Quantum Mathematics

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2022 - 2023

Foreword

Quantum physics is at the bleeding edge of science: its laws will dictate the next century of scientific and technological development. At the core of these concepts is math, which ultimately forms the fabric of the universe.

Quantum is a daunting term in pop culture and it's often invoked to patch plot holes in Hollywood blockbusters. Quantum physics has even entered the realm of "Rocket Science" and "Brain Surgery", as something that is beyond comprehension without the most sophisticated degrees. However, it's a firm belief of mine that complex topics shouldn't be gatekept: anyone armed with curiosity should be able to explore and learn. This, of course, includes the Quantum realm. I am someone often armed only with curiosity, and it can be hard to even begin to explore an topic on my own. This independent study, therefore, has a dual purpose. I want to learn about the quantum realm, and I want to make it easier for the next person to as well.

Why quantum? Why math? The easy answer is that I am interested in both of quantum physics and math. As most easy answers, this oversimplifies things. The more complex answer has two parts: quantum physics is weird, cool, and new, and I have been fortunate enough to be exposed to several applications of quantum physics. Quantum lies on the bleeding edge of human knowledge, and is our best attempt at describing this mysterious universe we have found ourselves inhabiting. The unknown has always captured my interest, and quantum is no different. Besides, it tells us that most of our fundamental perceptions of the universe are wrong (there's such thing as transportation, and communication without transmitting information, but no such thing as passive observation). Quantum math, specifically, covers a wide variety of topics, typically taught independently, including linear algebra, complex number, and a specific form of notion used in the quantum fields. Learned together, with the added context of quantum topics, their interconnections and relevance will be far more apparent, and a solid foundation for any future pursuit of the quantum fields will be developed.

In short, quantum physics is paving the way as we attempt to the understand

the universe. I am exploring the mathematical elements of quantum physics to set a foundation for future personal exploration, and along the way I want to make quantum more accessible.

1 Linear Algebra and Complex Numbers Crash Course

1.1 Complex Numbers

If i is the square root of -1, then $i^2 = -1$. $-1x - 1 = 1$. So far so good. This is illustrated below as a rotation. So, if multiplying by i rotates the arrow, and

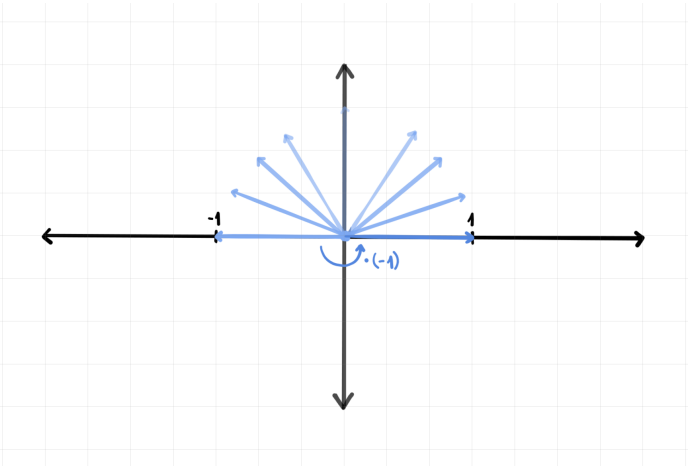

Figure 1: Rotation of -1

multiplying by i2 rotates the arrow from -1 to 1, multiplying by a single i will rotate the arrow halfway, as pictured below. An interesting development emerges! Imaginary numbers (we were using i in this example) act almost like a second dimension and axis. The numbers we use are actually two dimensional; we just tend to tend to use only the classic number line.

The name of these two dimensional numbers is "complex numbers". The formal definition of complex numbers is "any number written in from $z = a + bi$, where a and b are real numbers." a is called the real part of the complex number - $\text{Re}(z)$, and b is the imaginary part $-\text{Im}(z)$.

The graph above is called a "complex plane", which is used to visualize complex numbers using the x-axis to denote the real part, and the y-axis to denote the imaginary part. Complex numbers, $z = a + bi$, can be represented as a point on the complex plane where a is the x value and b is the y value.

