Quantum Dynamics

Tom Charnock

Contents

Chapter 1

Wave Mechanics

1.1 Wavefunction $\psi(x, y, z, t)$

The wavefunction of a quantum particle is defined by $\psi(x, y, z, t)$. It is a complex function which contains the most complete description available of the state of a particle. Physical interpretation of the wavefunction is given by the probability of finding a particle at a certain position.

$$\mathcal{P}(\underset{\sim}{r}, t)\delta^3\underset{\sim}{r} = |\psi(\underset{\sim}{r}, t)|^2\delta^3\underset{\sim}{r}$$

Where $\delta^3\underset{\sim}{r}$ is a volume element about $\underset{\sim}{r} = (x, y, z)$. Integrating this over all space must be equal to one and so the wavefunction must be integrable square, with a normalisation constant.

$$\int \delta^3\underset{\sim}{r}|\psi|^2 = 1$$

Any other integral which does not agree with this cannot be a wavefunction.

$$\psi \to 0 \, as \, x \to \pm\infty$$

1.2 Dynamics

The wavefunction evolves according the Schrdingers equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{\mathcal{H}}\psi$$

Where $\widehat{\mathcal{H}}$ is the Hamiltonian operator:

$$\widehat{\mathcal{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{r}, t)$$

The Schrdinger equation is linear so that is ψ_1 and ψ_2 are both solutions then $\psi = a\psi_1 + b\psi_2$, where a and b are complex numbers, must also be a solution. This is the principle of superposition. Since probability is conserved then:

$$\frac{\partial}{\partial t}\int \delta^3\underset{\sim}{r}|\psi|^2 = 0$$

This sets a condition on the form of $\widehat{\mathcal{H}}$. The complex conjugate of the Schrdinger equation is:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = \left[\widehat{\mathcal{H}}\psi\right]^*$$

This leads to:

$$\frac{\partial}{\partial t}\int \delta^3\underset{\sim}{r}\psi^*\psi = \int \delta^3\underset{\sim}{r}\left[\psi^*\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}\psi\right]$$

Schrdingers equation can be substituted in to give:

$$0 = \frac{1}{i\hbar}\int \delta^3\underset{\sim}{r}\left[\psi^*\widehat{\mathcal{H}}\psi - \left[\widehat{\mathcal{H}}\psi\right]^*\psi\right]$$

This means that the conjugate of the Hamiltonian must be equal and opposite to the Hamiltonian. In other words the Hamiltonian must be Hermitian. In wave mechanics a Hermitian operator $\widehat{\mathcal{O}}$ is one where:

$$\int \delta^3 \underset{\sim}{r} \psi_1^* \widehat{\mathcal{O}} \psi_2 = \int \delta^3 \underset{\sim}{r} \left[\widehat{\mathcal{O}} \psi_1 \right]^* \psi_2$$

Using the momentum operator $\widehat{p} = -i\hbar \frac{\delta}{\delta x}$ with any two physical wavefunctions ψ_1 and ψ_2:

$$\int_{-\infty}^{\infty} \delta x \psi_1^* \left(-i\hbar \frac{\delta}{\delta x} \right) \psi_2$$

Integrate by parts to give:

$$-i\hbar \int_{-\infty}^{\infty} \delta x \psi_1^* \frac{\delta \psi_2}{\delta x}$$

This can be expanded to:

$$-i\hbar \int_{-\infty}^{\infty} \delta x \frac{\delta}{\delta x} \left(\psi_1^* \psi_2 \right) + i\hbar \int_{-\infty}^{\infty} \delta x \left(\frac{\delta \psi_1^*}{\delta x} \right) \psi_2$$

This is the same as:

$$\int_{-\infty}^{\infty} \delta x \left[\widehat{p} \psi_1 \right]^* \psi_2$$

This is the definition of a Hermitian operator.

1.3 Operators and Expectation Values

Observable quantities are represented by linear, Hermitian operators in quantum mechanics. Some examples are the position operator $\widehat{\underset{\sim}{r}} = \underset{\sim}{r}$, the momentum operator $\widehat{\underset{\sim}{p}} = -i\hbar\nabla$ and the Hamiltonian operator $\widehat{\mathcal{H}}$. The ordering of operators must be followed because some of the operators may not commute. Average results of a series of measurements of an observable $\mathcal{A}$, is represented by $\widehat{\mathcal{A}}$ and is given by an expectation value:

$$\left\langle \widehat{\mathcal{A}} \right\rangle = \int \delta^3 \underset{\sim}{r} \psi^* \widehat{\mathcal{A}} \psi$$

The expectation value of an observable must be real. This means that:

$$\left\langle \widehat{\mathcal{A}} \right\rangle = \left[\left\langle \widehat{\mathcal{A}} \right\rangle \right]^*$$

It can be seen that:

$$\int \delta^3 \underset{\sim}{r} \psi^* \widehat{\mathcal{A}} \psi = \int \delta^3 \underset{\sim}{r} \left(\widehat{\mathcal{A}} \psi \right)^* \psi$$

This is the definition of a Hermitian operator. For an operator $\widehat{\mathcal{B}}$, a Hermitian conjugate operator can be defined as $\widehat{\mathcal{B}}^\dagger$. This is:

$$\int \delta^3 \underset{\sim}{r} \psi_1^* \widehat{\mathcal{B}}^\dagger \psi_2 = \int \delta^3 \underset{\sim}{r} \left[\widehat{\mathcal{B}} \psi_1 \right]^* \psi_2$$

For a Hermitian operator $\widehat{\mathcal{A}}^\dagger = \widehat{\mathcal{A}}$.

1.4 Time-Independent Schrdinger Equation

If the Hamiltonian Operator is independent of time then the wavefunction can be written as:

$$\Psi(\underset{\sim}{r}, t) = \psi(\underset{\sim}{r}) e^{-\frac{iEt}{\hbar}}$$

This means that the Schrdinger equation can be written as an eigenfunction equation, with $\psi_n(\underset{\sim}{r})$ as the eigenfunction and E_n as the corresponding eigenvalue.

$$i\hbar \frac{\partial \Psi}{\partial t} = E\psi(\underset{\sim}{r}) e^{-\frac{iEt}{\hbar}} = \widehat{\mathcal{H}} \psi(\underset{\sim}{r}) e^{-\frac{iEt}{\hbar}}$$

$$\widehat{\mathcal{H}} \psi_n = E_n \psi_n$$

As $\widehat{\mathcal{H}}$ is Hermitian then E_n is real.

Degeneracy

Sometimes there is more than one eigenfunction corresponding to the same eigenvalue. This is know as degeneracy.

Normalisation

The eigenfunctions can be normalised such that any two different eigenfunctions are orthonormal:

$$\int \delta^3 \underset{\sim}{r} \psi_n^* \psi_m = \delta_{nm}$$

This is true in both non-degenerate and degenerate cases. It can be seen by expanding the time-independent Schrdinger equation that:

$$(E_m - E_n) \int \delta^3 \underset{\sim}{r} \psi_n^* \psi_m = 0$$

All observable operators follow the rules that for an observable $\mathcal{A}$, the operator, $\widehat{\mathcal{A}}$, must be Hermitian, the eigenvalues, a_n must be real with eigenfunctions, u_n, which are orthonormal.

Dirac δ Function

For an operator with continuous eigenvalues (non-discrete) the Dirac δ function is used. As the Dirac δ function is:

$$\int_{-\infty}^{\infty} \delta q \delta(q - q_o) f(q) = f(q_o)$$

Then the orthonormal condition gives that:

$$\int \delta q \varphi_\beta^*(q) \varphi_{\beta'}(q) = \delta(\beta - \beta')$$

Eigenfunctions of an operator corresponding to an observable are postulated to form a complete set. This means that any physically acceptable wavefunction as a superposition of the eigenfunctions is $\widehat{\mathcal{H}} \psi_n = E_n \psi_n$. For any wavefunction $\Phi(\underset{\sim}{r}, t)$ then $\Phi(\underset{\sim}{r}, t) = \sum_n c_n(t) \psi_n(\underset{\sim}{r})$ can be written as the sum of the eigenfunction. $c_n(t)$ are the probability amplitudes, which are in general, time dependent and complex. The sum takes place over all the eigenfunctions of $\widehat{\mathcal{H}}$ when ψ_n is chosen to be orthonormal.

$$\int \delta^3 \underset{\sim}{r} \Phi^*(\underset{\sim}{r}, t) \Phi(\underset{\sim}{r}, t) = \sum_n \sum_m c_n^*(t) c_m(t) \int \delta^3 \underset{\sim}{r} \psi_n^*(\underset{\sim}{r}) \psi_m(\underset{\sim}{r})$$

As $\int \delta^3 \underset{\sim}{r} \psi_n^*(\underset{\sim}{r}) \psi_m(\underset{\sim}{r}) = \delta_{nm}$ then the only time the sum can occur is when $m = n$ and so the sum becomes:

$$\int \delta^3 \underset{\sim}{r} \Phi^*(\underset{\sim}{r}, t) \Phi(\underset{\sim}{r}, t) = \sum_n c_n^*(t) c_n(t) = \sum_n |c_n(t)|^2$$

For normalised wavefunctions $\sum_n |c_n(t)|^2 = 1$. Because ψ_n are orthonormal:

$$c_R(t) = \int \delta^3 \underset{\sim}{r} \psi_R^*(\underset{\sim}{r}) \Phi(\underset{\sim}{r}, t)$$

Where $\Phi(\underset{\sim}{r}, t) = \sum_n c_n(t) \psi_n(t)$. This can be substituted to give:

$$\Phi(\underset{\sim}{r}, t) = \sum_n \int \delta^3 \underset{\sim}{r}' \psi_n^*(\underset{\sim}{r}') \psi_n(\underset{\sim}{r}) \Phi(\underset{\sim}{r}', t)$$

From this can be found the completeness relation:

$$\sum_n \psi) n^*(\underset{\sim}{r}') \psi_n(\underset{\sim}{r}) = \delta(\underset{\sim}{r} - \underset{\sim}{r}')$$

1.5 Measurement Postulate

If an observable is measured with a Hermitian operator, $\widehat{\mathcal{A}}$, which has eigenfunctions u_n and eigenvalues a_n, the result will be one of the eigenvalues. For a system in a state $\psi(\underset{\sim}{r}, t) = \sum_n c_n(t)u_n$ and the probability of getting a particular result a_j is $\mathcal{P} = |c|^2$ for a normalised ψ. Immediately after getting a result a_j, the system will definitely be in the eigenstate u_j. The wavefunction is said to collapse. Non-commuting operations have different eigenfunctions. There cannot be a state where both quantities have a definite value.

1.6 Heisenberg's Uncertainty Principle

The product of uncertainty of any two, non-commuting quantities has a minimum value. Uncertainty is given by:

$$\Delta\mathcal{A} = \sqrt{\left\langle \widehat{\mathcal{A}}^2 \right\rangle - \left\langle \widehat{\mathcal{A}} \right\rangle^2}$$

The uncertainty depends on the state of the system $\psi = u_n$. For an eigenstate of an operator $\widehat{\mathcal{A}}$

$$\left\langle \widehat{\mathcal{A}} \right\rangle = \int u_n^* \widehat{\mathcal{A}} u_n \delta^3 \underset{\sim}{r} = a_n$$

$$\left\langle \widehat{\mathcal{A}}^2 \right\rangle = \int u_n^* \widehat{\mathcal{A}}^2 u_n \delta^3 \underset{\sim}{r} = a_n^2$$

$$\left\langle \widehat{\mathcal{A}}^2 \right\rangle - \left\langle \widehat{\mathcal{A}} \right\rangle^2 = a_n^2 - (a_n)^2 = 0$$

This means that there is no uncertainty in the state, where the state is an eigenfunction of the operator. It can be shown that for any two operators $\widehat{\mathcal{A}}$ and $\widehat{\mathcal{B}}$ then the uncertainty is:

$$\Delta\mathcal{A}^2\Delta\mathcal{B}^2 \geq -\frac{\left(\langle\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]\rangle\right)^2}{4}$$

For the position and momentum operators the commutator is $[\widehat{x}, \widehat{p}_x] = i\hbar$. This means that $\langle i\hbar\rangle = i\hbar$ and so the uncertainty is:

$$\Delta x^2 \Delta p_x^2 \geq -\frac{(i\hbar)^2}{4}$$

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Chapter 2

Dirac Notation

Dirac's notation allows both spin systems and wave mechanics to be described in the same formulation.

2.1 Spin

2.1.1 Ket and Bra

The state of a spin $\frac{1}{2}$ system is described by a spinor $\underset{\sim}{\psi} = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ where α and β are complex numbers. Dirac's notation describes the spinor as a "ket":

$$\underset{\sim}{\psi} = |\psi\rangle$$

The conjugate of the spinor is $\underset{\sim}{\psi}^\dagger = \begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}$, which is denoted by a "bra":

$$\underset{\sim}{\psi}^\dagger \equiv \langle\psi|$$

2.1.2 Scalar Product

The scalar product of two spinors $\underset{\sim}{\psi} = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ and $\underset{\sim}{\varphi} = \begin{pmatrix}a\\ b\end{pmatrix}$ is $\underset{\sim}{\varphi}^\dagger\underset{\sim}{\psi} = a^*\alpha + b^*\beta$. In Dirac notation the scalar product is given by a "bracket".

$$\underset{\sim}{\varphi}^*\underset{\sim}{\psi} \equiv \langle\varphi|\psi\rangle$$

Which is a complex number.

2.1.3 Operators

Operators on spinors are matrices $\widetilde{M}\underset{\sim}{\psi} = \underset{\sim}{(M\psi)}$, where a new spinor is created. The operator in Dirac notation is the same as an operator in wave mechanics.

$$\widehat{\mathcal{M}}|\psi\rangle = |\mathcal{M}\psi\rangle$$

If $\widehat{\mathcal{M}}|\psi\rangle = m|\psi\rangle$ then $|\psi\rangle$ is and eigenket of $\widehat{\mathcal{M}}$ and m is the associated eigenvalue.

