Symmetries in Quantum Mechanics

CM Hughes

Department of Mathematics and Statistics
University of Reading

March 6, 2014

Abstract

Quantum Mechanics was first conceived at the turn of the twentieth century, and since has shook the foundations of modern physics. It is a radically different viewpoint from classical physics, which works on the macroscopic scale, in contrast to quantum mechanics' microscopic domain. Though at first it was heavily debated by members of the scientific communit, it is and has been both theoretically and experimentally verified by the likes of Einstein, Heisenberg, Shrödinger, to name but a few. This being said, it is still an incomplete theory, and has yet not been concretely proved, despite strong experimental evidence for its truth.

The aim of this report is to introduce the field of quantum mechanics, and to investigate the notions of conservation/symmetry, familiar from classical mechanics. The transformations we consider here are parity/space-inversion, lattice translation and time reversal. We will build a knowledge base by analysng the operators that represent these transformation within a quantum mechanical framework.

This paper is presented for an audience that has completed a mathematics degree course up to and including second year. The specific feilds we draw upon include differential equations (MA1OD1, MA2OD2, MA2PD1), linear algebra (MA2LIN), and dynamics (MA2DY). These modules are assumed to be prior knowledge.

The main sources of information for this project are:

- An Introduction To Quantum Mechanics, D.J. Griffiths (1995), Second edition, Pearson Education ltd., 2005,
- Modern Quantum Mechanics, J.J. Sakurai (1994), First edition, Addison-Wesley Publishing Company inc. 1994.

which are referenced throughout. For specific pages, see the bibliography, which is found in section 6.

Contents

List of Tables

List of Figures

1 Fundamentals

1.1 The Wave Function

We begin by giving a basic overview of quantum theory.
The premise we are working is that, rather than the classical notion that a particle has a determinate position $x(t)$ at a given time t, said particle instead has an associated wave function, $\Psi(x,t)$, which gives the probability of finding a particle at a certain place at a given time.
For the one-dimensional case, this is obtained by Born's statistical interpretation (Griffiths, 1995):

$$\int_a^b |\Psi(t,x)|^2 \mathrm{d}x,$$

which obtains the probaility of finding particle between points $a\&b$ at time t, where the integrand is known as the probability denstity function.
This is the state that a particle is in when it is not being observed, it does not have a determinate position in space, but rather a probabilistic framework of where it is likely to be found (Figure 1).

However, upon obvservation, ie. when a measurement is taken, this wave function 'collapses' into an infintely high spike at the point where the particle is found to be (Figure 2).

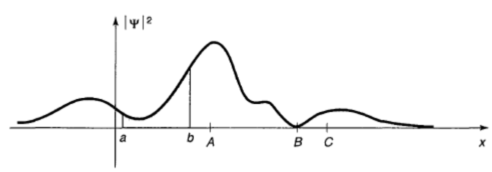

Figure 1: Open wave function (Griffiths, 1995).

There are two main ways to interpret this new way of approaching mechanics?;

- Realists believe that the particle was actually at the point at which it was found the whole time, and that quantum mechanics is an incomplete theory. They postulate that there is a 'hidden variable' as yet undiscovered, that would liquidise the inherent indeterminacy of the field.
- The orthodox position, also known as the Copenhagen interpretation, is that the

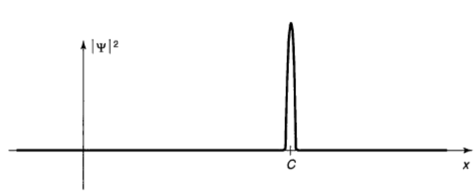

Figure 2: Collapsed Wave Function (Griffiths, 1995)

particle does not actually exist when it is not being observed, and that the act of measurement "compels the particle to assume a definite position" (Mermin, 1985). This is currently the most widely accepted view in physics.

This probabilistic approach to mechanics may seem counter intuitive, and indeed many physicists took an agnostic viewpoint in the early stages of the feild. That is until 1964, when Bell experimentally showed that these two interpretations were the only options (for details see Griffiths pg 423), annihilating agnosticism as a viable standpoint (Griffiths, 1995).
So how do we find this wave function?
Just as Newton's laws of motion form the backbone of classical mechanics, the quantum world finds similar structure, in the form of the time dependant Shröedinger equation**?** (shown here in one spatial dimension):

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi(t,x), \tag{1}$$

where $\hbar$:=Planck's constant, $m :=$ mass of our particle, and V :=potential term specific to each example of particle motion. This partial differential equation, along with the statistical interpretation, forms the fundamental foundation of quantum mechanics.

1.2 Normalisation

The first thing we must consider is a process known as normalisation. Due to the probabilistic nature of the statistical interpretation, it is clear that (Griffiths, 1995),

$$\int_{-\infty}^{\infty} |\Psi(t,x)|^2 \,\mathrm{d}x = 1, \tag{2}$$

ie. when the integral limits are infinite, the probability of finding the particle in that region is definite - it has to be found somewhere. This would be incompatible with Shrödinger's equation if it weren't for the property that, if we have $\Psi(x,t)$ as a solution, then $A\Psi(x,t)$ is also a solution, where A is any complex constant (Griffiths, 1995). The trick is to pick this constant so that equation 2 is satisfied, hence normalising the wave function. The amazing property of the Shrödinger equation is that, once a wave function has been normalised at time $t = 0$, it will stay normalised as time progresses. Let us confirm this, as without this property the entirety of Quantum Mechanics would break down.

To start, notice how the normalisation function changes with time (Griffiths, 1995):

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2\mathrm{d}x = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\Psi(t,x)|^2\,\mathrm{d}x, \tag{3}$$

$$= \int_{-\infty}^{\infty}\frac{\partial}{\partial t}(\Psi^*\Psi)\,\mathrm{d}x, \tag{4}$$

$$= \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi\right)\mathrm{d}x, \tag{5}$$

[via product rule],

$$= \int_{-\infty}^{\infty}\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)\mathrm{d}x, \tag{6}$$

[by Shrödinger equation & compex conjugation thereof],

$$= \int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right]\mathrm{d}x, \tag{7}$$

$$= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{x=-\infty}^{x=\infty}. \tag{8}$$

But, for our wave function to be normalisable in the first place, we require that $\Psi \to 0$ as $x \to \infty$ (Griffiths, 1995). Thus, we conclude that

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2\mathrm{d}x = 0,$$

ie. that the integral is constant in time. Hence, a normalised wave function stays normalised as time progresses. □

1.3 Expectation of Observables

So how do we approach this new way of doing things? If a particle's position is undeterminate, how do we even begin? Well, although we cannot say our particles definite position, we can certainly say where we expect the particle to be based on its wave function. This is given by

$$\langle x\rangle = \int_{\infty}^{\infty} x|\Psi(x,t)|^2\mathrm{d}x \text{ (Griffiths, 1995)} \tag{9}$$