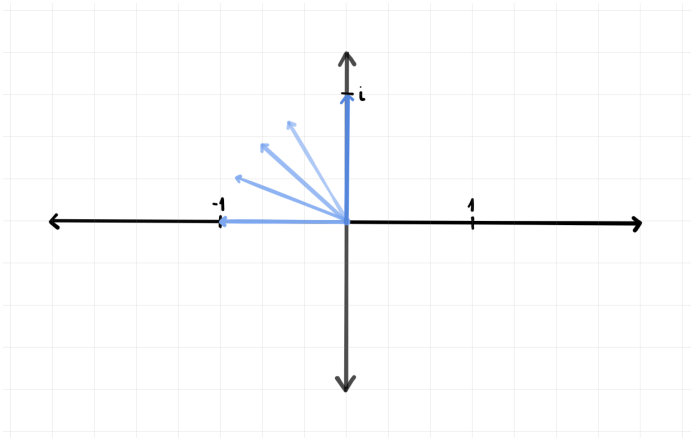

Figure 2: Rotation of i

Like with real numbers, there's a variety of operations that can be preformed on complex numbers. The summary of properties can be found in the notes below, but the general rule is that real and imaginary numbers cannot be combined. Real numbers can be combined with real numbers, and imaginary numbers can be combined with imaginary numbers, but they cannot be inter-combined.

There's a couple of other definitions that form the foundation of complex numbers:

- Complex Conjugate: the complex conjugate of a complex number $a + bi$ is $a - bi$.
- Modulus: the modulus of a complex number $a + bi$ is the square root of $a^2 + b^2$. This number will always be real and positive. The modulus represents the distance from the origin to the complex number on the complex plane.

Complex numbers, however, when represented as $a + bi$ can be hard to work with. Thankfully, the polar form of the equation offers some help. The polar form deals with the angle (θ) and length ($\bar{z}$) of the complex number, as shown below, instead of representing the number in terms of x and y values. Theta is known as the argument of the complex number. If we use this polar form, a can be expressed as the $\bar{z} * \cos$ and b can be expressed as $\bar{z} * \sin\theta$. Therefore, $z = a + bi$ can be rewritten as $z = \bar{z} * \cos\theta + \sin\theta i$. This is immensely helpful because of Euler's Formula: $e^{i(\theta)} = \cos\theta + \sin\theta i$. Putting all of this together, $z = \bar{z}e^{i\theta}$.

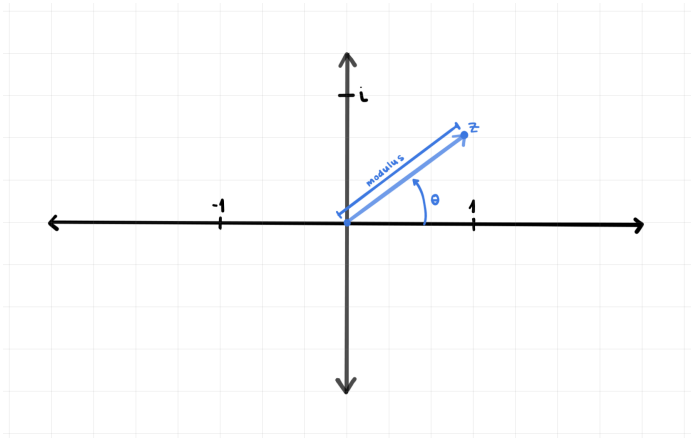

Figure 3: Modulus and Angle of a Complex Number

1.2 Linear Algebra Basics

Vectors

Most of Quantum Mathematics is linear algebra based, so it is absolutely essential to grasp the basics before moving on to more complex and niche mathematical topics. To quote The Mathematics of Quantum Mechanics, "the language of quantum mechanics - linear algebra".

Vectors are at the center of linear algebra. Vectors, basically, are a way of representing something that can't be described with a single number. Think about a coordinate system for example: A vector can be shown visually on the graph as an arrow starting at one point and going to another. For simplicity's sake, let's always place the "tail" (non-arrow) side of the vector on the origin. The point that the arrow lands on, let's call (x_1, y_1). To refer to this point, we have to use 2 numbers. Or, we can use the vector notation: $\left(\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \right)$. So, in essence, a vector is a way of representing multiple numbers.
There are two types of vectors: row vector and column vectors. The vector above is a column vector, which is a single column of numbers: $\left(\begin{bmatrix} x_1, y_1 \end{bmatrix} \right)$. A row vector, like a column vector, is exactly what it sounds like - a row of numbers: $\left(\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \right)$. Each number in a vector $\overrightarrow{v}$ is a component of $\overrightarrow{v}$, with the first number either in the row or column being the first component, v_1, the second number being the second component, v_2, and so on and so forth until the ith component, v_i. The total number of numbers, or components, in a vector is referred to

as the dimension of the vector. So, for instance, vector $\overrightarrow{v} = \left(\begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix} \right)$ has degree 3.