2.1.4 Expectation Values

For expectation values then:

$$\underset{\sim}{\psi}^\dagger\widetilde{M}\underset{\sim}{\psi} \equiv \langle\psi|\widehat{\mathcal{M}}|\psi\rangle = \langle\psi|\mathcal{M}\psi\rangle$$

Which more generally can be written for two different spinors:

$$\underset{\sim}{\varphi}^\dagger\widetilde{M}\underset{\sim}{\psi} \equiv \langle\varphi|\widehat{\mathcal{M}}|\psi\rangle$$

The ket can be thought of as a vector which is able to have an infinite number of components.

2.2 Wave Mechanics

2.2.1 Scalar Product

In wave mechanics the scalar product is given by:

$$\int \delta^3\underset{\sim}{r}\psi_1^*(\underset{\sim}{r})\psi_2(\underset{\sim}{r}) = \text{complex number}$$

Which is written in Dirac notation as it was for the scalar product in the spin system:

$$\int \delta^3\underset{\sim}{r}\psi_1^*(\underset{\sim}{r})\psi_2(\underset{\sim}{r}) \equiv \langle\psi_1|\psi_2\rangle$$

When finding the complex conjugate of the scalar product then:

$$[\langle\psi_1|\psi_2\rangle]^* = \langle\psi_2|\psi_1\rangle$$

And the scalar product of a state with itself is:

$$\int \delta^3\underset{\sim}{r}\psi^*\psi = \int \delta^3\underset{\sim}{r}|\psi|^2 \equiv \langle\psi|\psi\rangle$$

This must be a real, positive number which is equal to one when $|\psi\rangle$ is normalised.

2.2.2 Adding

When adding two kets then a third ket is made.

$$|\mathcal{A}\rangle = b|\mathcal{B}\rangle + c|\mathcal{C}\rangle$$

And the bra associated with $|\mathcal{A}\rangle$ is:

$$\langle\mathcal{A}| = b^*\langle\mathcal{B}| + c^*\langle\mathcal{C}|$$

It does not matter if the complex number is in front of or behind the bra or ket. The scalar product of the additions is:

$$\langle\mathcal{A}|\mathcal{A}\rangle = [b^*\langle\mathcal{B}| + c^*\langle\mathcal{C}|]\,[b|\mathcal{B}\rangle + c|\mathcal{C}\rangle]$$

This can be expanded by normal algebraic rules and rearranged to give:

$$\langle\mathcal{A}|\mathcal{A}\rangle = |b|^2\langle\mathcal{B}|\mathcal{B}\rangle + 2\Re\,[b^*c\langle\mathcal{B}|\mathcal{C}\rangle] + |c|^2\langle\mathcal{C}|\mathcal{C}\rangle$$

2.2.3 Hermitian Conjugation

The definition of a Hermitian conjugate in wave mechanic is:

$$\int \delta^3\underset{\sim}{r}\varphi^*(\underset{\sim}{r})\widehat{\mathcal{B}}^\dagger\psi(\underset{\sim}{r}) = \int \delta^3\underset{\sim}{r}\left[\widehat{\mathcal{B}}\varphi(\underset{\sim}{r})\right]^*\psi(\underset{\sim}{r})$$

This can be written much more easily using Dirac notation as:

$$\langle\varphi|\widehat{\mathcal{B}}^\dagger|\psi\rangle = \left[\langle\psi|\widehat{\mathcal{B}}|\varphi\rangle\right]^*$$

An operator is Hermitian if $\widehat{\mathcal{O}}^\dagger = \widehat{\mathcal{O}}$.

2.2.4 Eigenvalues to Eigenkets

Any operator $\widehat{\mathcal{A}}$ corresponding to an observable $\mathcal{A}$ is Hermitian and so has real eigenvalues a_n. The eigenket are $|u_n\rangle$ which corresponds to $u_n(\underset{\sim}{r})$ in wave mechanics.

$$\widehat{\mathcal{A}}|u_n\rangle = a_n|u_n\rangle$$

Eigenkets are orthogonal and can be normalised and this means that:

$$\langle u_n|u_m\rangle = \delta_{nm}$$

It also follows that eigenkets form a complete set so that:

$$|\psi\rangle = \sum_n c_m |u_n\rangle$$

This is equivalent to a set of unit vectors. The sum can be infinite. For a normalised state:

$$\langle\psi|\psi\rangle = \left[\sum_m c_m^* \langle u_n|\right]\left[\sum_n c_n |u_m\rangle\right] = \sum_n \sum_m c_n c_m^* \delta_{nm} = 1$$

Completeness Relation

In wave mechanics $\sum_n u_n^*(\underset{\sim}{r}')u_n(\underset{\sim}{r}) = \delta(\underset{\sim}{r} - \underset{\sim}{r}')$. The eigenfunctions of an observable follow this relation, which is why:

$$\int \delta^3 \underset{\sim}{r} \delta(\underset{\sim}{r} - \underset{\sim}{r}')\psi(\underset{\sim}{r}') = \sum_n c_n u_n(\underset{\sim}{r}) = \psi(\underset{\sim}{r})$$

The Dirac completeness relation is:

$$\sum_n |u_n\rangle\langle u_n| = \widehat{\mathbb{I}}$$

$\widehat{\mathbb{I}}$ is the identity operator where $\widehat{\mathbb{I}}|\psi\rangle = |\psi\rangle$ and $\langle\varphi|\widehat{\mathbb{I}}|\psi\rangle = \langle\varphi|\psi\rangle$. This is simpler than the wave mechanics version because there is no Dirac δ function. This is useful, for example:

$$|\psi\rangle = \sum_n |u_n\rangle\langle u_n|\psi\rangle = \sum_n c_n |u_n\rangle$$

This can be done because $\langle u_n|\psi\rangle$ is just a complex number and therefore moved arbitrarily.

$$\langle\varphi|\psi\rangle = \langle\varphi|\widehat{\mathbb{I}}|\psi\rangle = \sum_n \langle\varphi|u_n\rangle\langle u_n|\psi\rangle$$

2.2.5 Wavefunction

The position eigenkets are $|x\rangle, |x'\rangle, ...$ so that the position operators gives:

$$\widehat{x}|x\rangle = x|x\rangle$$

$$\widehat{x}|x'\rangle = x'|x'\rangle$$

$|x\rangle$ must form a complete set because $\widehat{\mathbb{I}} = \int \delta x |x\rangle\langle x|$.

$$\langle\psi|\psi\rangle = \int \langle\psi|x\rangle\langle x|\psi\rangle \delta x = \int \psi(x)^* \psi(x) \delta x$$

$$\psi(x) = \langle x|\psi\rangle$$

Bras and kets can be used as operators:

$$(|\varphi\rangle\langle\psi|)\,|\zeta\rangle = |\varphi\rangle\langle\psi|\zeta\rangle$$

A different ket is found, which means that $|\varphi\rangle\langle\psi|$ is an operator. For an operator $\widehat{\mathcal{A}}$ corresponding to an observable $\mathcal{A}$ with eigenkets $|u_n\rangle$ which form a complete set.

$$\widehat{\mathcal{A}} = \sum_n \sum_m |u_n\rangle\langle u_n| \underbrace{\widehat{\mathcal{A}}|u_m\rangle}_{a_m|u_m\rangle} \langle u_m|$$

$$\widehat{\mathcal{A}} = \sum_n \sum_m a_n |u_n\rangle \delta_{nm} \langle u_m| = \sum_n a_n |u_n\rangle\langle u_n|$$

For another operator $\widehat{\mathcal{B}}$ then:

$$\widehat{\mathcal{B}} = \sum_n \sum_m |u_n\rangle\langle u_n|\widehat{\mathcal{B}}|u_m\rangle\langle u_m| = \sum_n \sum_m \left(\langle u_n|\widehat{\mathcal{B}}|u_m\rangle\right)|u_n\rangle\langle u_m|$$

$|u_n\rangle$ is not an eigenket of $\widehat{\mathcal{B}}$ and so the result is slightly more complicated.

2.3 Schrodingers Equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \widehat{\mathcal{H}}|\psi\rangle$$

2.4 Operators

$$\left(\widehat{\mathcal{A}}\widehat{\mathcal{B}}\right)^{\dagger} = \widehat{\mathcal{B}}^{\dagger}\widehat{\mathcal{A}}^{\dagger}$$

This can be tested using Dirac notation using two arbitrary kets $|\varphi\rangle$ and $|\psi\rangle$.

$$\langle\varphi|\left(\widehat{\mathcal{A}}\widehat{\mathcal{B}}\right)^{\dagger}|\psi\rangle = \left[\langle\psi|\widehat{\mathcal{A}}\widehat{\mathcal{B}}|\varphi\rangle\right]^{*}$$

As this can be written $\left[\langle\psi|\widehat{\mathcal{A}}|\mathcal{B}\varphi\rangle\right]^{*}$ then it can be seen that:

$$\langle\mathcal{B}\varphi|\widehat{\mathcal{A}}^{\dagger}|\psi\rangle = \langle\mathcal{B}\varphi|\mathcal{A}^{\dagger}\psi\rangle$$

Taking the conjugate version of this gives:

$$\left[\langle\mathcal{A}^{\dagger}\psi|\mathcal{B}\varphi\rangle\right]^{*} = \left[\langle\mathcal{A}^{\dagger}\psi|\widehat{\mathcal{B}}|\varphi\rangle\right]^{*}$$

Finally conjugating this again to obtain the original equation gives:

$$\langle\varphi|\widehat{\mathcal{B}}^{\dagger}|\mathcal{A}^{\dagger}\psi\rangle = \langle\varphi|\widehat{\mathcal{B}}^{\dagger}\widehat{\mathcal{A}}^{\dagger}|\psi\rangle$$

This is always true.

Chapter 3

Two-Level System

A two level system is a system where the Hamiltonian has two eigenvalues. It is useful because the summations are only over two rather than over an infinite amount.

3.1 Spin $\frac{1}{2}$ Particles

The state is described by a spinor:

$$\underset{\sim}{\psi} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Which, when normalised, is such that $\underset{\sim}{\psi}^\dagger \underset{\sim}{\psi} = |\alpha|^2 + |\beta|^2 = 1$. Spin can be measured with respect to three axes, (x, y, z). The operators corresponding to the observables are given by:

$$\widetilde{S}_i = \frac{\hbar}{2}\widetilde{\sigma}_i$$

Where $\widetilde{\sigma}_i$ are the Pauli matrices:

$$\widetilde{\sigma}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \widetilde{\sigma}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \widetilde{\sigma}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

All of these matrices have eigenvalues of $\frac{\hbar}{2}$.

3.1.1 Dirac Notation

Each operator has two eigenvalues. Starting with $\widehat{S}_z$ gives eigenkets such that:

$$\widehat{S}_z|\uparrow\rangle = \frac{1}{2}\hbar|\uparrow\rangle \; and \; \widehat{S}_z|\downarrow\rangle = -\frac{1}{2}\hbar|\downarrow\rangle$$

Two eigenkets form a complete set:

$$\widehat{\mathbb{I}} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$$

The eigenkets are normalised so that $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$ and orthogonal so that $\langle\uparrow|\downarrow\rangle = 0$. A ket, $|\psi\rangle$ can be written in terms of $|\uparrow\rangle$ and $|\downarrow\rangle$.

$$|\psi\rangle = |\uparrow\rangle\langle\uparrow|\psi\rangle + |\downarrow\rangle\langle\downarrow|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

$\widehat{S}_z$ can also be written in terms of $|\uparrow\rangle$ and $|\downarrow\rangle$.

$$\widehat{S}_z = \frac{\hbar}{2}\left[|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\right]$$

If instead of using $\widehat{S}_z$, $\widehat{S}_x$ is used then a new set of eigenkets are needed, $|\rightarrow\rangle$ and $|\leftarrow\rangle$.

$$\widehat{S}_x|\rightarrow\rangle = \frac{\hbar}{2}|\rightarrow\rangle \quad and \quad \widehat{S}_x|\leftarrow\rangle = -\frac{\hbar}{2}|\leftarrow\rangle$$

These kets again are orthonormal so that $\langle \rightarrow \mid \rightarrow \rangle = \langle \leftarrow \mid \leftarrow \rangle = 1$ and $\langle \rightarrow \mid \leftarrow \rangle = 0$ and they form a complete set so that $\widehat{\mathbb{I}} = \mid \rightarrow \rangle\langle \rightarrow \mid + \mid \leftarrow \rangle\langle \leftarrow \mid$. This means that:

$$|\psi\rangle = \mid \rightarrow \rangle\langle \rightarrow |\psi\rangle + \mid \leftarrow \rangle\langle \leftarrow |\psi\rangle = a\mid \rightarrow \rangle + b\mid \leftarrow \rangle$$

As $|\psi\rangle$ is like a vector then $\mid \uparrow \rangle$, $\mid \downarrow \rangle$, $\mid \rightarrow \rangle$ and $\mid \leftarrow \rangle$ are comparable to unit vectors. To get to a vector using Cartesian coordinates $\underset{\sim}{v} = \alpha\underset{\sim}{i} + \beta\underset{\sim}{j}$ and then by rotating the axes to obtain different unit vectors $\underset{\sim}{v} = a\underset{\sim}{i}' + b\underset{\sim}{j}'$. To compare the two sets of unit vectors then $\underset{\sim}{i}' = c\underset{\sim}{i} + d\underset{\sim}{j}$ and $\underset{\sim}{j}' = e\underset{\sim}{i} + f\underset{\sim}{j}$. A particular change of a complete set of kets are called a representation. For the spin case $|\psi\rangle = \alpha\mid \uparrow \rangle + \beta\mid \downarrow \rangle$ is the $\widehat{S}_z$ representation and $|\psi\rangle = a\mid \rightarrow \rangle + b\mid \leftarrow \rangle$ is the $\widehat{S}_x$ representation. When a ket or operator is expanded in terms of a given complete set then it can be converted to a spinor or a matrix respectively.

$$\underset{\sim}{\psi} = \begin{pmatrix} \langle \uparrow |\psi\rangle \\ \langle \downarrow |\psi\rangle \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

The representation must be chosen previous to creating the spinor. The operator $\widehat{\mathcal{O}}$ can be written in terms of kets, again only in a previously chosen representation.