Note that this is not the average of many measurements on the same particle, but rather the average of the measurements on many different particles prepared in identical states. This distinction is crucial due to the collapsing nature of the wave function - once the first measurement has been performed upon a particle, its wave function becomes a spike at a particular value, and subsequent measurements will just return that same value. (Griffiths, 1995)

We can also derive the expectation value for the momentum of our partice (Griffiths, 1995):

$$\langle \rho \rangle = m\frac{d\langle x \rangle}{dt}, \tag{10}$$

$$= m\int_{-\infty}^{\infty} x\frac{\partial}{\partial t}|\Psi(x,t)|^2 \mathrm{d}x, \tag{11}$$

$$= \frac{i\hbar}{m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x, \tag{12}$$

[as before],

$$= \frac{i\hbar}{m}\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x \tag{13}$$

[via integration by parts],

$$= -i\hbar\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial \Psi}{\partial x}\right)\mathrm{d}x, \tag{14}$$

[by parts again].

These two quantities can in fact be used to generate any dynamical quantity we require, because all dynamical quantities of interest can be expressed in terms of these two variables. If we consider our two expectation equations in slightly different form (Griffiths, 1995), with ($\hat{\_}$) terms denoting operators:

$$\langle x \rangle = \int_{-\infty}^{\infty}\Psi^*(\hat{x})\Psi\mathrm{d}x, \tag{15}$$

$$\&\langle \rho \rangle = \int_{-\infty}^{\infty}\Psi^*\left(\frac{\hbar}{\imath}\frac{\partial}{\partial x}\right)\Psi\mathrm{d}x, \tag{16}$$

we see that the only difference between the two is the operator term between the wave function and its complex conjugate. We can therefore conclude that, because any dynamical observable Q can be expressed purely in terms of position and momentum, Q's expectation is given by

$$\langle Q(x,\rho)\rangle = \int_{-\infty}^{\infty}\Psi^* Q\left(\hat{x}, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\mathrm{d}x \text{ (Griffiths, 1995)}, \tag{17}$$

ie. we replace all the x's & p's in our Q formula with $\hat{x}$ & $\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$ operators respectively, 'sandwich' it between our wave function and its conjugate, and integrate through.

1.4 Time-Dependant Shrödinger Equation

Now, for a given particle in a particular state, how do we actually find its associated wave function $\Psi(x,t)$? This is of course the basic foundation of quantum mechanics, it would be helful to know how to obtain it. As such, we reconsider the time independant Shrödinger equation:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi(x,t), \text{ coupled with initial wave function } \Psi(x,0), \tag{18}$$

for a given potential V (which for now, we keep unspecified for the sake of arguement). This is a PDE of first order in t, second order in x. We therefore utilise the method of separation of variables (Griffiths, 1995). Both the equation and the method can easily be generalised to multiple dimensions **?**, but we work here in one dimension for conciseness and clarity So, we start out in the usual fashion, and let $\Psi(x,t) = \psi(x)\phi(t)$,

$$\implies \frac{\partial \Psi}{\partial t} = \psi \frac{d\phi}{dt}, \ \& \ \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \Psi}{dx^2}\phi, \tag{19}$$

so that Shrödinger now reads

$$i\hbar\psi\frac{d\phi}{dt} = -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2}\phi + V\psi\phi, \tag{20}$$

$$\implies i\hbar\frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V. \tag{21}$$

We now have the LHS in terms of ϕ only, and the RHS interms of ψ only. This can only be the case if both sides of the equation are constant, and we label this constant E:

$$E := i\hbar\frac{1}{\phi}\frac{d\phi}{dt} \qquad \implies \frac{d\phi}{dt} = -\frac{iE}{\hbar}, \tag{22}$$

$$\&E := -\frac{\hbar}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V \qquad \implies -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi, \tag{23}$$

we therefore now have two ODEs to solve, rather than one PDE. Equation (23) is a separable ODE and is therefore easy deal with. Its solution is given by

$$\phi(t) = Ce^{-\frac{iEt}{\hbar}} \text{ (Griffiths, 1995)}, \tag{24}$$

for constant C.

Equation (24) is known as the time-independant Shrödinger equation, and its solution method depends entirely on the potential V. As the only restriction on E is that it is constant, there is an infinite set $\{E_n\}$ of these constants, each with their own associated separable solution $\psi_n(x)$ (Griffiths, 1995). The full wave function solutions then take form

$$\Psi_n(x,t) = \psi_n(x)e^{\frac{iE_nt}{\hbar}}, \tag{25}$$

where the constant C has been asborbed into the ψ_n term. These separable solutions are known as stationary states, named for the property that their time-dependence cancels out under the probability density function (Griffiths, 1995). The same can be found for position and momentum expectations $\langle x\rangle$ & $\langle p\rangle$ respectively, and therefore for any dynamical quantity (Griffiths, 1995). For example, consider the classical Hamiltonian $H(x,p) = \frac{p^2}{2m} + V(x)$ for total energy. Under the transformation defined by $x \longrightarrow \hat{x}$ & $p \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$, this becomes the Hamiltonion operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x}) \text{ (Griffiths, 1995)}, \tag{26}$$

and we notice that the LHS of the time-independant Shrödinger equation is just this operator applied to ψ, The time-dependant Shrödinger equation can therefore be written

$$\hat{H}\psi = E\psi, \tag{27}$$

and the expectation value of the Hamiltonian is given by (Griffiths, 1995),

$$\langle H \rangle = E \int_{-\infty}^{\infty} \psi^* \hat{H} \psi \tag{28}$$

$$= E \int_{-\infty}^{\infty} |\psi(x)|^2 \mathrm{d}x, \tag{29}$$

$$= E \int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{d}x, \tag{30}$$

$$= E \text{ [by normalisation]} \tag{31}$$

It can be shown that the variance of this expectation is equivalent to 0 (Griffiths, 1995). This means that any Hamiltonian measurement on a separable solution ψ_0 will definitely return the corresponding contant E_0. This puts a useful restriction on the set $\{E_n\}$, and elements that satisfy this are called allowed energies (Griffiths, 1995).
Returning to our method, the way in which we construct the full general solution for our wave function is via a linear combination of these stationary states (Griffiths, 1995):

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t), \tag{32}$$

$$= \sum_{n=1}^{\infty} c_n \psi_n(x) e^{\frac{-iE_n t}{\hbar}} \tag{33}$$

with c_n's determined by Fourier's trick, which uses the given initial wave function:

$$c_n = \int_a^b \psi_n(x)^* \Psi(x,0) \mathrm{d}x \text{ (Griffiths, 1995).} \tag{34}$$