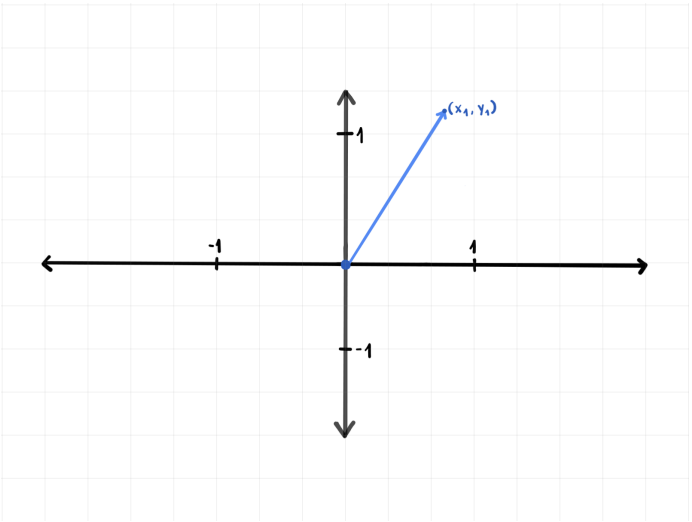

Figure 4: Vector $\left(\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \right)$.

Vectors, just like the numbers we use everyday, can be added, multiplied and otherwise manipulated. The rules, however, differ in some cases.

Vector addition is the process where two or more vectors are added together. If $\overrightarrow{v} = \left(\begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \right)$ and $\overrightarrow{w} = \left(\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \right)$, then $\overrightarrow{v} + \overrightarrow{w} = \left(\begin{bmatrix} v_1 + w_1 \\ v_2 + w_2 \end{bmatrix} \right)$. This can be abstracted to if $\overrightarrow{v}$ are arbitrary n-dimensional vectors, the jth component of $\overrightarrow{v} + \overrightarrow{w}$ denoted $(\overrightarrow{v} + \overrightarrow{w})_j$ is $v_j + w_j$.

Scalar multiplication happens between a scalar (such as 2 or π) and a vector. If $\overrightarrow{v} = \left(\begin{smallmatrix} v_1 \\ v_2 \end{smallmatrix} \right)$ and c is a scalar, $c\overrightarrow{v} = \left(\begin{bmatrix} cv_1 \\ cv_2 \end{bmatrix} \right)$. From a component view, for vectors of any dimension, $(c\overrightarrow{v})_j = cv_j$. Scalar multiplication of a vector by a positive integer will not change the direction of the vector, but scalar multiplication by a negative integer will invert a vector's direction.

The magnitude, or norm, of a vector ($|\vec{v}|$) is the length of that vector. Magnitude can be calculated using Pythagorean Theorem, as a vector can be thought of as the hypotenuse of a triangle where the x distance and y distance are the other two legs. The Pythagorean Theorem works for any number of dimensions, so it will work no matter how many elements the vector in question has. Therefore, $|\vec{v}| = \sqrt{v_1^2 + v_2^2 ... v_n^2}$. A vector with length 1 is called a unit vector. Any nonzero vector can be "normalized", or scaled to a unit

vector. To normalize a vector $\vec{v}$, multiply it by $\frac{1}{|\vec{v}|}$.

Linear independence is a quality of a group of vectors of the same dimension. If a set of vectors is linearly independent, no vector from the set is a scalar multiple of another. Mathematically, if c and d are nonzero scalars and $\vec{v}$ and $\vec{w}$ are vectors of the same dimension, then $\vec{v}$ and $\vec{w}$ are linearly independent if and only if $c\vec{v} \neq d\vec{w}$.

Lastly for vectors is **vector space**, which is the collection of all the complex numbers that can be formed from a set of vectors using vector addition and scalar multiplication. In order for a set (a collection of mathematical objects) to be considered a vector space, the set must be closed under addition and scalar multiplication, meaning any vector generated via scalar multiplication and vector addition using vectors in the set with also be in the set.

Matrices

Simply, a matrix is just a box of numbers. Matrices are very similar to vectors, and share a lot of the same properties; however, they can have both multiple rows and multiple columns: $\left(\begin{bmatrix} a, b \\ c, d \end{bmatrix} \right)$. To indicate an element of a matrix, that element's row and column in the matrix is used. So, for any matrix Q, Q_{ij} is the number in the ith row and jth column. If a matrix has m rows and n columns, it is a mxn dimensional matrix.

Matrices can be added and multiplied by scalars the exact same way vectors are. However, the process to multiple two matrices becomes a little more difficult. There are several requirements for matrix multiplication. For the case of MxN, M must have the same number of columns as N has rows. Additionally, the multiplication between the matrices is not communicative, and therefore MxN is much different than NxM. The multiplication itself follows the rule $(MN)_{ij} = \sum_{k=1}^{n} M_{ik}N_{kj}$. To the mechanics of this, see Figure 2 below.