$$\widehat{\mathcal{O}} = \left(\langle \uparrow |\widehat{\mathcal{O}}| \uparrow \rangle\right) \mid \uparrow \rangle\langle \uparrow \mid + \left(\langle \downarrow |\widehat{\mathcal{O}}| \uparrow \rangle\right) \mid \downarrow \rangle\langle \uparrow \mid + \left(\langle \uparrow |\widehat{\mathcal{O}}| \downarrow \rangle\right) \mid \uparrow \rangle\langle \downarrow \mid + \left(\langle \downarrow |\widehat{\mathcal{O}}| \downarrow \rangle\right) \mid \downarrow \rangle\langle \downarrow \mid$$

This can be written as a matrix:

$$\widetilde{O} = \begin{pmatrix} \langle \uparrow |\widehat{\mathcal{O}}| \uparrow \rangle & \langle \uparrow |\widehat{\mathcal{O}}| \downarrow \rangle \\ \langle \downarrow |\widehat{\mathcal{O}}| \uparrow \rangle & \langle \downarrow |\widehat{\mathcal{O}}| \downarrow \rangle \end{pmatrix}$$

This means that:

$$\widehat{S}_z = \frac{\hbar}{2}\left(\mid \uparrow \rangle\langle \uparrow \mid - \mid \downarrow \rangle\langle \downarrow \mid\right)$$

This is the same as $\widetilde{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The same can be carried out for the $\widetilde{S}_x$ direction:

$$\widetilde{\sigma}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \langle \uparrow |\widehat{\sigma}_x| \uparrow \rangle & \langle \uparrow |\widehat{\sigma}_x| \downarrow \rangle \\ \langle \downarrow |\widehat{\sigma}_x| \uparrow \rangle & \langle \downarrow |\widehat{\sigma}_x| \downarrow \rangle \end{pmatrix} = \widehat{\sigma}_x = [\mid \uparrow \rangle\langle \downarrow \mid + \mid \downarrow \rangle\langle \uparrow \mid]$$

The eigenvectors can be found by taking the determinant of the matrix, $\lambda = \pm 1$. This means that the eigenkets are:

$$\mid \rightarrow \rangle = \underset{\sim}{\psi}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \langle \uparrow \mid \rightarrow \rangle \\ \langle \downarrow \mid \rightarrow \rangle \end{pmatrix} = \left(\langle \uparrow \mid \rightarrow \rangle\right) \mid \uparrow \rangle + \left(\langle \downarrow \mid \rightarrow \rangle\right) \mid \downarrow \rangle = \frac{1}{\sqrt{2}}\left[\mid \uparrow \rangle + \mid \downarrow \rangle\right]$$

$$\mid \leftarrow \rangle = \underset{\sim}{\psi}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} \langle \uparrow \mid \leftarrow \rangle \\ \langle \downarrow \mid \leftarrow \rangle \end{pmatrix} = \left(\langle \uparrow \mid \leftarrow \rangle\right) \mid \uparrow \rangle + \left(\langle \downarrow \mid \leftarrow \rangle\right) \mid \downarrow \rangle = \frac{1}{\sqrt{2}}\left[\mid \uparrow \rangle - \mid \downarrow \rangle\right]$$

This now means that it is possible to convert between bases.

$$|\psi\rangle = a\mid \rightarrow \rangle + b\mid \leftarrow \rangle = \frac{a}{\sqrt{2}}\left[\mid \uparrow \rangle + \mid \downarrow \rangle\right] + \frac{b}{\sqrt{2}}\left[\mid \uparrow \rangle - \mid \downarrow \rangle\right] = \left(\frac{a+b}{\sqrt{2}}\right) \mid \uparrow \rangle + \left(\frac{a-b}{\sqrt{2}}\right) \mid \downarrow \rangle$$

Chapter 4

Quantum Harmonic Oscillators

If a particle has a mass, m and angular frequency ω then the Hamiltonian for a quantum harmonic oscillator is:

$$\widehat{\mathcal{H}} = \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega^2\widehat{x}^2$$

By introducing the ladder operators:

$$\widehat{a} = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}\widehat{x} + \frac{i}{(2\omega m\hbar)^{\frac{1}{2}}}\widehat{p}$$

$$\widehat{a} = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}\widehat{x} - \frac{i}{(2\omega m\hbar)^{\frac{1}{2}}}\widehat{p}$$

As these are not Hermitian then they cannot correspond to an observable. It can also be seen that:

$$\widehat{x} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a} + \widehat{a}^\dagger\right)$$

$$\widehat{p} = i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}\left(\widehat{a}^\dagger - \widehat{a}\right)$$

Testing this using the commutation relation gives:

$$\left[\widehat{a}, \widehat{a}^\dagger\right] = -\frac{i}{2\hbar}\left[\widehat{x}, \widehat{p}\right] + \frac{i}{2\hbar}\left[\widehat{p}, \widehat{x}\right] = -\frac{i}{\hbar}\left[\widehat{x}, \widehat{p}\right] = 1$$

$$\left[\widehat{a}, \widehat{a}^\dagger\right] = 1$$

The Hamiltonian can be written as:

$$\frac{p^2}{2m} = -\frac{\hbar\omega}{4}\left(\widehat{a}^\dagger\widehat{a}^\dagger + \widehat{a}\widehat{a} - \widehat{a}^\dagger\widehat{a} - \widehat{a}\widehat{a}^\dagger\right) \text{ and } \frac{1}{2}m\omega^2\widehat{x}^2 = \frac{\hbar\omega}{4}\left(\widehat{a}^\dagger\widehat{a}^\dagger - \widehat{a}\widehat{a} + \widehat{a}^\dagger\widehat{a} + \widehat{a}\widehat{a}^\dagger\right)$$

As $\widehat{a}\widehat{a}^\dagger = \widehat{a}^\dagger\widehat{a} + 1$ then:

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

By introducing a number operator $\widehat{n} = \widehat{a}^\dagger\widehat{a}$ then it is clear that $\widehat{n}$ is Hermitian with real eigenvalues.

$$\widehat{n}|n\rangle = n|n\rangle$$

The eigenkets of $\widehat{n}$ are also eigenkets of $\widehat{\mathcal{H}}$.

$$\widehat{\mathcal{H}}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$$

This shows that the energy eigenvalues are $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$. As the energy is observable then $|n\rangle$ must be orthonormal and form a complete set.

4.1 Ladder Operators

By acting on the state $|n\rangle$ with one of the ladder operators a different energy level can be obtained. For the raising operator, $\widehat{a}^\dagger$ then:

$$\widehat{n}\left(\widehat{a}^\dagger|n\rangle\right) = \widehat{a}^\dagger\widehat{a}\widehat{a}^\dagger|n\rangle = \left(\widehat{a}^\dagger\widehat{a}^\dagger\widehat{a} + \widehat{a}^\dagger\right)|n\rangle = (n+1)\,\widehat{a}^\dagger|n\rangle$$

As $\widehat{n}|n+1\rangle = \langle n+1|n+1\rangle$ then it is clear that;

$$\widehat{a}^\dagger|n\rangle = c_+(n)|n+1\rangle$$

Where $c_+(n)$ is a constant which generally depends on n. The lowering operator can be examined in the same way:

$$\widehat{n}\left(\widehat{a}|n\rangle\right) = \widehat{a}^\dagger\widehat{a}\widehat{a}^d agger|n\rangle = \left(\widehat{a}\widehat{a}^\dagger\widehat{a} - \widehat{a}^\dagger\right)|n\rangle = (n-1)\,\widehat{a}|n\rangle$$

This means that:

$$\widehat{a}|n\rangle = c_-(n)|n-1\rangle$$

Which lowers the energy level. It is also possible to get $\widehat{a}|n\rangle = 0$. To calculate the values of $c_\pm$ then:

$$\langle n|\widehat{n}|n\rangle = n\langle n|n\rangle = n$$

Which can be written as:

$$\langle n|\widehat{a}^\dagger\widehat{a}|n\rangle = c_-(n)\langle n|\widehat{a}^\dagger|n-1\rangle = c_-(n)\left[\langle n-1|\widehat{a}|n\rangle\right]^*$$

This shows that $|c_-(n)|^2 = n$ and so:

$$c_-(n) = \sqrt{n}$$

Now, because $c_-(n) = c_+(n-1)$ then:

$$c_+(n) = \sqrt{n-1}$$

The raising and lowering operators can now be redefined as

$$\widehat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$\widehat{a} = \sqrt{n}|n-1\rangle$$

The eigenvalues of the Hamiltonian must be non-negative because only $\widehat{x}^2$ and $\widehat{p}^2$ appear in the Hamiltonian so:

$$\langle n|\widehat{x}^2|n\rangle = \langle n|\widehat{x}|xn\rangle = \left[\langle xn|xn\rangle\right]^* = \langle xn|xn\rangle \geq 0$$

This is the modulus squared of xn which cannot be negative. The sum over $\widehat{p}^2$ is also zero so:

$$\langle n|\widehat{\mathcal{H}}|n\rangle \geq 0$$

There must also be a ground state where the lowest energy eigenvalue is $n = n_g$ so that:

$$E_g = \left(n_g + \frac{1}{2}\right)\hbar\omega$$

To calculate the lowest energy then the lowest state must be found. $\widehat{a}|n_g\rangle = 0$ so the eigenvalue equation gives:

$$\widehat{\mathcal{H}}|n_g\rangle = \hbar\omega\left(\widehat{a}^\dagger\widehat{a} + \frac{1}{2}\right)|n_g\rangle = \frac{\hbar\omega}{2}|n_g\rangle$$

This shows that $n_g = 0$ so $\widehat{a}|0\rangle = 0$. The other eigenkets can then be formed from $|0\rangle$.

$$\widehat{a}^\dagger|0\rangle = |1\rangle\ ,\ \widehat{a}^\dagger|1\rangle = \sqrt{2}|2\rangle\ ,\ \widehat{a}^\dagger|2\rangle = \sqrt{3}|3\rangle$$

It can be seen that to move from the ground state to the any other then:

$$|n\rangle = \frac{\left(\widehat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle$$

To work out the position uncertainty of a harmonic oscillator in a number state $|n\rangle$ then:

$$\Delta_x = \sqrt{\langle \widehat{x}^2 \rangle - \langle \widehat{x} \rangle^2}$$

As it is known that $\widehat{x} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \left(\widehat{a}^\dagger + \widehat{a}\right)$ then:

$$\langle \widehat{x} \rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \langle n|\widehat{a}^\dagger + \widehat{a}|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \left[\langle n|\widehat{a}^\dagger|n\rangle + \langle n|\widehat{a}|n\rangle\right] = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \left[\sqrt{n+1}\langle n|n+1\rangle + \sqrt{n}\langle n|n-1\rangle\right]$$

As $\langle i|j\rangle = \delta_{ij}$ then $\langle \widehat{x} \rangle = 0$. Now as $\langle n| \left(\widehat{a}^\dagger\right)^i (\widehat{a})^j |n\rangle = \delta_{ij}$ then:

$$\langle \widehat{x}^2 \rangle = \left(\frac{\hbar}{2m\omega}\right) \langle n| \left(\widehat{a}^\dagger + \widehat{a}\right)^2 |n\rangle = \left(\frac{\hbar}{2m\omega}\right) \langle n| \left(\widehat{a}^\dagger\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a} + \widehat{a}\widehat{a}^\dagger + \widehat{a}\widehat{a}\right) |n\rangle$$

As $\left[\widehat{a}, \widehat{a}^\dagger\right] = 1$ and $\widehat{a}^\dagger\widehat{a} = \widehat{n}$ then this becomes:

$$\langle \widehat{x}^2 \rangle = \left(\frac{\hbar}{2m\omega}\right) \langle n| \left(\widehat{a}^\dagger\widehat{a} + \widehat{a}\widehat{a}^\dagger\right) |n\rangle = \left(\frac{\hbar}{2m\omega}\right) \langle n| \left(2\widehat{a}^\dagger\widehat{a} + 1\right) |n\rangle = \left(\frac{\hbar}{2m\omega}\right) (2n+1)$$

This means the uncertainty in the position is:

$$\Delta_x = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (2n+1)^{\frac{1}{2}}$$

Chapter 5

Operator Dynamics

Normally the time evolution of a system is dictated by the wavefunction and the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{\mathcal{H}}|\psi(t)\rangle$$

This means that the expectation values also are time dependent. Instead of this view then the evolution can be written in terms of a time evolution operator, $\widehat{\mathcal{U}}(t)$. This defines $|\psi(t)\rangle = \widehat{\mathcal{U}}(t)|\psi(0)\rangle$. As this $|\psi(0)\rangle$ is arbitrary then the Schrödinger equation is:

$$\frac{\delta\widehat{\mathcal{U}}(t)}{\delta t} = -\frac{i}{\hbar}\widehat{\mathcal{H}}\widehat{\mathcal{U}}(t)$$

If the normal solution to a first order differential equation is taken then:

$$\widehat{\mathcal{U}}(t) = e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}$$

This is the correct form of the time evolution operator. By expanding the exponential into the power series $e^{\widehat{\mathcal{A}}} = 1 + \widehat{\mathcal{A}} + \frac{\widehat{\mathcal{A}}^2}{2!} + \frac{\widehat{\mathcal{A}}^3}{3!} + ...$ then:

$$\frac{\delta\widehat{\mathcal{U}}(t)}{\delta t} = \frac{\delta}{\delta t}\left(1 - \frac{i\widehat{\mathcal{H}}t}{\hbar} + \left(\frac{i\widehat{\mathcal{H}}t}{\hbar}\right)^2\frac{t^2}{2} + \left(\frac{i\widehat{\mathcal{H}}t}{\hbar}\right)^3 + ...\right) = -\frac{i\widehat{\mathcal{H}}}{\hbar} + \left(\frac{i\widehat{\mathcal{H}}}{\hbar}\right)^2 t + \left(\frac{i\widehat{\mathcal{H}}}{\hbar}\right)^3\frac{t^2}{2} + ... = -\frac{i\widehat{\mathcal{H}}}{\hbar}e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}$$