1.5 Dirac Notation

We now recall linear algebra, and introduce Dirac notation, along with the notion of Hilbert Space. For N-dimensional vector spaces,

- a vector, denoted $|\alpha\rangle$ is represented by $\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$
- The inner product of two vectors $|\alpha\rangle$ and $|\beta\rangle$ is defined as $\langle \alpha | \beta \rangle = a_1 b_1 + a_2 b_2 + \ldots + a_N b_N$, a complex number, (ref)
- Linear transformations take matrix form:

$$|\beta\rangle = \hat{T}|\alpha\rangle \longrightarrow \boldsymbol{b} = \boldsymbol{T}\boldsymbol{a} = \begin{pmatrix} t_{1,1} & t_{1,2} & \cdots & t_{1,N} \\ t_{2,1} & t_{2,2} & \cdots & t_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ t_{N,1} & t_{N,2} & \cdots & t_{N,N} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \text{ (Griffiths, 1995)}$$

However, due to quantum vectors being infinitely dimensional, issues arise such as inner product existence **?**. We therefore only work within Hilbert space, which is defined as the set of functions $f(x)$ that satisfy

$$\int_a^b |f(x)|^2 \mathrm{d}x < \infty, \tag{35}$$

ie. all square-integrable functions for which normalisation is possible (Griffiths, 1995). The vectors, $|\alpha\rangle$, that reside in this space are known as kets, and every ket has a corresponding bra, which is denoted

$$\langle\alpha| = (a_1^*, a_2^*, \ldots, a_n^*), \tag{36}$$

for N dimensions, existing in bra space (Griffiths, 1995). Operators act upon kets from the right, while upon bras from the right. These two vector spaces have a one-to-one relation, or dual correspondance with each other, and together they make up dual space (Griffiths, 1995). The inner product is still denoted $\langle\alpha|\beta\rangle$, and all the usual inner product identities apply, namely $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$ and that $\langle\alpha|\beta\rangle$ is real.

An important result is the associative axiom, which says that, for operator $\hat{A}$,

$$(\langle\beta|)(\hat{A}|\alpha\rangle) = (\langle\beta|\hat{A})(|\alpha\rangle), \tag{37}$$

and we denote these two equivalent products as $\langle\beta|\hat{A}|\alpha\rangle$ (Sakuraii, 1994).

1.6 Hermitian Operators

We can express expectation values of dynamical quantities with inner product notation:

$$\langle Q(x,p)\rangle = \langle\Psi|\hat{Q}\Psi\rangle, \tag{38}$$

again where $\hat{Q}$ is the operator formed from Q under the transformation $x \longrightarrow \hat{x}$ and $p \longrightarrow \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$. Because measurements of observables must return real values, we have that

$$\langle Q\rangle \in \mathbb{R} \implies \langle Q\rangle = \langle Q\rangle^*, \tag{39}$$

but as complex conjugation reverses the order of terms in inner product notation, this means that we have

$$\langle\Psi|\hat{Q}\Psi\rangle = \langle\hat{Q}\Psi|\Psi\rangle, \tag{40}$$

for all possible Ψ. Thus, all operators that physically represent observables have the property

$$\langle\alpha|\hat{Q}\alpha\rangle = \langle\hat{Q}\alpha|\alpha\rangle, \tag{41}$$

for general ket $|\alpha\rangle$ and we define Hermitian operators as operators which satisfy this requirement (Griffiths, 1995).

1.7 Eigenstates, Eigenkets and Eigenvalues

A determinate state is the situation where any Q measurement is certain to return a specific value q (Griffiths, 1995). We have seen such a situation - the stationary states of the Hamiltonian, and we generalise this by noting that the variance of such an expectation would be equivalent to zero (Griffiths, 1995):

$$\begin{aligned} 0 = \sigma^2 &= \left\langle(\hat{Q} - \langle Q\rangle^2\right\rangle && (42)\\ &= \left\langle\Psi|(\hat{Q} - q)^2\Psi\right\rangle && (43)\\ &= \left\langle(\hat{Q} - q)\Psi|(\hat{Q} - q)\Psi,\right. && (44) \end{aligned}$$

but, as the only function whose inner product with itself is 0, we therefore have

$$\hat{Q}\Psi = q\Psi, \tag{45}$$

which we recognise as the eigenvalue equation for operator $\hat{Q}$, where Ψ is an eigenfunction of $\hat{Q}$, and q is its corresponding eigenvalue (Griffiths, 1995). Thus, we conclude that determinate states are simply eigenfunctions (also known as eingenkets) of $\hat{Q}$. For general ket $|\alpha\rangle$, these eigenkets are denoted $|\alpha'\rangle$, with a' representing the corresponding eigenvalue. The physical situations that they represent are defined as eigenstates.

1.8 Commutation Relation

We now define the commutation relation of two operators. In general, operators do not commute under inner products, that is that for operators $\hat{A}$ and $\hat{B}$ acting on general ket $|\alpha\rangle$,

$$\langle \hat{A}\alpha|\hat{B}\alpha\rangle \neq \langle \hat{B}\alpha|\hat{A}\alpha\rangle. \tag{46}$$

We denote the difference between these two quantities by

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}, \tag{47}$$

and is defined as the commutation relation between operators. If this value is equivalent to zero, then we say that the operators commute, and that they are invariant. Invariant operators, $\hat{Q}$, have the property

$$\hat{A}^{\dagger}\hat{Q}\hat{A} = \hat{Q}, \text{ and that } \hat{Q}|\alpha'\rangle \tag{48}$$

for $\hat{A}^{\dagger}$ defined as the dual corresponding bra space operator to $\hat{A}$, which operates on general bras from the right; $\hat{A}|\alpha\rangle = \langle\alpha|\hat{A}^{\dagger}$.

1.9 Symmetry Operators

We represent transformations like parity or lattice translation with symmetry operators which we define as

$$\hat{\xi} = 1 - \frac{i\epsilon}{\hbar}\hat{G}, \tag{49}$$

where $\hat{G}$ is defined as the Hermitian generator of $\hat{\xi}$ (Sakuraii, 1994). If the Hamiltonion operator is invariant under $\hat{\xi}$, ie. if

$$\hat{\xi}^{\dagger}\hat{H}\hat{\xi} = \hat{H} \tag{50}$$

$$\implies [\hat{G}, \hat{H}] = 0, \tag{51}$$

then it follows from the Heisenberg equation of motion that

$$\frac{dG}{dt} = 0, \tag{52}$$

ie. that $\hat{G}$ is a constant of motion **?**.