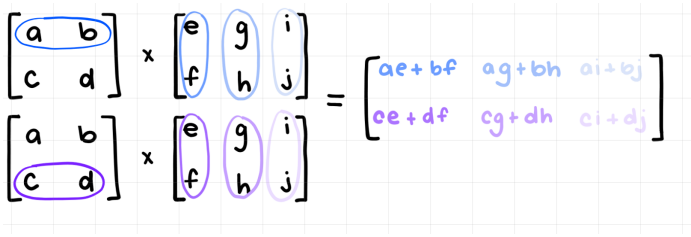

Figure 5: Matrix Multiplication

There are several special matrices that we will use later on: the identity

matrix and the unitary matrix. The identity matrix where every element is zeros except for the left top to bottom right diagonal. The more formal definition is a matrix $\mathbf{I}$ defined such that for every $n * n$ matrix M and any $\vec{v}$ in $\mathbf{C}^n$, $\mathbf{I}M = M\mathbf{I} = M$ and $\mathbf{I}v = \vec{v}$. Some examples include: $\left(\begin{bmatrix} 1, 0 \\ 0, 1 \end{bmatrix} \right)$, $\left(\begin{bmatrix} 1, 0, 0 \\ 0, 1, 0 \\ 0, 0, 1 \end{bmatrix} \right)$, and $\left(\begin{bmatrix} 1, 0, 0, 0 \\ 0, 1, 0, 0 \\ 0, 0, 1, 0 \\ 0, 0, 0, 1 \end{bmatrix} \right)$. Identities are special because, as pointed out by the formal definition, because, when multiplied by a matrix with the same number of rows, it does not change the matrix. Same goes for a vector - it will not alter the vector.

The second special matrix is the unitary matrix, U, which is a matrix that satisfies $UU^\dagger = U^\dagger U = \mathbf{I}$, where signifies a complex conjugate.

Matrices end up being very important in Quantum Mechanics (and Linear Algebra overall) due to the fact that they can be thought of as linear functions! A linear function, f is a function that satisfies: 1. $f(x + y) = f(x) + f(y)$ for any input x and y and 2. $f(cx) = cf(x)$ for any input x and any scalar c. Matrices satisfy both of these requirements, and therefore, serve as linear functions when manipulated.

Dot Product and Basis

The dot product, or inner product, is way of combining two vectors. The dot product works by summing up the product of the corresponding elements in each vector: $\vec{v} \cdot \vec{w} = \sum_{j=1}^{n} v_j w_j$. The two vectors (in this case $\vec{v}$ and $\vec{w}$) must have the same dimension. Another way of computing the dot product of two vectors is with the magnitudes of each vector: $\vec{v} \cdot \vec{w} = |\vec{v}||\vec{w}| \cos\theta$, where θ is the angle between the two vectors. Because the dot product involves the angle, computing it can reveal information about the two vectors. Most notably, if the dot product of two vectors is zero, then the two vectors must be perpendicular, as $\cos 90 = 0$.
The dot product can be used for projection of one vector onto another. Projection is visually explained in Figure 3 below. The projection of vector $\vec{v}$ onto vector $\vec{w}$ is the vector along $\vec{w}$ until point on $\vec{w}$ that corresponds with a line perpendicular to the x-axis dropped down from the end of $\vec{v}$.
Projection can be calculated using dot product and norms: $P_{\vec{v}\vec{w}} = \frac{1}{|\vec{w}|}\vec{w} \cdot \vec{v}$. $P_{\vec{v}\vec{w}}$ is a scalar and gives the component of the projection along $\vec{w}$ - the magnitude.

A basis is a finite set of vectors that can be used to describe any other vectors of the same dimension. Essentially, a basis is a group of vectors that can form any other vector with the same number elements through linear combination (vector addition or scalar multiplication). In order to qualify as a basis, the