This shows that the operator acts as expected when differentiated with respect to time. For an energy eigenstate $|\varphi_i\rangle$ then $\widehat{\mathcal{H}}^n|\varphi_i\rangle = E_i^n|\varphi_i\rangle$. This can be seen by multiplying by the Hamiltonian:

$$\widehat{\mathcal{H}}|\varphi_i\rangle = E_i|\varphi_i\rangle$$
$$\widehat{\mathcal{H}}^2|\varphi_i\rangle = \widehat{\mathcal{H}}\widehat{\mathcal{H}}|\varphi_i\rangle = E_i\widehat{\mathcal{H}}|\varphi_i\rangle = E_i^2|\varphi_i\rangle$$
$$\widehat{\mathcal{H}}^3|\varphi_i\rangle = \widehat{\mathcal{H}}\left(\widehat{\mathcal{H}}^2|\varphi_i\rangle\right) = E_i^2\widehat{\mathcal{H}}|\varphi_i\rangle = E_i^3|\varphi_i\rangle$$

Now if $|\psi(0)\rangle = |\varphi_i\rangle$ then:

$$|\psi(t)\rangle = \widehat{\mathcal{U}}(t)|\varphi_i\rangle = e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}|\varphi_i\rangle = \sum_{n=0}^{\infty}\frac{\left(-\frac{it}{\hbar}\right)^n\widehat{\mathcal{H}}^n}{n!}|\varphi_i\rangle = e^{-\frac{iE_it}{\hbar}}|\varphi_i\rangle$$

This shows how an energy eigenstate evolves in time. Due to linearity then $|\psi(0)\rangle = \sum_n c_n|\varphi_n\rangle$ becomes:

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{iE_nt}{\hbar}}|\varphi_n\rangle$$

$\mathcal{U}(t)$ can also be used in the expectation values:

$$\langle\widehat{\mathcal{A}}\rangle_t = \langle\psi(t)|\widehat{\mathcal{A}}|\psi(t)\rangle = \langle\psi(0)|\widehat{\mathcal{U}}^\dagger(t)\widehat{\mathcal{A}}\widehat{\mathcal{U}}(t)|\psi(0)\rangle$$

Where $\widehat{\mathcal{A}}\widehat{\mathcal{U}}(t) = |\psi(t)\rangle$. This can be seen by introducing an arbitrary ket $|\varphi\rangle$ then:

$$\langle\psi(t)|\varphi\rangle = [\langle\varphi|\psi(t)\rangle]^* = \left[\langle\varphi|\widehat{\mathcal{U}}(t)|\psi(0)\rangle\right]^* = \langle\psi(0)|\widehat{\mathcal{U}}^\dagger(t)|\varphi\rangle$$

As this is true for any ket then $\langle\psi(t)| = \langle\psi(0)|\widehat{\mathcal{U}}^\dagger(t)$.

5.1 Heisenberg Picture

By combining $\widehat{\mathcal{U}}^\dagger(t)\widehat{\mathcal{A}}\widehat{\mathcal{U}}(t) = \widehat{\mathcal{A}}_H(t)$ to get:

$$\langle\widehat{\mathcal{A}}\rangle_t = \langle\psi_H|\widehat{\mathcal{A}}_H(t)|\psi_H\rangle$$

Where the operator $\widehat{\mathcal{A}}_H$ is an operator which evolves in time, and the state is a constant given by $|\psi_H\rangle = |\psi(0)\rangle$. The answer from of the expectation value is the same as the description in the Schrödinger picture, but it is easier to understand in the classical sense. The equation of motion in Heisenberg's picture is given by:

$$\frac{\delta\widehat{\mathcal{A}}_H}{\delta t} = \frac{\delta\widehat{\mathcal{U}}^\dagger(t)}{\delta t}\widehat{\mathcal{A}}\widehat{\mathcal{U}}(t) + \widehat{\mathcal{U}}^\dagger(t)\widehat{\mathcal{A}}\frac{\delta\widehat{\mathcal{U}}(t)}{\delta t}$$

As $\frac{\delta\widehat{\mathcal{U}}(t)}{\delta t} = -\frac{i\widehat{\mathcal{H}}}{\hbar}e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}$ and $\frac{\delta\widehat{\mathcal{U}}^\dagger(t)}{\delta t} = \frac{i\widehat{\mathcal{H}}}{\hbar}e^{\frac{i\widehat{\mathcal{H}}t}{\hbar}}$, and because $\mathcal{U}$ is unitary such that:

$$\widehat{\mathcal{U}}(t)\widehat{\mathcal{U}}^\dagger(t) = \widehat{\mathcal{U}}^\dagger(t)\widehat{\mathcal{U}}(t) = \widehat{\mathbb{I}}$$

Which means that as long as the state is normalised then the probability of finding a particle in space at any time must always be 1, the equation of motion is:

$$\frac{\delta\widehat{\mathcal{A}}_H(t)}{\delta t} = \frac{i\widehat{\mathcal{H}}}{\hbar}\widehat{\mathcal{A}}_H - \widehat{\mathcal{A}}_H\frac{i\widehat{\mathcal{H}}}{\hbar} = \frac{i}{\hbar}\left[\widehat{\mathcal{H}}, \widehat{\mathcal{A}}_H\right]$$

$$i\hbar\frac{\delta\widehat{\mathcal{A}}_H(t)}{\delta t} = \left[\widehat{\mathcal{A}}_H(t), \widehat{\mathcal{H}}\right]$$

The position operator, $\widehat{x}_H(t)$, is given by:

$$\widehat{x}_H(t) = \widehat{\mathcal{U}}^\dagger(t)\widehat{x}\widehat{\mathcal{U}}(t)$$

As $x = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a} + \widehat{a}^\dagger\right)$ then:

$$\widehat{x}_H(t) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a}_H(t) + \widehat{a}_H^\dagger(t)\right)$$

As $\widehat{\mathcal{U}} = e^{-i\omega t}$ and $\widehat{a}_H(t) = \widehat{a}\widehat{\mathcal{U}}$ then this is:

$$\widehat{x}_H(t) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a}e^{-\omega t} + \widehat{a}^\dagger e^{i\omega t}\right)$$

This has an oscillating position, as expected for a simple harmonic oscillator. The expectation value for a state $|n\rangle$ in an energy eigenstate is:

$$\langle\widehat{x}\rangle_t = \langle n|\widehat{x}_H(t)|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left[\langle n|\widehat{a}|n\rangle e^{-i\omega t} + \langle n|\widehat{a}^\dagger|n\rangle e^{i\omega t}\right] = 0$$

As $\langle n_i|n_j\rangle = \delta_{ij}$. There is no evidence of a harmonic oscillator system in the expectation value, due to the energy eigenvalues of the quantum harmonic oscillator being more quantum than normal.

5.1.1 Harmonic Oscillator

The Hamiltonian is given by:

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

Where $\left[\widehat{a}, \widehat{a}^\dagger\right] = 1$. The equation of motion in the Heisenberg picture is:

$$i\hbar\frac{\delta\widehat{a}_H(t)}{\delta t} = \left[\widehat{a}_H(t), \widehat{\mathcal{H}}\right]$$

By definition $\widehat{a}_H(t) = \widehat{\mathcal{U}}^\dagger(t)\widehat{a}\widehat{\mathcal{U}}(t)$ so:

$$\left[\widehat{a}_H(t), \widehat{\mathcal{H}}\right] = \widehat{\mathcal{U}}^\dagger(t)\widehat{a}\widehat{\mathcal{U}}(t)\widehat{\mathcal{H}} - \widehat{\mathcal{H}}\widehat{\mathcal{U}}^\dagger(t)\widehat{a}\widehat{\mathcal{U}}(t)$$

Because both $\widehat{\mathcal{U}}(t)$ and $\widehat{\mathcal{U}}^{\dagger}(t)$ always commute with the Hamiltonian then:

$$\widehat{\mathcal{U}}^{\dagger}(t)\left(\widehat{a}\widehat{\mathcal{H}}-\widehat{\mathcal{H}}\widehat{a}\right)\widehat{\mathcal{U}}(t)=\hbar\omega\widehat{\mathcal{U}}^{\dagger}(t)\left(\widehat{a}\widehat{a}^{\dagger}\widehat{a}-\widehat{a}^{\dagger}\widehat{a}\widehat{a}\right)\widehat{\mathcal{U}}(t)$$

Now by substituting in $\widehat{a}\widehat{a}^{\dagger}=1+\widehat{a}^{\dagger}\widehat{a}$ found from $\left[\widehat{a},\widehat{a}^{\dagger}\right]=1$ and using $\widehat{\mathcal{U}}^{\dagger}\widehat{a}\widehat{\mathcal{U}}(t)=\widehat{a}_H(t)$ then:

$$\frac{\delta\widehat{a}_H(t)}{\delta t}=-i\omega\widehat{a}_H(t)$$

If the initial condition is $\widehat{a}_H(0)=\widehat{a}$ then:

$$\widehat{a}_H(t)=\widehat{a}e^{-i\omega t}$$

5.2 Interaction Picture

Another way of handling time-dependence in which both states and operators evolve in time is the interaction picture. It is useful when the Hamiltonian has two parts, $\widehat{\mathcal{H}}=\widehat{\mathcal{H}}_o+\widehat{\mathcal{H}}'$, where $\widehat{\mathcal{H}}_o$ is simple in the sense that the eigenstates and eigenvalues can be known. $\widehat{\mathcal{H}}'$ is a small additional term which makes the total Hamiltonian more difficult to deal with. This is known as a perturbation. The states in the interaction picture evolve as:

$$|\psi_I(t)\rangle=e^{-\frac{i\widehat{\mathcal{H}}_o t}{\hbar}}|\psi_S(t)\rangle$$

The operators evolve as:

$$\widehat{\mathcal{A}}_I(t)=e^{\frac{i\widehat{\mathcal{H}}t}{\hbar}}\widehat{A}_S e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}$$

This means that if there was no perturbation then the Heisenberg picture would be recovered for operators. The equations of motion in the interaction picture are:

$$\frac{\delta\widehat{\mathcal{A}}_I(t)}{\delta t}=\frac{i}{\hbar}\left[\widehat{\mathcal{H}}_o,\widehat{\mathcal{A}}_I(t)\right]$$

And:

$$i\hbar\frac{\delta|\psi_I(t)\rangle}{\delta t}=\widehat{\mathcal{H}}'_I(t)|\psi_I(t)\rangle$$

The states evolve due to the perturbation, which, when small, occurs very slowly.

Chapter 6

Perturbation Theory

There are very few systems where the differential equations can be analytically solved. For other systems then approximations must be made to get indications of the eigenvalues and eigenstates. An example of an approximation made to a system is for the vibration of a diatomic molecule, which is generally approximated as a harmonic oscillator system, but the potential is not truly harmonic. To find out what happens to the eigenvalues and eigenfunctions due to higher order terms in the Hamiltonian then perturbation theory can be used. For a Hamiltonian $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_o + \widehat{\mathcal{H}}'$ where the eigenkets and eigenvalues of $\widehat{\mathcal{H}}_o$ are known by:

$$\widehat{\mathcal{H}}_o|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle$$

$|\psi_n^{(0)}\rangle$ are orthonormal and form a complete set so that $\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle = \delta_{nm}$ and $\sum_n |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}| = \widehat{\mathbb{I}}$. $\widehat{\mathcal{H}}'$ is a small correction to the known Hamilton, and is known as a weak perturbation. To calculate the eigenkets and eigenvalues of the full problem as a power series in $\widehat{\mathcal{H}}'$ then a *book keeping operator*, λ is introduced.

$$\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_o + \lambda\widehat{\mathcal{H}}'$$

This is introduced because it acts as a handle to keep track of terms of $\widehat{\mathcal{H}}'$. If in an equation there is a term $\lambda^3\chi$ where χ includes lots of other members then, within these members, there must be $\widehat{\mathcal{H}}'^3$. Whenever λ is set to zero then the normal $\widehat{\mathcal{H}}_o$ must be recovered, and whenever λ is set to one then the total Hamiltonian is found. The eigenkets and eigenvalues of $\widehat{\mathcal{H}}$ can be written arbitrarily in symbolic form, although the values are unknown.

$$\widehat{\mathcal{H}}|\psi_n\rangle = \left(\widehat{\mathcal{H}}_o + \lambda\widehat{\mathcal{H}}'\right)|\psi_n\rangle = E_n|\psi_n\rangle$$

$|\psi_n\rangle$ and E_n can be written as a power series in λ:

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + ...$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$$

Calculating the first few terms of the power series, when $\widehat{\mathcal{H}}'$ is weak, whould give the values of E_n and $|\psi_n\rangle$ to a good approximation. Starting with $\left(\widehat{\mathcal{H}}_o + \lambda\widehat{\mathcal{H}}'\right)|\psi_n\rangle = E_n|\psi_n\rangle$ and substituting into the series expansion of E_n and $|\psi_n\rangle$ gives:

$$\left(\widehat{\mathcal{H}}_o + \lambda\widehat{\mathcal{H}}'\right)\left(|\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + ...\right) = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_m^{(2)} + ...\right)\left(|\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + ...\right)$$

As the coeffiecients of λ must be the same on either side, due to the above equation holding for a range of λ then:

$$\begin{array}{lcrcl}
\lambda^{(0)} & : & \widehat{\mathcal{H}}_o|\psi_n^{(0)}\rangle & = & E_n^{(0)}|\psi_n^{(0)}\rangle \\
\lambda & : & \widehat{\mathcal{H}}_o|\psi_n^{(1)}\rangle + \widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle & = & E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(2)}\rangle \\
\lambda^2 & : & \widehat{\mathcal{H}}_o|\psi_n^{(2)}\rangle + \widehat{\mathcal{H}}'|\psi_n^{(1)}\rangle & = & E_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle
\end{array}$$

6.1 First Order Perturbation

The first order correction to the energy $E_n^{(1)}$ can be found by multiplying both sides of the λ equation by $\langle\psi_n^{(0)}|$.

$$\langle\psi_n^{(0)}|\widehat{\mathcal{H}}_o|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle = E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle$$

Now as the first term $\langle\psi_n^{(0)}|\widehat{\mathcal{H}}_o|\psi_n^{(1)}\rangle$ can be written as:

$$\left[\langle\psi_n^{(1)}|\widehat{\mathcal{H}}_o|\psi_n^{(0)}\rangle\right]^* = \left[E_n^{(0)}\langle\psi_n^{(1)}|\psi_n^{(0)}\rangle\right]^* = E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle$$

Then this can be cancelled from both sides of the equation to give the first order correction to the energy.

$$E_n^{(1)} = \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle$$

The value of $|\psi_n^{(1)}\rangle$ is unknown, but must be orthonormal and because the unperturbed eigenstates form a complete set, $\widehat{\mathbb{I}} = \sum_m |\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|$ then:

$$|\psi_n^{(1)}\rangle = \widehat{\mathbb{I}}|\psi_n^{(1)}\rangle = \sum_m |\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle = \sum_m c_{mn}^{(1)}|\psi_m^{(0)}\rangle$$

So the coefficient given by $|\psi_n^{(1)}\rangle$ is $c_{mn}^{(1)} = \langle\psi_m^{(0)}|\psi_n^{(1)}\rangle$. This is the general way to calculate the value of a perturbed eigenstate. For the second order perturbation then:

$$|\psi_n^{(2)}\rangle = \sum_m |\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\psi_n^{(2)}\rangle = \sum_m c_{mn}^{(2)}|\psi_m^{(0)}\rangle$$

Where $c_{mn}^{(2)} = \langle\psi_m^{(0)}|\psi_n^{(2)}\rangle$.