Now, consider an eigenvalue of g'. If a system is in the corresponding eigenstate represented by $|g'\rangle$ at a time, t_0, then under the time evolution operator, which is defined by

$$|g', t_0; t\rangle = \hat{U}(t, t_0)|g'\rangle \text{ (Sakuraii, 1994)}, \tag{53}$$

then the ket we obtain is also an eigenket of $\hat{G}$, with the same eigenvalue g' (Sakuraii, 1994). This is confirmed by the fact that $\hat{G}$ and time evolution commute:

$$\begin{aligned} \hat{G}|g', t_0; t\rangle &= \hat{G}[\hat{U}(t, t_0)|g' & (54)\\ &= \hat{U}(t, t_0)\hat{G}|g'\rangle & (55)\\ &= g'[\hat{U}(t, t_0)|g'\rangle]. & (56) \end{aligned}$$

1.10 Unitary Operators

If a symmetry operator, $\hat{U}$, satisfies the condition that

$$\begin{aligned} \hat{U}^\dagger \hat{U} &= \hat{U}\hat{U}^\dagger & (57)\\ &= \hat{I}, & (58) \end{aligned}$$

where $\hat{I}$ is the identity operator, then we define $\hat{U}$ as a unitary operator.

1.11 Degeneracies

The set of an operator's eigenvalues is known as the operator's spectrum. We define a degenerate spectrum as a spectrum for which there is not a one-to-one correspondence between the eigenvalues and the corresponding eigenfunctions **?**.

An important result on degeneracies is that, if

$$[\hat{H}, \hat{\xi}] = 0, \tag{59}$$

ie. if $\hat{H}$ and $\hat{\xi}$ commute, and we have $|n\rangle$ as an energy eigenket with corresponding eigenvalue, E_n, then $\hat{\xi}|n\rangle$ is also an energy eigenket (Sakuraii, 1994). To prove this we apply the Hamiltonian operator to $\hat{\xi}|n\rangle$:

$$\begin{aligned} \hat{H}(\hat{\xi}|n\rangle) &= \hat{\xi}\hat{H}|n\rangle & (60)\\ &= E_n(\hat{\xi}|n\rangle) \text{ (Sakuraii, 1994).} \qquad \square & (61) \end{aligned}$$

If $|n\rangle$ and $\hat{\xi}|n\rangle$ represent different states, then we have degeneracy **?**.

1.12 Quantum Mechanical Tunnelling

We now introduce the Heisenberg Uncertainty Principle, which asserts that the standard deviations of a particle's position and momentum expectation values, σ_x and σ_ρ respectively, satisfy the inequality

$$\sigma_x \sigma_\rho \geq \frac{\hbar}{2} \text{ (Griffiths, 1995)}, \tag{62}$$

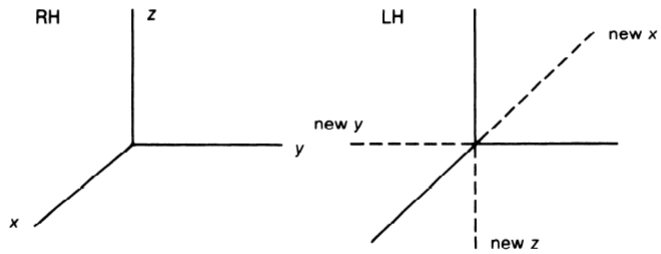

Figure 3: Left hand and right hand coordinate systems **?**

which we take as axiom (for proof, see Griffiths pg 114-116). We see from equation (62) that, if we decrease σ_x by a substantial amount, in order to be more certain of a particle's position, then σ_ρ must increase in order for (61) to still hold.

A result of this is quantum tunnelling. This is when a particle passes through a higher finite energy barrier than classical mechanics would allow.
However, this does not occur if said energy barrier is infinite.

2 Space Inversion/Parity

The Parity operator, which we denote $\hat{\pi}$, represents the space inversion transformation, which effectively takes a right hand coordinate system and transforms it into a left hand system (Figure 3). For general ket $|\alpha\rangle$, the space inverted state is denoted $\hat{\pi}|\alpha\rangle$, in usual operator fashion.

2.1 Parity Observable Expectations

Now, for the transformation we are defining, we require that

$$\langle\alpha|\hat{\pi}^\dagger\hat{x}\hat{\pi}|\alpha\rangle = -\langle\alpha|x|\alpha\rangle, \tag{63}$$

ie. that the expectation of position takes the opposite sign. This necessitates the requirement that

$$\hat{\pi}^\dagger\hat{x}\hat{\pi} = \text{-}\hat{x}, \tag{64}$$

that is that $\hat{x}$ and $\hat{\pi}$ must anticommute:

$$\hat{x}\hat{\pi} = \text{-}\hat{\pi}\hat{x}. \tag{65}$$

We now claim that the expectation of position under parity takes the form

$$\hat{\pi}|x'\rangle = e^{i\delta}|\text{-}\hat{x}'\rangle, \mathrm{d}x \tag{66}$$

where $e^{i\delta}$ is defined as a phase factor. To prove this assertion, we apply $\hat{x}\hat{\pi}$ to our eigenket (Sakuraii, 1994):

$$\hat{x}\hat{\pi}|x'\rangle = \text{-}\hat{\pi}\hat{x}|x'\rangle \tag{67}$$
$$= (\text{-}x')\hat{\pi}|x'\rangle, \tag{68}$$

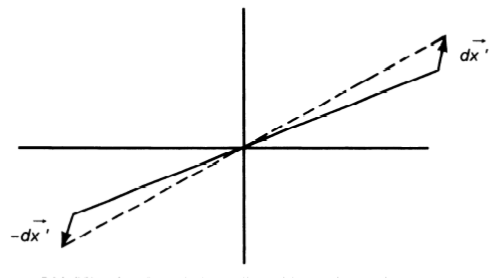

Figure 4: Parity followed by translation, and vice versa (Sakuraii, 1994)

and therefore see that $\pi|x'\rangle$ is also an eigenket of $\hat{x}$, with eigenvalue -x', so it must be the same as our position eigenket, $|\text{-}x'\rangle$, up to a phase factor. □
If we set $e^{i\delta}$, without loss of generality, we have that

$$\hat{\pi}^2|x'\rangle = |x'\rangle, \tag{69}$$

$$\implies \hat{\pi}^2 = 1 \tag{70}$$

which implies that $\hat{\pi}$ is Hermitian, and has the property that

$$\hat{\pi}^{\text{-}1} = \hat{\pi}^{\dagger} = \hat{\pi}, \tag{71}$$

with eigenvalues ± 1 (Sakuraii, 1994).

For momentum, we also expect our expectation value to be opposite in sign under space inversion (Sakuraii, 1994). To show this, we consider how parity behaves when parity is combined with translation (Figure 4). We see that applying followed by parity is equivalent to applying parity followed by opposite translation.

