\alpha x^2}\end{aligned} \tag{4.74}$$

by inspection. By normalising the wavefunction, we find that the ground energy eigenfunction is given by,

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}. \tag{4.75}$$

Subsequent energy eigenfunctions can be found by using the raising operator.

4.7.2 Matrix Treatment of the Simple Harmonic Oscillator

We can find the matrix form of the raising and lowering operators by considering,

$$\begin{aligned}\langle n|\,\hat{a}_-\,|m\rangle &= \langle n|\,\sqrt{m}\,|m-1\rangle \\ &= \sqrt{m}\,\langle n|m-1\rangle \\ &= \sqrt{m}\delta_{n(m-1)}\end{aligned} \tag{4.76}$$

which we can write in matrix form,

$$a_- = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{4.77}$$

Similarly for the raising operator,

$$a_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & \ddots & \\ \vdots & \vdots & \vdots & & \ddots \end{pmatrix} \tag{4.78}$$

From this, we can find the matrix form of the momentum operator by eq. (4.61),

$$p = \sqrt{\frac{\hbar m\omega}{2}} \begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & \cdots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & \cdots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & \cdots \\ 0 & 0 & i\sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & & \ddots \end{pmatrix} \tag{4.79}$$

4.8 First Order Perturbation Theory

For non-trivial potentials, we can make a first order approximation if the potential can be described as a trivial potential summed with a perturbation. For a potential with energy levels E_n which can be approximated some 0^{th} order potential with energy levels $E_n^{(0)}$ and energy eigenstates $\left|n^{(0)}\right\rangle$, plus some perturbation $\hat{H}$, the energy levels of the potential is given by,

$$E_n = E_n^{(0)} + \left\langle n^{(0)} \right| \hat{H} \left| n^{(0)} \right\rangle . \tag{4.80}$$

Appendix A

Matrix Mathematics

A.1 Eigenvalues and Eigenvectors

For a matrix A, there exists a set of eigenvectors $\{\mathbf{v}_i\}$ which are *invariant* under the transformation by the matrix, other than by scaling of the set of eigenvalues $\{\lambda_j\}$. This can be satisfied by,

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{A.1}$$

If two or more eigenvectors share an eigenvalue they are *degenerate*.

Suppose a matrix A with eigenvalue $\{\lambda_j\}$ and eigenvectors $\{\mathbf{v}_i\}$. $\forall$ scalars a,

$$A\mathbf{v} + aI\mathbf{v} = (\lambda + a)\,\mathbf{v}. \tag{A.2}$$

We can then calculate eigenvalues by,

$$\det\{A - \lambda I\} = 0 \tag{A.3}$$

from which the corresponding eigenvectors can be found.

If a matrix A and its eigenvalues λ is raised to some power n, then the eigenvalues of the exponentiated matrix correspond to λ raised to the power n. Or,

$$A^n\mathbf{v} = \lambda^n\mathbf{v}. \tag{A.4}$$

For a diagonalised matrix, its eigenvalues correspond to the values on the diagonal, and its eigenvectors are the basis vectors of the space.

A.2 Hermitian Matrices

A Hermitian matrix H is one that is invariant under a Hermitian conjugate, i.e.,

$$H^\dagger = H. \tag{A.5}$$

Property 1: *The eigenvalues of a Hermitian matrix are real.*

Proof. Consider a Hermitian matrix H. Take the Hermitian conjugate of its eigenvectors,

$$H^\dagger\mathbf{v}^\dagger = \lambda^*\mathbf{v}^\dagger. \tag{A.6}$$

Since H is hermitian, then,

$$\mathbf{v}^\dagger H = \lambda^*\mathbf{v}^\dagger. \tag{A.7}$$

Now consider,

$$\mathbf{v}^\dagger H\mathbf{v} = \lambda\mathbf{v}^\dagger\mathbf{v} \tag{A.8}$$

and taking the conjugate,

$$\mathbf{v}^\dagger H\mathbf{v} = \lambda^*\mathbf{v}^\dagger\mathbf{v}. \tag{A.9}$$

We can equate eqs. (A.8) and (A.9),

$$\lambda\mathbf{v}^\dagger\mathbf{v} = \lambda^*\mathbf{v}^\dagger\mathbf{v}. \tag{A.10}$$

If $\mathbf{v}$ is non-trivial, $\lambda = \lambda^* \therefore \lambda \in \mathbb{R}$. □

Property 2: *The eigenvectors of a Hermitian matrix corresponding to different eigenvalues are orthogonal.*

Proof. Let λ_1 and λ_2 be the eigenvalues of a Hermitian matrix H, with eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$ respectively. We have,

$$\mathbf{v}_2^\dagger H \mathbf{v}_1 = \lambda_1 \mathbf{v}_2^\dagger \mathbf{v}_1 \tag{A.11}$$

$$\mathbf{v}_1^\dagger H \mathbf{v}_2 = \lambda_2 \mathbf{v}_1^\dagger \mathbf{v}_2. \tag{A.12}$$

Taking the Hermitian conjugate of eq. (A.12),

$$v_2^\dagger H \mathbf{v}_1 = \lambda_2 \mathbf{v}_2^\dagger \mathbf{v}_1. \tag{A.13}$$

Equating eqs. (A.11) and (A.13),

$$\lambda_1 \mathbf{v}_2^\dagger \mathbf{v}_1 = \lambda_2 \mathbf{v}_2^\dagger \mathbf{v}_1. \tag{A.14}$$

Given $\lambda_1 \neq \lambda_2$, we require $\mathbf{v}_2^\dagger \mathbf{v}_1 = 0 \therefore \mathbf{v}_1$ and $\mathbf{v}_2$ are orthogonal. □

A consequence of of property 2 is that a Hermitian matrix can always be diagonalised under a basis transformation.

Appendix B

Postulates of Quantum Mechanics

Below are all the postulates of quantum mechanics, stated in full.

1. The quantum state $|\psi\rangle$ of a system is represented by a normalised vector witih complex elements.

2. A measurement $\mathcal{M}$ of a quantum system is a set of Hermitian linear operators $\left\{\hat{M}_i\right\}$ with non-negative eigenvalues taht satisfy
$$\sum_i \hat{M}_i = \hat{I}. \tag{B.1}$$
The born rule states that the probability of obtaining an outcome i when in state ψ is,
$$P(i) = \langle\psi| \hat{M}_i |\psi\rangle . \tag{B.2}$$

3. The time evolution of a closed quantum system is governed by the Schroedinger equation,
$$i\hbar \frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = \hat{H}|\psi\rangle \tag{B.3}$$
where $\hat{H}$ is a Hermitian operator known as the Hamiltonian. The Schroedinger equation has solution,
$$|\psi(t)\rangle = \exp\left(-i\frac{\hat{H}(t-t_0)}{\hbar}\right)|\psi(t_0)\rangle . \tag{B.4}$$

4. The state space of a composite physical system is the tensor product $\otimes$ of the component physical systems.