6.2 Second Order Perturbation

Now for higher order terms the equations are more untidy. For the second order then the λ^2 equation gets multiplied by $\langle\psi_n^{(0)}|$ to give:

$$\langle\psi_n^{(0)}|\widehat{\mathcal{H}}_o|\psi_n^{(2)}\rangle + \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(1)}\rangle = E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(2)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle$$

In a similar way to the first order perturbation $\langle\psi_n^{(0)}|\widehat{\mathcal{H}}_o|\psi_n^{(2)}\rangle$ cancels out with $E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle$. By placing the values of $|\psi_n^{(1)}\rangle$ and $|\psi_n^{(2)}\rangle$ in, as calculated earlier:

$$\sum_m \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_m^{(0)}\rangle c_{mn}^{(1)} = E_n^{(1)}c_{nn}^{(1)} + E_n^{(2)}$$

As $E_n^{(1)} = \langle\psi_n^{(0)}|\widehat{\mathcal{H}}|\psi_n^{(0)}\rangle$ then:

$$\sum_m \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_m^{(0)}\rangle c_{mn}^{(1)} - \langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle c_{nn}^{(1)} = E_n^{(2)}$$

If only $|\psi_n^{(0)}\rangle$ is placed into the λ^2 equation, along with a second unperturbed eigenstate $\langle\psi_k^{(0)}|$ then:

$$E_k^{(0)}c_{nk}^{(1)} + \langle\psi_k^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle = E_n^{(0)}c_{nk}^{(1)} + E_n^{(1)}\langle\psi_k^{(0)}|\psi_n^{(0)}\rangle$$

This means that when $n \neq k$ then:

$$c_{nk}^{(1)} = \frac{\langle\psi_k^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$$

This only works when there are no degeneracies and so $E_n^{(0)} \neq E_k^{(0)}$. This is because $c_{nk}^{(1)}$ would become infinite and not a small correction. This can be used when the for $m = k$ to give the energy of the second perturbation as:

$$E_n^{(2)} = \sum_{m\neq n} \frac{\langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$$

As $\langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_m^{(0)}\rangle$ is the complex conjugate of $\langle\psi_m^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle$ due to $\widehat{\mathcal{H}}'$ being Hermitian then:

$$E_n^{(2)} = \sum_{m\neq n} \frac{\left|\langle\psi_n^{(0)}|\widehat{\mathcal{H}}'|\psi_m^{(0)}\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}$$

6.2.1 $c_{nn}^{(1)}$

$\langle\psi_n|\psi_n\rangle = 1$ for all of the terms in the infinite series then $|\psi_n\rangle$ is required to be normalised up to the power of λ to the order of the perturbation. For the first order calculation $|\psi_n\rangle \approx |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle$ then it is required that $\langle\psi_n|\psi_n\rangle = 1 + O(\lambda^2)$.

$$\langle\psi_n|\psi_n\rangle = \left[\langle\psi_n^{(0)}| + \lambda\langle\psi_n^{(1)}|\right]\left[|\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle\right] = \langle\psi_n^{(0)}|\psi_n^{(0)}\rangle + \lambda\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \lambda\langle\psi_n^{(1)}|\psi_n^{(0)}\rangle + \lambda^2\langle\psi_n^{(1)}|\psi_n^{(1)}\rangle$$

$\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle = 1$ and terms of λ^2 are not included which means that $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_n^{(1)}|\psi_n^{(0)}\rangle$ must be zero. As $c_{nn}^{(1)} = \langle\psi_n^{(0)}|\psi_n^{(1)}\rangle$ then $c_{nn}^{(1)} + \left(c_{nn}^{(1)}\right)^* = 0$, which is satisfied when $c_{nn}^{(1)} = 0$. This means that up tp first order:

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \sum_{m\neq n}\left[\frac{\langle\psi_m^{(0)}|\widehat{\mathcal{H}}'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}\right]|\psi_m^{(0)}\rangle$$

6.3 Harmonic Oscillator

A harmonic oscillator with angular frequency ω, mass m has a Hamiltonian:

$$\widehat{\mathcal{H}} = \frac{\widehat{p}^2}{2m} + \frac{m\omega^2\widehat{x}^2}{2} = \hbar\omega\left(\widehat{a}^\dagger\widehat{a} + \frac{1}{2}\right)$$

6.3.1 Perturbation of $\widehat{\mathcal{H}}' = k\widehat{x}^2$

If the harmonic oscillator is subject to a perturbation of $\widehat{\mathcal{H}}' = k\widehat{x}^2$, where $\widehat{x} = \left(\frac{\hbar k}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a}^\dagger + \widehat{a}\right)$ so:

$$\widehat{\mathcal{H}}' = \frac{\hbar k}{2m\omega}\left(\widehat{a}^\dagger + \widehat{a}\right)^2$$

The first order correction to the ground state energy is:

$$E_o^{(1)} = \langle 0|\widehat{\mathcal{H}}'|0\rangle = \frac{\hbar k}{2m\omega}\langle 0|(\widehat{a}^\dagger + \widehat{a})^2|0\rangle$$

$(\widehat{a}^\dagger + \widehat{a})^2$ can be expanded and using $\widehat{a}|0\rangle = 0$, $\langle 0|\widehat{a}^\dagger\widehat{a}^\dagger|0\rangle = \langle 0|\widehat{a}^\dagger|1\rangle = \sqrt{2}\langle 2|0\rangle = 0$ due to orthonormality then:

$$E_o^{(0)} = \frac{\hbar k}{2m\omega}\langle 0|\widehat{a}\widehat{a}^\dagger|0\rangle$$

$\langle 0|\widehat{a}\widehat{a}^\dagger|0\rangle = 1$ and so the first order correction is:

$$E_o^{(1)} = \frac{\hbar k}{2m\omega}$$

This problem can actually be solved exactly using:

$$\widehat{\mathcal{H}} + \widehat{\mathcal{H}} = \frac{\widehat{p}^2}{2m} + \frac{m\omega^2\widehat{x}^2}{2} + k\widehat{x}^2 = \frac{\widehat{p}^2}{2m} + \frac{m\widetilde{\omega}^2\widehat{x}^2}{2}$$

Where $\widetilde{\omega}^2 = \omega^2\left(1 + \frac{2k}{m\omega^2}\right)$. This means that the ground state energy is:

$$E_o = \frac{\hbar\widetilde{\omega}}{2} = \frac{\hbar\omega}{2}\left(1 + \frac{2k}{m\omega^2}\right)^{\frac{1}{2}}$$

As this perturbation must be small to carry out the perturbation calculation then $k \ll \frac{m\omega^2}{2}$, which means $\frac{2k}{m\omega^2} \ll 1$ and Taylor expansion can be used to obtain:

$$\left(1 + \frac{2k}{m\omega^2}\right)^{\frac{1}{2}} \approx 1 + \frac{k}{m\omega^2}$$

When this is included in the energy then:

$$E_o = \frac{\hbar\omega}{2} + \frac{\hbar k}{2m\omega}$$

Which is indeed exactly the same answer as obtained from the perturbation calculation.

6.3.2 Perturbation of $\widehat{\mathcal{H}}' = k\left(\widehat{a}^\dagger + \widehat{a}\right)$

The first and second order corrections to the ground and first excited states energy levels can be obtained as such.

First Order

$$E_n^{(1)} = \langle n|\widehat{\mathcal{H}}'|n\rangle = k\langle n|(\widehat{a}^\dagger + \widehat{a})|n\rangle = 0$$

This is zero because the number of $\widehat{a}^\dagger$ and $\widehat{a}$ is never equal to each other and so all the first order corrections are zero.

Second Order

Ground State, $|0\rangle$

$$E_o^{(2)} = \sum_{m\neq 0} \frac{\left|\langle m|\widehat{\mathcal{H}}'|0\rangle\right|^2}{E_0^{(0)} - E_m^{(0)}}$$

As $E_0^{(0)} = \frac{\hbar\omega}{2}$ and $E_m^{(0)} = \hbar\omega\left(m + \frac{1}{2}\right)$ then $E_o^{(0)} - E_m^{(0)} = -m\hbar\omega$ to give:

$$E_0^{(2)} = -k^2 \sum_{m\neq 0} \frac{\left|\langle m|(\widehat{a}^\dagger + \widehat{a})|0\rangle\right|^2}{m\hbar\omega}$$

Again $\widehat{a}|0\rangle = 0$ so $\langle m|\widehat{a}^\dagger|0\rangle = \langle m|1\rangle$ which is only non-zero for $m = 1$ so:

$$E_0^{(2)} = -\frac{k^2}{\hbar\omega}$$

First Excited State, $|1\rangle$ The same formulation can be taken as for the ground state, except the energy in the denominator is that of the energy of the first excited level $E_1^{(0)} - E_m^{(0)} = \hbar\omega(1-m)$.

$$E_1^{(2)} = k^2 \sum_{m\neq 1} \frac{\left|\langle m|(\widehat{a}^\dagger + \widehat{a})|1\rangle\right|^2}{\hbar\omega(1-m)}$$

There are two terms in the sum $\langle m|(\widehat{a}^\dagger + \widehat{a})|1\rangle = \sqrt{2}\langle m|2\rangle + \langle m|0\rangle$. When $m = 0$ then the energy is $E_1 0^{(2)} = \frac{k^2}{\hbar\omega}$ and when $m = 2$ then $E_1 2^{(2)} = -\frac{2k^2}{\hbar\omega}$. The second order correction on the energy is therefore:

$$E_1^{(0)} = -\frac{k^2}{\hbar\omega}$$

There is a shift in the energy due moving the system by kx.

Chapter 7

Time-Dependent Perturbation Theory

For a system with a perturbation applied at $t = 0$, which can be constant or can have time dependence. The probability of finding a system in a different state at a later time can be calculated using time-dependent perturbation theory. A system has an initial Hamiltonian $\widehat{\mathcal{H}}_o$, with eigenkets $|l\rangle$ and eigenvalues E_k, so that $\widehat{\mathcal{H}}_o|k\rangle = E_k|k\rangle$. The perturbation $\widehat{\mathcal{H}}'$ is applied when $t = 0$ and so the Hamiltonian for $t > 0$ is $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_o + \widehat{\mathcal{H}}'(t)$ where $\widehat{\mathcal{H}}'$ may depend explicitly on time. If the system starts at $t = 0$ in $|i\rangle$ the probability of finding the system in $|f\rangle$ at a later time can be found, where the state of they system for $t > 0$ can be written as:

$$|\psi(t)\rangle = \sum_k c_k(t) e^{-\frac{iE_k t}{\hbar}} |k\rangle$$

This uses the fact that the states, $|k\rangle$, form a complete set and are orthonormal. The coefficient is written as $c_k(t)e^{-\frac{iE_k t}{\hbar}}$ to simplify the working out later. Substituting $|\psi(t)\rangle$ into the Schrödinger equation gives:

$$i\hbar \sum_k \left(\dot{c}_k e^{-\frac{iE_k t}{\hbar}} - \frac{iE_k}{\hbar} c_k e^{-\frac{iE_k t}{\hbar}} \right) |k\rangle = \left(\widehat{\mathcal{H}}_o + \widehat{\mathcal{H}}' \right) \sum_k c_k e^{-\frac{iE_k t}{\hbar}} |k\rangle$$

This simplifies due to $\widehat{\mathcal{H}}_o|k\rangle = E_k|k\rangle$ and therefore $E_k c_k e^{-\frac{iE_k t}{\hbar}}$ cancels on both sides. This gives:

$$\sum_k i\hbar c_k e^{-\frac{iE_k t}{\hbar}} |k\rangle = \sum_k c_k e^{-\frac{iE_k t}{\hbar}} \widehat{\mathcal{H}}'|k\rangle$$

Both sides can be multiplied by $\langle f|e^{-\frac{iE_k t}{\hbar}}$ where $\sum_k \langle f|k\rangle c_k = c_f$. If the difference in energies is defined as $\omega_{fk} = \frac{E_f - E_k}{\hbar}$ then this becomes:

$$i\hbar \dot{c}_f = \sum_k c_k e^{i\omega_{fk} t} \langle f|\widehat{\mathcal{H}}'|k\rangle$$

Now if it is assumed that $\widehat{\mathcal{H}}'$ is a weak perturbation then the coefficient can be expanded in terms of the powers of the perturbation, again using the book keeping parameter, λ.

$$c_k(t) = c_k^{(0)}(t) + \lambda c_k^{(1)}(t) + \lambda^2 c_k^{(2)}(t) + ...$$

It is known what $c_k^{(0)}(t)$ is at $t = 0$ because it describes the system without any perturbation. The initial conditions are that:

$$c_k(t) = \begin{cases} c_i^{(0)}(0) = 1 \\ c_f^{(0)}(0) = 0 \end{cases}$$

Schrödingers equation now becomes:

$$i\hbar \left[\dot{c}_f^{(0)} + \lambda \dot{c}_f^{(1)} + \lambda^2 \dot{c}_f^{(2)} + ... \right] = \sum_k \langle f|\lambda \widehat{\mathcal{H}}'|k\rangle \times \left[c_k^{(0)} + \lambda c_k^{(1)} + \lambda^2 c_k^{(2)} + ... \right] e^{i\omega_{fk} t}$$