Mathematically, this is formulated as the requirement that (Sakuraii, 1994),

$$\hat{\pi}\hat{\Lambda}(dx') = \hat{\Lambda}(\text{-}dx')\hat{\pi}, \tag{72}$$

where $\Lambda(\lambda)$ is the translation operator, $e^{\frac{i\lambda\hat{p}}{\hbar}}$ (Sakuraii, 1994). It follows that

$$\hat{\pi}\left(1 - \frac{i\hat{p}(dx')}{\hbar}\right)\hat{\pi}^{\dagger} = 1 + \frac{i\hat{p}(dx)}{\hbar}, \tag{73}$$

from which it is clear that

$$[\hat{\pi}, \hat{p}] = 0, \tag{74}$$

ie. that $\hat{\pi}$ and $\hat{p}$ commute, so that

$$\hat{\pi}\hat{p}\hat{\pi} = \text{-}\hat{p}. \tag{75}$$

With these two expectation values, we can construct the expectation of any dynamical observable, $\hat{Q}(x, p)$, in the manner discussed in section 1.

2.2 Wave Function Behaviour Under Parity

For our wave function, $\psi(x,t)$, for a state represented by $|\alpha\rangle$, which we henceforth denote by

$$\psi(x') = \langle x'|\alpha\rangle. \tag{76}$$

When parity is applied, our wave function takes the form

$$\psi(\text{-}x') = \langle \text{-}x'|\hat{\pi}|\rangle = \langle \text{-}x'|\alpha\rangle \text{ (Sakuraii, 1994)} \tag{77}$$

If we have $|\alpha\rangle$ as an eigenket of parity with eigenvalues ± 1, then

$$\hat{\pi}|\alpha\rangle = \pm|\alpha\rangle \text{ (Sakuraii, 1994)}, \tag{78}$$

and its corresponding wave function is

$$\langle x'|\hat{\pi}|\alpha\rangle, \tag{79}$$

and we say that the state represented by $|\alpha\rangle$ is even or odd under parity respectively, based on the sign choice its wave function takes in the equation

$$\psi(\text{-}x') = \pm\psi(x'). \tag{80}$$

However, because momentum and parity anticommute, a momentum eigenket will not nessecarily be an eigenket of parity (Sakuraii, 1994).

For the hamiltonian operator, we have the following theorem (Sakuraii, 1994):

For $[\hat{H},\hat{\pi}] = 0$ ($\hat{H}$ and $\hat{\pi}$ commute) and $\hat{H}|n\rangle = E_n|n\rangle$ ($|n\rangle$ is a non-degenerate eigenket of $\hat{H}$ with eigenvalue E_n), $|n\rangle$ is also an eigenket of the parity operator, $\hat{\pi}$.

To prove this theorem (Sakuraii, 1994), first notice that $\frac{1}{2}(1 \pm \hat{\pi}|n\rangle$ is a parity eigenket with eigenvalues ± 1.
But this is also an energy eigenket, with eigenvalue E_n, and this means that $|n\rangle$ and $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ must represent the same state (REF). Otherwise, we would have a degeneracy that contradicts our assumption. We therefore conclude that $|n\rangle$ must also be an eigenket of parity, with corresponding eigenvalues ± 1. □

2.3 Symmetric Double Well Potential

Figure 5 shows the symmetric double wave potential for the two lowest lying states. We denote the symmetric case $|S\langle$ and $|A\rangle$.

It can be shown (see Sakurai pg 257 for details), and indeed inferred from the figure, that

$$E_A > E_S. \tag{81}$$

We can form the kets:

$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) \tag{82}$$

$$\&|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle), \tag{83}$$

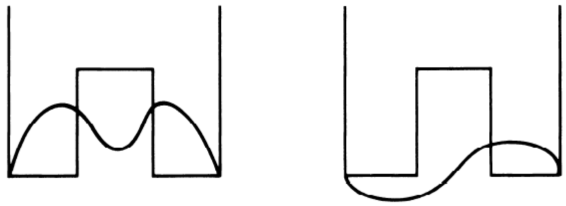

Figure 5: Symmetric Double Well Potential (Sakuraii, 1994)

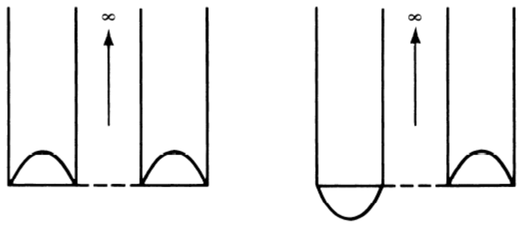

Figure 6: Symmetric Double Well Potential with infinite energy barrier (Sakuraii, 1994)

whose wave functions are respectively concentrated in the right hand well and left hand well (Sakuraii, 1994). Now, under parity, $|R\rangle$ and $|L\rangle$ are unchanged, ie. they are not $\hat{\pi}$ eigenstates, and they are also not eigenstates of $\hat{H}$ (Sakuraii, 1994). To see this, we consider a system represented by $|R\rangle$ at $t = 0$ (Sakuraii, 1994). By applying the time evolution operator, we see that at a later time, δt, we have

$$|R, t_0 = 0; t\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{iE_S t}{\hbar}}|S\rangle + e^{-\frac{iE_A t}{\hbar}}|A\rangle\right) \tag{84}$$

$$= \frac{1}{\sqrt{2}}e^{\frac{-iE_S t}{\hbar}}\left(|S\rangle + e^{\frac{-(E_A - E_S)t}{\hbar}}|A\rangle\right). \tag{85}$$

When time, $T \equiv \frac{2\pi\hbar}{2(E_A - E_S)}$, is subbed into this equation, the system evolves to a point where it is represented by $|L\rangle$ (REF). At time $t = 2T$, the system has reverted back to $|R\rangle$ state. We therefore have oscilatory behavior, with angular frequency $\omega = \frac{E_A - E_S}{\hbar}$.If we make the barrier in between the wells in finite (Figure 6), this behaviour ceases, suggesting that the oscillation is a result of quantum tunneling. In this case, a state represented by $|R\rangle$ will stay unchanged as time progresses, ie. oscillation time is equivalent to ∞ (REF). This example shows a state which is antisymmetrical despite the symmetry of the Hamiltonian under space inversion - where there is degeneracy, symmetry is not necessarily observed by $|S\rangle$ and $|A\rangle$.

2.4 Parity Selection Rule

We now claim that, when $\hat{\pi}|\alpha\rangle = \epsilon_\alpha|\alpha\rangle$ and $\hat{\pi}|\beta\rangle = \epsilon_\beta|\beta\rangle$, ie. if $|\alpha\rangle$ and $|\beta\rangle$ are parity eigenvalues with respective eigenvalues ϵ_α and ϵ_β, we have that $\epsilon_\alpha = -\epsilon_\beta$. (Sakuraii, 1994)

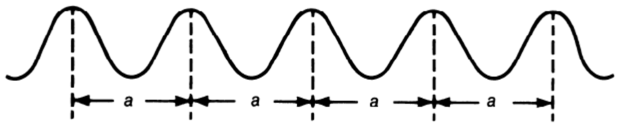

Figure 7: Potential $V(x \pm a) = V(x)$ for finite energy barriers between lattice sites (Sakuraii, 1994)

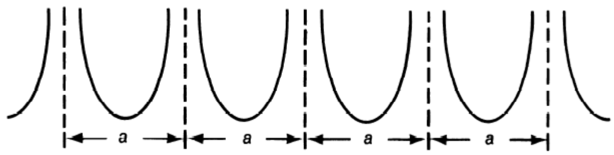

Figure 8: Potential $V(x \pm a) = V(x)$ for infinite energy barriers between lattice sites (Sakuraii, 1994)

To prove this assertion, we notice that

$$\langle\beta|\hat{\pi}^{-1}\hat{\pi}\hat{x}\hat{\pi}^{-}1\hat{\pi}|\alpha\rangle = \langle\beta|\hat{x}|\alpha\rangle \tag{86}$$

$$= \epsilon_\alpha\epsilon_\beta\,(\text{-}\langle\beta|\hat{x}|\alpha\rangle)\,, \tag{87}$$

which cannot happen for finite nonzero $\langle\beta|\hat{x}|\alpha\rangle$, unless ϵ_α and ϵ_β are sign opposite. □

This means that the parity odd operator, $\hat{x}$, connects states of opposite parity. this can in fact be generalised for any parity odd operator (REF), and similarly for parity even operators connecting states of the same parity.

3 Lattice Translation

3.1 Lattice Translation Operator

Lattice translation is the operator equivalent to the classical equivalent of the same name.

Now, consider a one-dimensional a-periodic potential, $V(x \pm a) = V(x)$ for (a) finite energy barriers between lattice sites (Figure 3), and (b) infinite energy barriers (Figure 4) (Sakuraii, 1994).

The lattice translation operator, $\hat{\tau}(l)$, has the property that (Sakuraii, 1994):

$$\hat{\tau}(l)x\hat{\tau}(l) = x + l \tag{88}$$

$$\implies \hat{\tau}^\dagger(a)V(x)\hat{\tau}(a) = V(x+a) \tag{89}$$

$$= V(x) \text{ in our case.} \tag{90}$$

Kinetic energy is invariant under translation (Sakuraii, 1994), and therefore the Hamiltonian satisfies

$$\hat{\tau}^\dagger(a)H\hat{\tau}(a) = H, \tag{91}$$

and this together with the fact that $\tau(a)$ is unitary (show & ref) implies that

$$[\hat{H}, \hat{\tau}(a)] = 0. \tag{92}$$

This means that the matrix representations of $\tau(\hat{a})$ and $\hat{H}$ can be diagonalised simultaneously (ref). However, though $\hat{\tau}$ is unitary, it is not Hermitian, and we therefore expect it's eigenvalues to be complex numbers of modulus 1 (Sakuraii, 1994).

We first consider case (b), where the energy boundaries between lattice sites are infinite, and there is no possibility of quantum tunnelling. We denote $|n\rangle$ as the ket corresponding to the n'th lattice site. This is an eigenket of total energy, and we denote the corresponding eigenvalue as E_0:

$$\hat{H}|n\rangle = E_0|n\rangle. \tag{93}$$

It's wave function $\langle x'|n\rangle$ is only finite in the lattice site it is localised in (Sakuraii, 1994). However, note that all lattice sites are identical when they are assumed to be distinct, and therefore all of these states have the same corresponding eigenvalue E_0, there therefore exists an infinitefold degeneracy (Sakuraii, 1994). Now, notice that

$$\hat{\tau}(a)|n\rangle = |n+1\rangle, \tag{94}$$

which means that $|n\rangle$ is not an eigenket of the lattice translation operator, despite the fact is it an eigenket of the Hamitonian. This fits in with out earlier theorem on symmetry and degeneracy. For symmetry, we must find a simultaneous eigenket of $\hat{H}$ and $\hat{\tau}(a)$ (Sakuraii, 1994).

We can accomplish this, as before, by forming the linear combination ,

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle, \tag{95}$$

for $\theta \in [-\pi, \pi]$ is a real paramater (Sakuraii, 1994). Due to the fact that $|n\rangle$ is an n-independant energy eigenket with corresponding θ-independant eigenvalue. We then apply $\tau(a)$ to show that

$$\tau(a) = \sum_{n=-\infty}^{\infty} e^{in\theta}|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}, \tag{96}$$

$$= e^{-i\theta}|\theta\rangle \tag{97}$$

ie. that $|n\rangle$ is also an eigenket of $\hat{\tau}(a)$.

We now approach the (a) case, a much more physically realistic situation. As before, we represent the n'th lattice site as localised ket $|n\rangle$, with the property defined by equation 53 still holding. But now, due to the fact the energy barriers between sites are not infinite, there is a possibility of quantum tunnelling occurring, ie. that the wave function $\langle x'|n\rangle$ could be finite in lattice sites other than that represented by $|n\rangle$. For the $|n\rangle$ basis, the Hamiltonian matrix has equal diagonal elements due to $\tau(l)$ invariance:

$$\langle n|H|n\rangle = E_0 \tag{98}$$

where E_0 is still n-independant (Sakuraii, 1994). Due to the possibility of tunnelling, this matrix may not be completely diagonal. However if we set the energy barriers high, we can legitimately assume that non-diagonal elements are negligible (Sakuraii, 1994). We formulate this mathematically as the requirement that

$$\langle n'|\hat{H}|n\rangle \neq 0 \Longleftrightarrow n' = 1 \text{ or } n' = n+1 \tag{99}$$

This is known as the tight binding approximation. We now, as before, define the linear combination

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle, \tag{100}$$

which is clearly a $\tau(l)$ eigenket for energy, by the same arguement as before. To check for energy, we apply $\hat{H}$ (Sakuraii, 1994):

$$\hat{H}\sum e^{in\theta}|n\rangle = E_0\sum e^{in\theta}|n\rangle - \triangle\sum e^{in\theta}|n+1\rangle - \triangle\sum e^{in\theta}|n-1\rangle, \tag{101}$$

$$[\text{for the substitution } -\triangle = \langle n\pm 1|\hat{H}|n\rangle],$$

$$= E_0\sum e^{in\theta}|n\rangle - \triangle\sum\left(e^{in\theta-i\theta} + e^{in\theta+i\theta}\right)|n\rangle, \tag{102}$$

$$= (E_0 - 2\triangle\, cos\theta)\sum e^{in\theta}|n\rangle, \tag{103}$$

and we see that our energy eigenket is now θ-dependant. As $\triangle$ becomes finite, our previous degeneracy no longer applies (Sakuraii, 1994), and we therefore have a continuous spectrum of eigenvalues in the interval $[(E_0 - 2\triangle)(E_0 + 2\triangle)]$.