The number of powers of λ must be the same on both sides. Because $i\hbar \dot{c}_f^{(0)} = 0$ then $c_f^{(0)}(t)$ does not

$$\begin{aligned}
\lambda^0 &= i\hbar\dot{c}_f^{(0)} &&= 0 \\
\lambda^1 &= i\hbar\dot{c}_f^{(1)} &&= \textstyle\sum_k \langle f|\widehat{\mathcal{H}}'|k\rangle c_k^{(0)} e^{i\omega_{fk}t} \\
\lambda^n &= i\hbar\dot{c}_f^{(n)} &&= \textstyle\sum_k \langle f|\widehat{\mathcal{H}}'|k\rangle c_k^{(n-1)} e^{i\omega_{fk}t}
\end{aligned}$$

depend on time and so $c_f^{(0)}(t) = c_f^{(0)}(0) = 0$ when $f \neq i$ or $c_f^{(0)}(t) = c_i^{(0)}(0) = 1$ when $f = i$. The first power of the λ equation becomes much simpler because there is only one state which has an initial coefficient.

$$i\hbar\dot{c}_f^{(1)} = \langle f|\widehat{\mathcal{H}}'|i\rangle e^{i\omega_{fi}t}$$

For the lowest order of perturbation then $c_f(t) = c_f^{(0)}(t) + \lambda c_f^{(1)}(t)$, then for $f \neq i$, $c_f(t) = \lambda c_f^{(1)}(t) = c_f^{(1)}(t)$. This means that:

$$\dot{c}_f = -\frac{i}{\hbar}\widehat{\mathcal{H}}'_{fi}(t)e^{i\omega_{fi}t}$$

Where $\widehat{\mathcal{H}}'_{fi}(t) = \langle f|\widehat{\mathcal{H}}'|i\rangle$. For an initial condition of $c_f^{(0)} = 0$, then the initial state cannot be $|f\rangle$ and the probability of finding the system in $|f\rangle$ at a time t is:

$$\mathcal{P}_{if}(t) = \left|c_f(t)e^{-\frac{iE_f t}{\hbar}}\right|^2 = |c_f(t)|^2$$

The value of $c_f(t)$ can be calculated by solving the differential equation with the initial condition:

$$\dot{c}_f = -\frac{i}{\hbar}\widehat{\mathcal{H}}'_{fi}(t)e^{i\omega_{fi}t}$$

7.1 Constant Perturbation

For a constant perturbation switched on at $t = 0$ then the matrix element $\widehat{\mathcal{H}} = V_o$ which is constant. Placing this into the differential equation and solving using $c_f(0) = 0$ gives:

$$c_f(t) = -\frac{iV_o}{\hbar}\int_0^t \delta t' e^{i\omega_{fi}t'} = -\frac{V_o}{\hbar}\frac{e^{i\omega_{fi}t} - 1}{\omega_{fi}}$$

This means the probability is:

$$\mathcal{P}_{if}(t) = |c_f(t)|^2 = \frac{V_o^2}{\hbar^2\omega_{fi}^2}\left(e^{i\omega_{fi}t} - 1\right)\left(e^{-i\omega_{fi}t} - 1\right) = \frac{2V_o^2}{\hbar^2\omega_{fi}^2}\left(1 - \cos\omega_{fi}t\right)$$

Using the trigonometric identity $2\sin^2\vartheta = 1 - \cos 2\vartheta$ then:

$$\mathcal{P}_i f(t) = \frac{4V_o^2}{\hbar^2\omega_{fi}^2}\sin^2\frac{\omega_{fi}t}{2}$$

There is an oscillation which is scaled by V_o which must be $V_o \ll \hbar\omega_{fi}$ because the perturbation is weak.

7.2 Harmonic Perturbation

If the perturbation has the form $\widehat{\mathcal{H}}'_{fi} = V_o\cos\omega t$ where V_o is constant. This can be placed into the differential equation with an initial condition of $c_f(0) = 0$.

$$c_f(t) = -\frac{iV_o}{\hbar}\int_0^t \delta t' e^{i\omega_{fi}t'}\cos\omega t'$$

The cos can be expanded in terms of exponentials to give:

$$c_f(t) = -\frac{iV_o}{2\hbar}\int_0^t \delta t'\left(e^{i(\omega+\omega_{fi})t'} + e^{-i(\omega-\omega_{fi})t'}\right) = \frac{V_o}{2\hbar}\left(\frac{e^{i(\omega+\omega_{fi})t} - 1}{\omega + \omega_{fi}} - \frac{e^{-(\omega-\omega_{fi})t} - 1}{\omega - \omega_{fi}}\right)$$

There are two frequencies in the system, $\omega_{fi} = \frac{E_f - E_i}{\hbar}$ which can be positive or negative depending on the states $|i\rangle$ and $|f\rangle$.

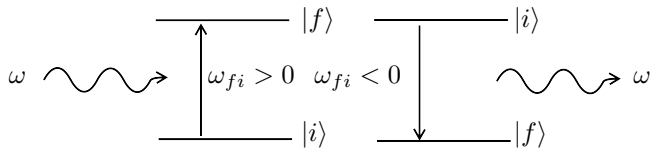

Figure 7.1: Different Frequencies of Different Transitions

If the final state has a higher energy than the initial state, then the system must absorb energy, or if the initial state has higher energy than the final state, then the system must emit energy. This means that the oscillation frequency, ω, must be positive. If there is an energy difference between $|i\rangle$ and $|f\rangle$ which allows $\omega \approx |\omega_{fi}|$ then the coefficient becomes large and therefore satisfies a resonance condition. Transitions are much more likely to occur when ω matches the level separation. The $c_f(t)$ equation can be greatly simplified during resonance, depending on the sign of $\omega_f i$.

For $\omega_{fi} < 0$ then $\frac{1}{\omega - \omega_{fi}} \ll \frac{1}{\omega + \omega_{fi}}$ and so the second term in the $c_f(t)$ equation can be neglected.

For $\omega_{fi} > 0$ then $\frac{1}{\omega - \omega_{fi}} \gg \frac{1}{\omega + \omega_{fi}}$ and so the first term in the $c_f(t)$ equation can be neglected. Defining $\Delta = \omega - \omega_{fi}$ then the equation becomes:

$$c_f(t) \approx \frac{V_o}{2\hbar} \frac{e^{-i\Delta t} - 1}{\Delta}$$

This is called the rotating wave approximation. The approximation could have been made before solving the differential equation because:

$$\dot{c}_f = -\frac{iV_o}{\hbar} \cos\omega t e^{i\omega_{fi} t} = -\frac{iV_o}{2\hbar} \left(\underbrace{e^{i(\omega + \omega_{fi})t}}_{fast} + \underbrace{e^{-i\Delta t}}_{slow} \right)$$

For a weak perturbation then the fast term, which oscillates rapidly, can be neglected as it makes very little difference on average. This cannot be done unless V_o is very small and the perturbation is very weak. The probability can now be found:

$$\mathcal{P}_{if} = |c_f(t)|^2 = \frac{V_o^2}{4\hbar^2\Delta^2} \left(e^{i\Delta t} - 1\right)\left(e^{-i\Delta t} - 1\right) = \frac{V_o^2}{\hbar^2\Delta^2} \sin^2 \frac{\Delta t}{2}$$

This is almost the same as the constant case, except the frequency is given by Δ. The value of Δ has to be constrained such that when $\Delta \neq 0$ then $\mathcal{P}_{if}$ oscillates in time if $V_o \ll \hbar\Delta$ so that $\mathcal{P}_{if} \ll 1$, but when $\Delta \to 0$ then $\mathcal{P}_{if} = \frac{V_o^2 t^2}{4\hbar^2}$. Eventually this breaks down for $t \approx \frac{2\hbar}{V_o}$, and so only short times can be studied at resonance.

7.3 Two-Level System

For a quantum two-level system with the unperturbed Hamiltonian $\widehat{\mathcal{H}}_o = E_a|a\rangle\langle a| + E_b|b\rangle\langle b|$, where $|a\rangle$ and $|b\rangle$ are the orthonormal eigenkets. The energy is $\hbar\omega_{ba} = E_b - E_a > 0$ so that $|a\rangle$ is the ground state. The system is subject to a perturbation of $\widehat{\mathcal{H}}' = V_o(|b\rangle\langle a| + |a\rangle\langle b|)$ which is turned on at $t = 0$ and where V_o is real. Perturbation theory shows that at a time, t:

$$|\psi(t)\rangle = c_a e^{-\frac{iE_a t}{\hbar}} |a\rangle + c_b e^{-\frac{iE_b t}{\hbar}} |b\rangle$$

Where $\dot{c}_b = -\frac{i}{\hbar}\langle b|\widehat{\mathcal{H}}'|a\rangle e^{i\omega_{ba}t}$. If the system starts in a state $|a\rangle$ at $t = 0$ then the probability of finding it in $|b\rangle$ at a later time is:

$$c_b(t) - c_b(0) = -\frac{i}{\hbar} \int_0^t \delta t' \langle b|\widehat{\mathcal{H}}'|a\rangle e^{i\omega_{ba}t'}$$

Where $c_a(0) = 1$ and $c_b(0) = 0$. The matrix element $\langle b|\widehat{\mathcal{H}}'|a\rangle = V_o(\langle b|b\rangle\langle a|a\rangle + \langle b|a\rangle\langle b|a\rangle)$ and due to orthonormality $\langle b|\widehat{\mathcal{H}}'|a\rangle = V_o$ so:

$$c_b(t) = -\frac{iV_o}{\hbar}\int_0^t \delta t' e^{i\omega_{ba}t'} = -\frac{V_o\left(e^{i\omega_{ba}t}-1\right)}{\hbar\omega_{ba}}$$

The probability of going from $|a\rangle \to |b\rangle$ is:

$$\mathcal{P}_{ab}(t) = |c_b|^2 = \frac{V_o^2}{\hbar^2\omega_{ba}^2}\left(e^{i\omega_{ba}t}-1\right)\left(e^{-i\omega_{ba}t}-1\right) = \frac{4V_o^2}{\hbar^2\omega_{ba}^2}\sin^2\frac{\omega_{ba}t}{2}$$

7.4 Rabi Oscillations

If there is a two-level system with orthonormal eigenkets $|0\rangle$ and $|1\rangle$ the Hamiltonian is $\widehat{\mathcal{H}}_o = E_o|0\rangle\langle 0| + E_1|1\rangle\langle 1|$. E_o and E_1 are the eigenvalues where $E_1 > E_o$ so that $|0\rangle$ is the ground state. If an extra oscillating potential is added with the form $\widehat{\mathcal{H}}' = V\cos\omega t(|0\rangle\langle 1| + |1\rangle\langle 0|)$, where V_o is a real constant. It does not have to be assumed that this is weak as the system is going to be solved without using a power series. The state is given by:

$$|\psi(t)\rangle = c_o e^{-\frac{iE_o t}{\hbar}}|0\rangle + c_1 e^{-\frac{iE_1 t}{\hbar}}|1\rangle$$

Now substituting this into the Schrödinger equation, with $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_o + \widehat{\mathcal{H}}'$ gives:

$$\left[i\hbar\dot{c}_o e^{-\frac{iE_o t}{\hbar}} + E_o c_o e^{-\frac{iE_o t}{\hbar}}\right]|0\rangle + \left[i\hbar\dot{c}_1 e^{-\frac{iE_1 t}{\hbar}} + E_1 c_1 e^{-\frac{iE_1 t}{\hbar}}\right]|1\rangle = E_o c_o e^{-\frac{iE_o t}{\hbar}}|0\rangle + E_1 c_1 e^{-\frac{iE_1 t}{\hbar}}|1\rangle + V_o\cos\omega t\left[c_o e^{-\frac{iE_o t}{\hbar}}\widehat{\mathcal{H}}'|0\rangle -$$

The $E_o c_o e^{-\frac{iE_o t}{\hbar}}|0\rangle$ and $E_1 c_1 e^{-\frac{iE_1 t}{\hbar}}|1\rangle$ cancel out, and by multiplying both sides of the equation by $\langle 0|e^{\frac{iE_o t}{\hbar}}$ then:

$$i\hbar\dot{c}_o = V_o\cos\omega t c_1 e^{-\omega_{10}t}$$

Where $\omega_{10} = E_1 - E_o$ since $\langle 0|\widehat{\mathcal{H}}'|0\rangle = 0$ and $\langle 0|\widehat{\mathcal{H}}'|1\rangle = V_o\cos\omega t$. This equation can be expanded to:

$$i\hbar\dot{c}_o = \frac{V_o c_1}{2}\left(e^{i(\omega-\omega_{10})t} + e^{-i(\omega+\omega_{10})t}\right)$$

The Schrödinger equation can also be multiplied by $\langle 1|e^{\frac{iE_1 t}{\hbar}}$ instead of $\langle 0|e^{\frac{iE_o t}{\hbar}}$ to give:

$$i\hbar\dot{c}_1 = V_o\cos\omega t c_o e^{i\omega_{10}t}$$

Where the energy difference is the opposite way around since $\langle 1|\widehat{\mathcal{H}}'|1\rangle = 0$ and $\langle 1|\widehat{\mathcal{H}}'|-\rangle = V_o\cos\omega t$. Writing this out in terms of the exponentials gives:

$$i\hbar\dot{c}_1 = \frac{V_o}{2}c_o\left(e^{-i(\omega+\omega_{10})t} + e^{-i(\omega-\omega_{10})t}\right)$$

As $c_o(0) = 1$ and $c_1(0) = 0$ then the equations can be solved exactly, but this is very difficult and long-winded. If it can be assumed that $\omega \approx \omega_{10}$ then it can be seen that each equation has a fast oscillating term and a slow oscillating term. The rotating wave approximation can be made to obtain:

$$\dot{c}_o = -\frac{iV_o}{2\hbar}c_1 e^{-i\Delta t} \quad and \quad \dot{c}_1 = -\frac{iV_o}{2\hbar}c_o e^{i\Delta t}$$

Where $\Delta = \omega_{10} - \omega$. Using the initial conditions and differentiating the $\dot{c}_o$ equation then a second order differential can be made, which can be solved exactly.

$$c_1(t) = \frac{iV_o}{\hbar\Omega_R}e^{i\Delta t}\sin\frac{\Omega_R t}{2}$$

Where $\Omega_R = \sqrt{\Delta^2 - \left(\frac{V_o}{\hbar}\right)^2}$ is the Rabi frequency. The probability of being in state $|1\rangle$ after starting in state $|0\rangle$ is:

$$\mathcal{P}_{01}(t) = |c_1|^2 = \frac{V_o^2}{\hbar^2\Omega_R^2}\sin^2\frac{\Omega_R t}{2}$$

Applying a periodic potential which oscillates harmonically in times to a quantum two-level system leads to oscillations in the probability of finding the system in one of the states, called Rabi Oscillations.