3.2 Wave Function Behaviour Under Lattice Translation

We now investigate the behavior of a wave function under lattice transformation. For the lattice translated state $\hat{\tau}(a)|\theta\rangle$, we have the wave function

$$\langle x'|\hat{\tau}(a)|\theta\rangle = \langle x'-a|\theta\rangle \text{ REF} \tag{104}$$

This, together with our earlier substitution, results in

$$\langle x'|\hat{\tau}(a)|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle, \tag{105}$$

$$\Longrightarrow \langle x'-a|\theta\rangle = \langle x'|\theta\rangle e^{-i\theta} \text{ (Sakuraii, 1994).} \tag{106}$$

To solve this equation we set

$$\langle x'|\theta\rangle = e^{ikx'}u_k(x') \tag{107}$$

with $\theta = ka$, for a-periodic function $u_k(x')$ (Sakuraii, 1994). Thus, we see that the wave function of $|\theta\rangle$, eigenket of $\hat{\tau}$ can be written in the form of a product between plane-wave $e^{ikx'}$ and an a-periodic function. This result is known as Bloch's Theorem, and it holds even if the tight binding approximation is lifted (Sakuraii, 1994).

Now, having established our previous result, we now see that as we vary θ in the range $[-\pi,\pi]$, our k $(\equiv \frac{\theta}{a})$ varies from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$, and the energy eigenvalue is now k-dependant:

$$E(k) = E_0 - 2\triangle\, cos(ka), \tag{108}$$

which we also notice is independant of the shape of our potential when the tight binding approximation is applied (Sakuraii, 1994). Due to quantum tunnelling, the infinitefold degeneracy is lifted entirely (Sakuraii, 1994), and our allowed energies form a continuous spectrum in the range $[(E-2\triangle),(E+2\triangle)]$, which is known as the Brillouin Zone (Sakuraii, 1994).

4 Time Reversal

4.1 Antiunitary Operators

Before we can consider the time reversal, or reversal of motion operator, we must first establish some important results. Consider the general symmetry operations, for unitary operator $\hat{U}$,

$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle = \hat{U}|\alpha\rangle, \text{ and } |\beta\rangle \longrightarrow |\tilde{\beta}\rangle = \hat{U}|\beta\rangle. \tag{109}$$

For unitary operations, such as parity or lattice translation, inner products are preserved (Sakuraii, 1994), ie that

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle. \tag{110}$$

This is due to the fact that if $\hat{U}$ is unitary, then

$$\hat{U}\langle\beta|\alpha\rangle = \langle\beta|\hat{U}^{\dagger}\hat{U}|\alpha\rangle \tag{111}$$

$$= \langle\beta|\alpha\rangle. \tag{112}$$

However, time-reversal is not unitary (Sakuraii, 1994), and this means that this property does not hold. We therefore impose the slightly weaker restriction:

$$|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|, \tag{113}$$

whose non-trivial satisfaction implies that

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* \tag{114}$$

$$= \langle\alpha|\beta\rangle, \tag{115}$$

and if this is the case we define our transformation as antiunitary, with $\hat{U}$ defined as the corresponding antiunitary operator (Sakuraii, 1994). If $\langle\tilde{\beta}|\tilde{\alpha}\rangle \neq \langle\beta|\alpha\rangle^*$, but the operator satisfies

$$\hat{U}\left(c_1|\alpha\rangle + c_2|\beta\rangle\right) = c_1\hat{U}|\alpha\rangle + c_2\hat{U}|\beta\rangle, \tag{116}$$

for constants c_1 and c_2, then we say that $\hat{U}$ is antilinear (Sakuraii, 1994). Note that, for antilinear operators, we avoid bra operations, because Dirac's ket and bra notation was intended for use with linear operators, not antilinear (Sakuraii, 1994). However, we can still use triple inner product notation, as long as we define this as, for antilinear operator $\hat{S}$

$$\langle\beta|\hat{S}|\alpha\rangle = (\langle\beta|)(\hat{S}|\alpha\rangle|), \tag{117}$$

$$\neq (\langle\beta|\hat{S})(|\alpha\rangle) \text{ (Sakuraii, 1994)}, \tag{118}$$

Now, antiunitary operators can be written in the form

$$\hat{S} = \hat{U}\hat{K}, \tag{119}$$

ie. as the product of a unitary operator, $\hat{U}$, and the complex conjugation operator, $\hat{K}$ (Sakuraii, 1994). The complex conjugation operator has the property that, for general ket $|\alpha\rangle$:

$$\hat{K}c_1|\alpha\rangle = c_1^*\hat{K}|\alpha\rangle \text{ (Sakuraii, 1994)}, \tag{120}$$

and therefore it follows that under the complex conjugation operation, for corresponding $|\alpha\rangle$ eigenvalue a',

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle = \sum_{a'} \langle a'|\alpha\rangle^* \hat{K}|\alpha\rangle \tag{121}$$

$$= \sum_{a'} \langle a'|\alpha\rangle|a'\rangle. \tag{122}$$

This property allows us to confirm our earlier equation:

$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle = \sum_{a'} \langle a'|\alpha\rangle^* \hat{U}\hat{K}|a'\rangle, \tag{123}$$

$$= \sum_{a'} \langle a'|\alpha\rangle^* \hat{U}|a'\rangle, \tag{124}$$

$$= \sum_{a'} \langle a'|\alpha\rangle \hat{U}|a'\rangle. \tag{125}$$

Similarly,

$$|\beta\rangle = \sum_{a'} \langle a'|\beta\rangle^* \hat{U}|a'\rangle \longleftrightarrow |\tilde{\beta}\rangle = \sum_{a'} \langle a'|\beta\rangle\langle a'|\hat{U}^*\rangle, \tag{126}$$

with $\longleftrightarrow$ denoting dual correspondance, and therefore the inner product of $|\tilde{\beta}\rangle$ and $|\tilde{\alpha}\rangle$ is given by

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a''}\sum_{a'} \langle a''|\beta\rangle\langle a''|\hat{U}^\dagger\hat{U}|a'\rangle\langle\alpha|a'\rangle, \tag{127}$$

$$= \sum_{a'} \langle\alpha|a'\rangle\langle a'|\beta\rangle \tag{128}$$

$$= \langle\alpha|\beta\rangle \tag{129}$$

$$= \langle\beta|\alpha\rangle^*, \tag{130}$$

so our requirements hold. For our purposes, we need only consider transformations that are unitary or antiunitary (Sakuraii, 1994).

4.2 Time Reversal Operator

We now turn to the time reversal operator, denoted $\hat{\Theta}$. Let us first consider the classical situation that this operator represents. Figure 7 shows a particle halting its motion at time $t = 0$, and reversing its trajectory along the same path as before.

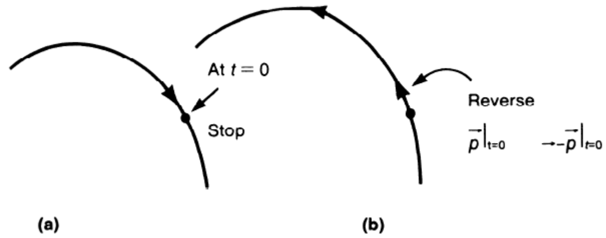

Figure 9: Classical time reversal representation (Sakuraii, 1994)

This is mathematically formulated by the requirement that, if we have $\boldsymbol{x}(t)$ as a solution to

$$m\ddot{\boldsymbol{x}} = -\bigtriangledown V(\boldsymbol{x}) \tag{131}$$

Then we also have -$\boldsymbol{x}(t)$ as a possible solution (Sakuraii, 1994).

For the quantum sitiuation, our Shrödinger equation reads

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\bigtriangledown + \hat{V}\right)\psi. \tag{132}$$

It is clear from the first order time derivative that $\psi(x,t)$ is not a solution, however complex conjugation of our Shrödinger equation reveals $\psi^*(x,-t)$ as a solution (Sakuraii, 1994). We therefore conclude that applying the time reversal operator to a wave function is equivalent to taking its complex conjugate:

$$\hat{\Theta}\psi = \hat{\Theta}\langle x'|\alpha\rangle \tag{133}$$
$$= \langle x'|\alpha\rangle^*. \tag{134}$$

So, let us now analyse the actual behaviour of the time reversal operator, $\hat{\Theta}$. Consider the time reversed system represented by

$$|\alpha\rangle \longrightarrow \hat{\Theta}|\alpha\rangle, \tag{135}$$

given for an initial time $t = 0$. At a slightly later time, δt, our system is found in the state represented by

$$|\alpha, t_0 = 0; t = \delta t\rangle = \left(1 - \frac{i\bar{H}}{\hbar}\delta t\right)|\alpha\rangle, \tag{136}$$

for $\hat{H}$ denoting the Hamiltonion operator that defines time reversal (Sakuraii, 1994). First, we subject $|\alpha\rangle$ at $t = 0$ to the time reversal operator:

$$\hat{\Theta}|\alpha, t_0 = 0; t = \delta t\rangle = \hat{\Theta}\left(1 - \frac{i\bar{H}}{\hbar}\delta t\right)|\alpha\rangle, \tag{137}$$
$$= \left(1 - \frac{i\bar{H}}{\hbar}\delta t\right)\hat{\Theta}|\alpha\rangle, \text{ if motion is symmetrical.} \tag{138}$$

For symmetrical motion in time, this must hold for any ket, $|\gamma\rangle$, ie. we must have the identity (Sakuraii, 1994):

$$-i\hat{H}\hat{\Theta}|\gamma\rangle = \hat{\Theta}i\hat{H}|\gamma\rangle. \tag{139}$$

Now, if $\hat{\Theta}$ is unitary, it follows from here that

$$-\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H}, \tag{140}$$

which implies that an energy eigenket with corresponding eigenvalue E_0 would satisfy the condition

$$\hat{H}\hat{\Theta}|n\rangle = -\hat{\Theta}\hat{H}|n\rangle \tag{141}$$

$$= (-E_n)\hat{\Theta}|n\rangle, \tag{142}$$

ie. that $\hat{\Theta}|n\rangle$ is an energy eigenket with corresponding eigenvalue E_n (Sakuraii, 1994). This is a clear contradiction, and to see this consider a free particle (for details, see Griffiths section 2.4). The lowest energy that it can possibly have is zero (representing the particle at rest (Sakuraii, 1994). this means that the $(-\infty, 0)$ of the E_n spectrum would have to be discarded, and this issue forces us to draw the conclusion that the time reversal operator must not be unitary.
On the other hand, if $\hat{\Theta}$ is antiunitary, we instead have the situation;

$$\hat{\Theta}\hat{H} = \hat{H}\hat{\Theta}. \tag{143}$$

This equation does not to lead to the contradiction found above, and the solutions it admits are physically sensible. We therefore take the time reversal operator to be antiunitary (Sakuraii, 1994).

5 Conclusion

We have seen the that the operators that represent quantum mechanical symmetry transformation behave very differently to their classical counterparts. This is due to the inherent indeterminacy of the field, discussed in section 1.

This radical shift in physics is extremely counter-intuitive. Though it has not been concretely proved as yet, it has strong support from experimental evidence and theoretical logic alike, and though we have only sratched the surface of the feild in this paper, the author hopes that it will initiate the reader into this new way of doing things.

6 Bibliography

An Introduction To Quantum Mechanics, Second Edition, pg 3, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 3, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 5, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 3-4, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 423, Pearson Education ltd., 2005

Is the Moon Really There When Nobody Looks?, pg 38, Physics Today, 1985

An Introduction To Quantum Mechanics, Second Edition, pg 12, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 12-13, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 13-14, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 14, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 15, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 15, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 16, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 17, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 17, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 24-29, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 28, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 99, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 26, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 26, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 27, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 27, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 27, Pearson Education ltd., 5005

An Introduction To Quantum Mechanics, Second Edition, pg 27, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 28, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 28, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 93-94, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 94, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 112, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 112, Pearson Education ltd., 2005

Modern Quantum Mechanics, pg 16-17, Addison-Wesley Publishing Company inc., 1994

An Introduction To Quantum Mechanics, Second Edition, pg 97, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 99, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 99, Pearson Education ltd., 2005

An Introduction To Quantum Mechanics, Second Edition, pg 99, Pearson Education ltd., 2005

Modern Quantum Mechanics, pg 249, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 250, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 16-17, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 250, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 250, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 250, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 16-17, Addison-Wesley Publishing Company inc., 1994

An Introduction To Quantum Mechanics, Second Edition, pg 19, Pearson Education ltd., 2005

Modern Quantum Mechanics, pg 252, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 252, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 252, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 252-253, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 253, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 253, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 352, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 254, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 254, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 255, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 255-256, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 256, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 257, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 257, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 257, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 257, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 258, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 259-260, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 261, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 261, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 261, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 262, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 263, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 264, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 264, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 265, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 268, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 269, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 269, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 269, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 273, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 273, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 269, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 269, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 271, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 267, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 266, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 271-272, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 272, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 272, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 272, Addison-Wesley Publishing Company inc., 1994

Modern Quantum Mechanics, pg 273, Addison-Wesley Publishing Company inc., 1994