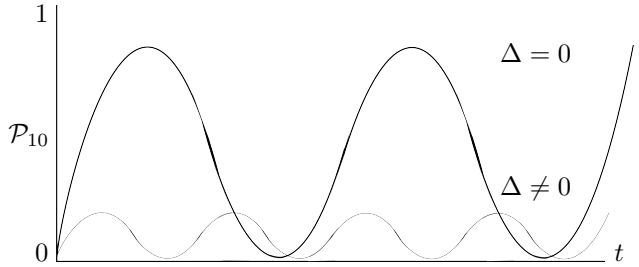

Figure 7.2: Rabi Oscillations

In resonance then the system is driven so that $\mathcal{P}_{01}(t)$ goes from zero to one, but when the system is off resonance then the oscillations are smaller so $\mathcal{P}_{01}(t) < 1$.

7.4.1 Perturbation Theory

For weak excitation then $V_o \ll \hbar\Delta$ so that $\Omega_R \approx \Delta$. This means that the probability is:

$$\mathcal{P}_{01}(t) \approx \frac{V_o^2}{\hbar^2\Delta^2} \sin^2 \frac{\Delta t}{2}$$

Which is the same probability as given by Perturbation theory.

7.4.2 Quantum Control

By applying a pulsed field on the system for a time $t = \frac{\pi}{\Omega_R}$ then the system can be pushed from a definite initial state to a definite final state. This has been done for a superconducting circuit with Josephson Junctions to make a two level system, with microwave light incident on it with a Rabi frequency of $\Omega_R = \frac{V_o}{\hbar}$ where V_o is the amplitude of the microwave radiation. By increasing the Rabi frequency then the rate of probability switching increases.

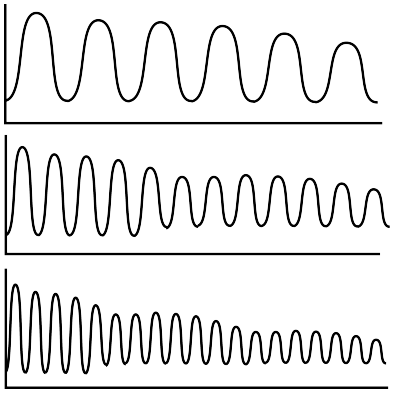

Figure 7.3: Probability Switching vs. Time at Different Rabi Frequencies

There is an exponential decay in the probability due to energy escaping from the system.

Chapter 8

Oscillator Dynamics and Coherent States

A classical harmonic oscillator has an angular frequency, ω, and mass, m. The equation of motion is $\ddot{x}+\omega^2 x = 0$ with a solution of $x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t$, where $\dot{x}(0) = \frac{p(0)}{m}$. If either $x(0)$ or $p(0)$ are non-zero then the system oscillates. In the case of a quantum harmonic oscillator then the Hamiltonian is $\widehat{\mathcal{H}} = \hbar\omega(\widehat{a}^\dagger\widehat{a} + \frac{1}{2})$, with energy eigenstates given by the number states $|n\rangle$ so that $\widehat{\mathcal{H}}|n\rangle = \hbar\omega(n+\frac{1}{2})|n\rangle$. The position expectation value is:

$$\langle\widehat{x}\rangle_t = \langle\psi(t)|\widehat{x}|\psi(t)\rangle = \langle\psi(0)|\widehat{x}_H(t)|\psi(0)\rangle$$

As it is known that:

$$\widehat{x}_H(t) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a}(t) + \widehat{a}^\dagger(t)\right) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\widehat{a}e^{-i\omega t} + \widehat{a}^\dagger e^{i\omega t}\right)$$

The for any number state $|\psi(0)\rangle = |n\rangle$ then:

$$\langle\widehat{x}\rangle_t = \langle n|\widehat{x}_H(t)|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\langle n|\widehat{a}|n\rangle e^{-i\omega t} + \langle n|\widehat{a}^\dagger|n\rangle e^{i\omega t}\right) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\langle n|n-1\rangle e^{-i\omega t} + \langle n|n+1\rangle e^{i\omega t}\right) = 0$$

This is zero due to orthonormality. For the quantum harmonic oscillator, none of the number states oscillate, which is very different to the classical harmonic oscillator, where everything above initial conditions of zero, there are oscillations.

8.1 Coherent States

By defining a coherent state $|\alpha\rangle$ which is an eigenstate of $\widehat{a}$, with an eigenvalue α so that:

$$\widehat{a}|\alpha\rangle = \alpha|\alpha\rangle$$

α in general is a complex number due to $\widehat{a}$ not being Hermitian. This means that the eigenvalues do not have to be real. Calculating $\widehat{a}^\dagger|\alpha\rangle$ is difficult, so it is easier to find the conjugation relation. For any ket $|\psi\rangle$ then $\langle\psi|\widehat{a}|\alpha\rangle = \alpha\langle\psi|\alpha\rangle$ so that $\langle\alpha|\widehat{a}^\dagger|\psi\rangle = \alpha^*\langle\alpha|\psi\rangle$. As this is true for any $|\psi\rangle$ then it can be seen that $\langle\alpha|\widehat{a}^\dagger = \langle\alpha|\alpha^*$. By writing $|\alpha\rangle$ as a superposition of number states, $|n\rangle$, then the wavefunction can be found. This is because $|n\rangle$ form a complete set and are orthonormal.

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$$

c_n now needs to be calculated. There are two answers for $\alpha|\alpha\rangle$:

$$\widehat{a}|\alpha\rangle = \alpha|\alpha\rangle$$

And:

$$\widehat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_n\widehat{a}|n\rangle = \sum_{n=1}^{\infty} c_n\sqrt{n}|n-1\rangle$$

Where $n \neq 0$ because $\widehat{a}|0\rangle = 0$. The first and second equations are equal and so by multiplying by $\langle m|$, which is another number state, it is found that:

$$\langle m| \{\alpha|\alpha\rangle\} = \langle m| \left\{ \sum_{n=1}^{\infty} c_n \sqrt{n}|n-1\rangle \right\}$$

This can be rewritten as:

$$\alpha\langle m| \left\{ \sum_{n=0}^{\infty} c_n |n\rangle \right\} = \langle m| \left\{ \sum_{n=1}^{\infty} c_n \sqrt{n}|n-1\rangle \right\}$$

On the left hand side $m = n$, but on the right $m = n-1$. The equation now becomes $\alpha c_m = c_{m+1}\sqrt{m+1}$. This shows that:

$$c_{m+1} = \frac{\alpha c_m}{\sqrt{m+1}}$$

If $\langle m-1|$ was used then:

$$c_m = \frac{\alpha c_{m-1}}{\sqrt{m}}$$

And if $\langle m-2|$ was used then

$$c_{m-1} = \frac{\alpha c_{m-2}}{\sqrt{m-1}}$$

This is a recursion relation between the coefficients. By taking the states back to $|0\rangle$ then the value of c_m is:

$$c_m = \frac{\alpha^m c_o}{\sqrt{m!}}$$

The value of c_o can be found in two ways either using:

$$\langle\alpha| = c_o^* \sum_{n'=0}^{\infty} \frac{(\alpha^*)^{n'}}{\sqrt{n'!}} \langle n'|$$

This means that:

$$\langle\alpha|\alpha\rangle = c_o c_o^* \sum_n \sum_{n'} \frac{(\alpha^*)^{n'}}{\sqrt{n'!}} \frac{\alpha^n}{\sqrt{n!}} = |c_o|^2 \sum_n \frac{(|\alpha|^2)^n}{n!}$$

Using the expansion $e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!}$ and making sure the state is normalised $\langle\alpha|\alpha\rangle = 1$.

$$\langle\alpha|\alpha\rangle = |c_o|^2 e^{|\alpha|^2} = 1$$

This can now be used to find:

$$c_o = e^{-\frac{|\alpha|^2}{2}}$$

The other way of calculating this is to use $|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$ and recall that for a normalised state $\sum_n |c_n|^2 = 1$. Expanding this gives $\sum_n \left|\frac{c_o \alpha^2}{\sqrt{n!}}\right|^2 = 1$ which can be again mapped onto the exponential function to give $c_o = e^{-\frac{|\alpha|^2}{2}}$. The result of this is that the coherent state can now be expressed as:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

8.1.1 Two Different Coherent States

As $\widehat{a}$ is not Hermitian then the eigenvalues do not have to be real and the eigenstate do not have to be orthogonal. For two coherent states, $|\alpha\rangle$ and $|\beta\rangle$ then the overlap can calculated using:

$$\langle\alpha| = e^{-\frac{|\alpha|^2}{2}} \sum_{n'=0}^{\infty} \frac{(\alpha^*)^{n'}}{\sqrt{n'1}} \langle n'|$$

And:

$$|\beta\rangle = e^{-\frac{|\beta|^2}{2}} \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{n!}} |n\rangle$$

The overlap is:

$$\langle\alpha|\beta\rangle = e^{-\frac{|\alpha|^2}{2}} e^{-\frac{|\beta|^2}{2}} \sum_{n=0}^{\infty}\sum_{n=0}^{\infty} \frac{(\alpha^*)^{n'}}{\sqrt{n'!}} \frac{\beta^n}{\sqrt{n!}} \langle n'|n\rangle$$

As the number states are orthonormal then the overlap can be written as:

$$\langle\alpha|\beta\rangle = e^{-\frac{|\alpha-\beta|^2}{2}} e^{\alpha^*\beta} = e^{-\frac{|\alpha-\beta|^2}{2}} e^{\frac{(\alpha^*\beta-\alpha\beta^*)}{2}}$$

$\alpha^*\beta - \alpha\beta^*$ is imaginary and so determines the phase of the exponential, but not the size. $\frac{|\alpha-\beta|^2}{2}$ shows that when $\alpha \approx \beta$ then $\langle\alpha|\beta\rangle \approx 1$, but when α and *beta* are different then $\langle\alpha|\beta\rangle \to 0$, so the coherent states are not orthogonal.

8.2 Classical Relation

8.2.1 Position Expectation Value

The position expectation value is:

$$\langle\alpha|\widehat{x}|\alpha\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \langle\alpha|(\widehat{a}+\widehat{a}^\dagger)|\alpha\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (\alpha\langle\alpha|\alpha\rangle + \alpha^*\langle\alpha|\alpha\rangle) = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} 2\mathbb{R}[\alpha]$$

This shows that $\langle\alpha|\widehat{x}|\alpha\rangle$ will be non-zero almost all of the time, unless α is purely imaginary, and so this is much closer to the classical dynamics or a harmonic oscillation. As a function of time the expectation value of the position is:

$$\langle\widehat{x}\rangle_t = \langle\alpha|\widehat{x}_H(t)|\alpha\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \langle\alpha|(\widehat{a}e^{-i\omega t} + \widehat{a}^\dagger e^{i\omega t})|\alpha\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t})$$

8.2.2 Momentum Expectation Value

The momentum expectation value can be calculated in a very similar way to the position to obtain:

$$\langle\widehat{p}\rangle = i\left(\frac{m\hbar}{2}\right)^{\frac{1}{2}} (\alpha^* - \alpha)$$

And the expectation value of the momentum as a function of time is:

$$\langle\widehat{p}\rangle_t = i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}} \langle\alpha|(\widehat{a}^\dagger e^{i\omega t} - \widehat{a}e^{-i\omega t})|\alpha\rangle = i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}} (\alpha^* e^{i\omega t} - \alpha e^{-i\omega t})$$

8.2.3 Classical Comparison

The quantum harmonic oscillator equation for coherent states is:

$$\langle\widehat{x}\rangle_t = \langle x(0)\rangle \cos\omega t + \frac{\langle p(0)\rangle}{m\omega} \sin\omega t$$

The classical harmonic oscillator equation is:

$$x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t$$

There is an exact comparison in the general form, with the only difference being that in the quantum system there is uncertainty on the expectation value given by the Heisenberg Uncertainty Principle.

8.2.4 Uncertainty

Coherent states minimise the uncertainty so that $\Delta x \Delta p = \frac{\hbar}{2}$. This can be found using $\Delta = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ and $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$. For this reason coherent states are also known as the minimum uncertainty states.

8.2.5 Properties

A coherent state evolves in time according to the Schrödinger equation in such a way as to remain a coherent state, although the eigenvalue changes.

$$\underset{\sim}{\widehat{U}}(t)|\alpha\rangle = e^{-\frac{i\widehat{\mathcal{H}}t}{\hbar}}|\alpha\rangle = e^{-\frac{i\omega t}{2}}|\beta\rangle$$

Where the eigenvalue $\beta = \alpha e^{-i\omega t}$ and $\widehat{a}\left(e^{-\frac{i\omega t}{2}}|\beta\rangle\right) = \beta\left(e^{-\frac{i\omega t}{2}}\right)|\beta\rangle$. The wavefunction of a coherent state is also a Gaussian of the form:

$$\psi_\alpha(x) = \langle x|\alpha\rangle = N_o e^{-\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}x - \frac{(\sqrt{2}\alpha)^2}{2}}$$

Due to a coherent state always evolving into another coherent state then the wavefunction must always be the same shape over time, which moves according to the phase factor $e^{-\frac{i\omega t}{2}}$.

Chapter 9

Density Operator

If the state vector of a system is known, then the most information possible is known about the results of any measurements. The expectation value for any observable can be calculated by $\langle\widehat{\mathcal{A}}\rangle = \langle\psi|\widehat{\mathcal{A}}|\psi\rangle$. The state of a system can alternatively be described by a density operator $\widehat{\varrho} = |\psi\rangle\langle\psi|$. The expectation values using the density operator are obtained by introducing the identity operator and a complete set of orthonormal states, such that:

$$\widehat{\mathbb{I}} = \sum_n |u_n\rangle\langle u_n|$$

This means the expectation becomes:

$$\langle\widehat{\mathcal{A}}\rangle = \sum_n \langle\psi|\widehat{\mathcal{A}}|u_n\rangle\langle u_n|\psi\rangle$$

As the brackets are just complex numbers then the order can be changed to obtain $\sum_n \langle u_n|\psi\rangle\langle\psi|\widehat{\mathcal{A}}|u_n\rangle$ which allows the density to be introduced:

$$\langle\widehat{\mathcal{A}}\rangle = \sum_n \langle u_n|\widehat{\varrho}\widehat{\mathcal{A}}|u_n\rangle$$

This is a trace operation and can be written as:

$$\langle\widehat{\mathcal{A}}\rangle = \mathrm{Tr}[\widehat{\varrho}\widehat{\mathcal{A}}]$$

The density operator has several advantages over using the state of the system, $|\psi\rangle$. It is particularly useful when the state of the system is not initially known for sure. If a system has a probability, p_1 that it is in a state $|\psi_1\rangle$ and a probability p_2 of being in $|\psi_2\rangle$ then the expectation value is:

$$\langle\widehat{\mathcal{A}}\rangle = p_1\langle\psi_1|\widehat{\mathcal{A}}|\psi_1\rangle + p_2\langle\psi_2|\widehat{\mathcal{A}}|\psi_2\rangle$$

This must be true because $p_1 + p_2 = 1$, and using classical thought, this is the expected value. It can be proved using the density operator $\widehat{\varrho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$ so the expectation value becomes:

$$\langle\widehat{\mathcal{A}}\rangle = \mathrm{Tr}[\widehat{\varrho}\widehat{\mathcal{A}}]$$

By introducing a complete set of orthonormal states then:

$$\langle\widehat{\mathcal{A}}\rangle = \sum_n \langle u_n|\widehat{\varrho}\widehat{\mathcal{A}}|u_n\rangle = \sum_n (p_1\langle u_n|\psi_1\rangle\langle\psi_1| + p_2\langle u_n|\psi_2\rangle\langle\psi_2|)\widehat{\mathcal{A}}|u_n$$

This can be expanded and reordered to get:

$$\langle\widehat{\mathcal{A}}\rangle = \sum_n p_1\langle\psi_1|\widehat{\mathcal{A}}|u_n\rangle\langle u_n|\psi_1\rangle + \sum_n p_2\langle\psi_2|\widehat{\mathcal{A}}|u_n\rangle\langle u_n|\psi_2\rangle$$

Now removing the identity, leaves the expectation value originally postulated:

$$\langle\widehat{\mathcal{A}}\rangle = p_1\langle\psi_1|\widehat{\mathcal{A}}|\psi_1\rangle + p_2\langle\psi_2|\widehat{\mathcal{A}}|\psi_2\rangle$$

When a system is in thermal equilibrium at a temperature T then the probability of the system being in a state with energy E_i is:

$$\frac{e^{-\frac{E_i}{k_B T}}}{Z}$$

Where $Z = \sum_i e^{-\frac{E_i}{k_B T}}$. The state with energy E_i is an energy eigenstate, $|\psi_i\rangle$ with an eigenvalue of E_i, so $\widehat{\mathcal{H}}|\psi_i\rangle = E_i|\psi_i\rangle$ In this case $\widehat{\varrho} = \sum_i p_i^{th}|\psi_i\rangle\langle\psi_i|$ where $p_i^{th} = \frac{e^{-\frac{E_i}{k_B T}}}{Z}$. If a system has a density operator of the form $\widehat{\varrho} = \sum_k p_k|\varphi_k\rangle\langle\varphi_k|$, where the states $|\varphi_k\rangle$ are normalised then the system has a probability, p_k of begin found in the state $|\varphi_k\rangle$. The trace of the density operator on its own is:

$$\mathrm{Tr}[\widehat{\varrho}] = \sum_n \langle u_n|\widehat{\varrho}|u_n\rangle = \sum_n \sum_k p_k \langle u_n|\varphi_k\rangle\langle\varphi_k|u_n\rangle$$

This can be rearranged, and the identity operator be removed to give:

$$\mathrm{Tr}[\widehat{\varrho}] = \sum_k p_k \langle\varphi_k|\varphi_k\rangle = \sum_k p_k = 1$$

It is always true that $\mathrm{Tr}[\widehat{\varrho}] = 2$. $\widehat{\varrho}$ does not have to be diagonal which can be seen in the case of spin-$\frac{1}{2}$ particles. $\widehat{\varrho} = |\psi\rangle\langle\psi|$ is diagonal, but since $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ then it can also be written as:

$$\widehat{\varrho} = \frac{1}{2}\left[|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right]$$

Which is not diagonal and not the same as $\widehat{\varrho} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\uparrow|$.

9.1 Properties

The density operator is Hermitian with eigenvalues, λ_i, which are real and non-negative. The eigenkets are $|j\rangle$ are orthonormal. As with all operators the density operator can be written in terms of its eigenvalues and eigenkets as:

$$\widehat{\varrho} = \sum_j \lambda_j |j\rangle\langle j|$$

λ_i is the probability of finding the system in the corresponding state $|j\rangle$ so that $\sum_j \lambda_j = 1$.

9.2 Pure and Mixing States

There are only two effects which the density operator can dictate. The first is that there is only one non-zero eigenvalue, such that $\lambda_k = 1$ and so the system is definitely in the quantum state $|k\rangle$ so that $\widehat{\varrho} = |k\rangle\langle k|$. This is called a *pure state*. The second effect is that the state is unknown and so λ_j has several non-zero eigenvalues, and so the state is called a mixed state.

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

For spin-$\frac{1}{2}$ particles a pure state can be written as $\widehat{\varrho} = |\uparrow\rangle\langle\uparrow|$, $\widehat{\varrho} = |\downarrow\rangle\langle\downarrow|$ or even $\widehat{\varrho} = \frac{1}{2}\left[|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow\right.$ which is less obvious. A mixed state for spin-$\frac{1}{2}$ particles could be $\widehat{\varrho} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$.

9.3 Expectation Values

As $\widehat{S}_z = |\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$ and $\widehat{S}_=|\downarrow\rangle = \frac{\hbar}{2}|\downarrow\rangle$ then is can be seen that:

$$\widehat{S}_z = \frac{\hbar}{2}\left[|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\right]$$

This can be written as an operator of the form $\widehat{O} = \sum_i \lambda_i |i\rangle\langle i|$. For a density operator:

$$\widehat{\varrho} = \frac{1}{4}|\uparrow\rangle\langle\uparrow| + \frac{3}{4}|\downarrow\rangle\langle\downarrow|$$

It can be seen that the kets are orthonormal and diagonal and that the probability sums to one and so the density operator seems sensible. The expectation value is:

$$\langle \widehat{S}_z \rangle = \mathrm{Tr}[\widehat{\varrho}\widehat{S}_z] = \langle \uparrow | \widehat{\varrho}\widehat{S}_z | \uparrow \rangle + \langle \downarrow | \widehat{\varrho}\widehat{S}_z | \downarrow \rangle$$

The first terms can be calculated as:

$$\langle \uparrow | \widehat{\varrho}\widehat{S}_z | \uparrow \rangle = \langle \uparrow | \left\{ \frac{1}{4} | \uparrow \rangle\langle \uparrow | + \frac{3}{4} | \downarrow \rangle\langle \downarrow | \right\} \widehat{S}_z | \uparrow \rangle = \frac{1}{4} \langle \uparrow | \widehat{S}_z | \uparrow \rangle = \frac{1}{4} \frac{\hbar}{2} \langle \uparrow | \left(| \uparrow \rangle\langle \uparrow | - | \downarrow \rangle\langle \downarrow | \right) | \uparrow \rangle = \frac{\hbar}{8}$$

The second term can be calculated in the same way:

$$\langle \downarrow | \widehat{\varrho}\widehat{S}_z | \downarrow \rangle = \frac{3}{4} \langle \downarrow | \widehat{S}_z | \downarrow \rangle = -\frac{3\hbar}{8}$$

This means the expectation value is $\langle \widehat{S}_z \rangle = \frac{\hbar}{8} - \frac{3\hbar}{8} = -\frac{\hbar}{4}$. For the non-diagonal state then this can be found in exactly the same way, but now using:

$$\langle \widehat{S}_z \rangle = \begin{pmatrix} \langle \uparrow | \widehat{S}_z | \uparrow \rangle & \langle \downarrow | \widehat{S}_z | \uparrow \rangle \\ \langle \uparrow | \widehat{S}_z | \downarrow \rangle & \langle \downarrow | \widehat{S}_z | \downarrow \rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Chapter 10

Composite Quantum Systems

Composite systems have more the one subcomponent. Examples of this type of system include atoms, molecules, solids and so on. It is simpler to focus on distinguishable particles, such as two different spin-$\frac{1}{2}$ particles. Each particle has its own ket, which describes its state. Particle 1 has $|\psi_1\rangle$ and particle 2 has $|\psi_2\rangle$. The overall state of the composite system is given by:

$$|\psi_{tot}\rangle = |\psi_1\rangle|\psi_2\rangle$$

This can also be written in shorthand as $|\psi_{tot}\rangle = |\psi_1, \psi_2\rangle$. As the magnetic moment of either spin along any set, x, y, z of axes, then there are six corresponding operators $\widehat{S}_z^{(1)}$, $\widehat{S}_x^{(1)}$, $\widehat{S}_y^{(1)}$ and $\widehat{S}_z^{(2)}$, $\widehat{S}_x^{(2)}$, $\widehat{S}_y^{(2)}$. $\widehat{S}_z^{(1)}$ only operates on kets of particle 1, and likewise for $\widehat{S}_z^{(2)}$ on particle 2. All of the operators on particle 1 commute with the operators on particle 2, such that $[\widehat{S}_z^{(1)}, \widehat{S}_x^{(2)}] = 0$, etc. Each operator has its own eigenkets and eigenvalues so for $\widehat{S}_z^{(1)}|\uparrow_1\rangle = \frac{\hbar}{2}|\uparrow_1\rangle$ and $\widehat{S}_z^{(1)}|\downarrow_1\rangle = -\frac{\hbar}{2}|\downarrow_1\rangle$. Similarly for $\widehat{S}_z^{(2)}|\uparrow_2\rangle = \frac{\hbar}{2}|\uparrow_2\rangle$ and $\widehat{S}_z^{(2)}|\downarrow_2\rangle = -\frac{\hbar}{2}|\downarrow_2\rangle$. There can also be operators, which act on booth of the particles, such as $\widehat{S}_z^{(1)}\widehat{S}_z^{(2)}|\uparrow_1\rangle|\uparrow_2\rangle = \frac{\hbar^2}{2}|\uparrow_1\rangle|\uparrow_2\rangle$, where the order of the operators does not matter as for $\widehat{S}_z^{(2)}\widehat{S}_z^{(1)}|\uparrow_1\rangle|\downarrow_2\rangle = \frac{\hbar}{2}\left(-\frac{\hbar}{2}\right)|\uparrow_1\rangle|\downarrow_1\rangle$.

10.1 Entanglement

Composite quantum systems have total states which involves kets of all the subsystems. For the two spin-$\frac{1}{2}$ system then $|\Psi_u\rangle = |\uparrow_1\rangle|\uparrow_2\rangle$ or $|\Psi_d\rangle = |\downarrow_1\rangle|\downarrow_2\rangle$. The superposition principle states that $|\Psi_{en}\rangle = \frac{1}{\sqrt{2}}[|\Psi_u\rangle + |\Psi_d\rangle]$ is also a possible state. A state that does not factorise into a product of states of its components is said to be entangled. The $|\Psi_u\rangle$ and $|\Psi_d\rangle$ states are not entangled, whereas $|\Psi_{en}\rangle$ is, because $|\Psi_{en}\rangle \neq |\varphi_1\rangle|\varphi_2\rangle$ for any states $|\varphi_1\rangle$ and $|\varphi_2\rangle$. $|\psi_c\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\uparrow_2\rangle + |\uparrow_1\rangle|\downarrow_2\rangle]$ is not entangle as it can be written $|\psi_c\rangle = |\uparrow_1\rangle \times \frac{1}{\sqrt{2}}(|\uparrow_2\rangle + |\downarrow_2\rangle)$.

10.2 Measurement

If a system begins in an entangled state $|\Psi_{en}\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\uparrow_2\rangle + |\downarrow_1\rangle|\downarrow_2\rangle]$ then by measuring the z-component of the magnetic moment of particle 1 the possible results are $\pm\frac{\hbar}{2}$. If the state is $\frac{\hbar}{2}$ then it must be $|\uparrow_1\rangle|\uparrow_2\rangle$ and so the state of particle 2 in known for certain. The same is true for a result of $-\frac{\hbar}{2}$ which confirms that particle 2 is given by the $|\downarrow_1\rangle|\downarrow_2\rangle$ state. Now because of the kets of the $\widehat{S}_x$ operator can be written as kets of the $\widehat{S}_z$ operator then by rewriting the entangled system as $|\Psi_{en}\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\uparrow_2\rangle + |\downarrow_1\rangle|\downarrow_2\rangle] = \frac{1}{\sqrt{2}}[|\rightarrow_1\rangle|\rightarrow_2\rangle + |\leftarrow_1\rangle|\leftarrow_2\rangle]$ then it can be seen that there is still uncertainty in the second particle if another direction is measured. So a particle 1 in the $|\uparrow_1\rangle|\uparrow_2$ state can have a particle 2 with equal probability of obtaining $\pm\frac{\hbar}{2}$ in the x direction. If two detectors are placed in front of particle 1 and particle 2 respectively, which measures $\widehat{S}$ in a particular direction and lights red for a value of $\frac{\hbar}{2}$ and green for a value of $-\frac{\hbar}{2}$. The detectors can be placed far enough away that there is no possible way that any communication can be made between the detectors, and the direction measured, only picked after the particles released and still there will always be a green light on one detector when there is a green light on the other, or red on one detector if the other one is red. If the

directions measured are different then the colour of the second detector will only be the same as the first detector half of the time as there is uncertainty in the second direction.