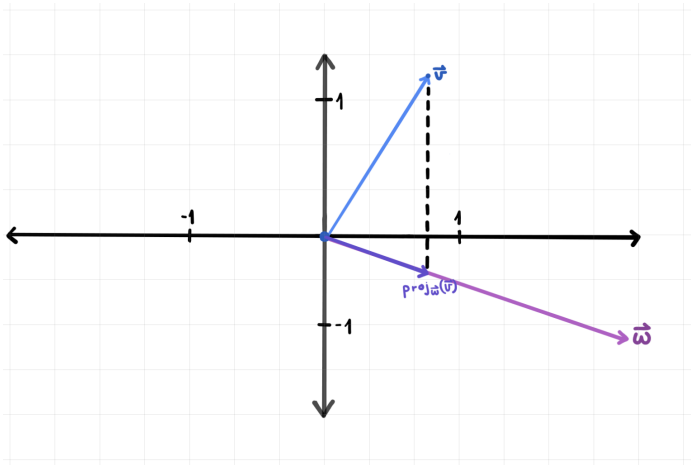

Figure 6: Vector Projections

group of vectors must be linearly independent. The most familiar basis in 2 dimensions is the standard basis: $\vec{v} = \begin{pmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \end{pmatrix} = v_1 \begin{pmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{pmatrix} + v_2 \begin{pmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{pmatrix}$. An orthogonal basis is a basis where each vector has a magnitude of 1 and every vector is perpendicular (or orthogonal) to every other vector. The basis example above is a orthogonal basis because $\begin{pmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{pmatrix}$ and $v_2 \begin{pmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{pmatrix}$ are perpendicular, as their dot product is equal to 0.

Vectors and matrices are at the heart of linear algebra, as well as form the core of quantum mechanics. Now that we've established a strong background in several of the linear algebra concepts, we can move on to the basics of quantum mechanics!

1.3 Quantum Mechanics Basics

Double Slit Experiment

In 1802, a British mathematician named Thomas Young came up with an experiment to prove how light was shaped. He directed a stream of light to hit a piece of material with two slits in it. Behind the material was another board. If the light behaved as a particle, only the areas directly behind the slits would be illuminated in discrete spots. However, if they behaved as a wave, there would be an "interference pattern" - strips would be illuminated on the back plate, with the strips near the center much brighter. Young's experiment showed strips, causing him to believe the wave theory of light was correct. However, within the next hundred years, the same double slit experiment was

used to show that light actually behaved like a particle *and* a wave. In 1927, Clinton Davisson and Lester Germer proved that electrons behave the same way. Shortly after, experiments proved that atoms and molecules also show properties of both waves and particles.

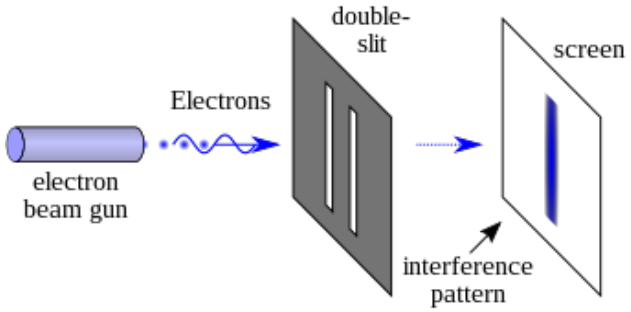

Figure 7: Double Slit Experiment

Wave Particle Duality

This idea that atoms, photons, molecules, and electrons act as both waves and particles is a key part of Quantum Mechanics called Wave Particle Duality. Classical physics dictates that small objects either acted as a particle or a wave. However, the double slit experiment proved otherwise; it is incomplete to describe an atom, photon, molecule or electron as only a particle or a wave - instead, these small objects contain proprieties of both. In fact, according to wave particle duality, all objects exhibit this behavior, however macroscopic objects (objects we can see) have such short wavelengths, there is no way to observe or measure large object's wavelengths.

Probability Density Function and Superposition

Because of the unique properties of quantum physics, it is impossible to tell exactly where an electron is at any giving moment! Although this seems a little un-intuitive, an electron can be in multiple places at once, and until an electron is 'measured' it does not exist in a specific place (or state). Physicist Erwin Schrodinger came up with his famous "Schrodinger's Box" experiment in order to highlight how ridiculous the idea of being in two places/states at once is. The thought experiment goes as follows: pretend you put a cat into a box with a vial of poison (it's a fairly gruesome thought experiment). The vial has a 50 percent chance of breaking and killing the cat and a 50 percent chance of not breaking, keeping the poison contained and the cat alive. You have no way of knowing if the poison vial has broken or not until you open the box. Therefore, according to the thought experiment, the cat must be both dead *and* alive, until you open the box, at which point both possible states

(dead and alive) coalesce into one: either dead or alive. In quantum mechanics, the electron is the cat - it exists in multiple places/states, until it is measured, in which case it collapses into a singular state. Just because it collapsed into one state, doesn't mean it was that state before it was measured. Instead, it was in multiple states at once - this is called superposition. Thus, the act of measuring fundamentally changes an electron.

In order to predict where an electron (or any other quantum sized object) will be, each object has a probability amplitude and a probability density function, which gives information about the probability of that object being in a given place. The probability amplitude is a complex number (see! they are useful in quantum mechanics) that uses the quantum state vector of an object to predict where the object can be found when measured. A quantum state vector is just a mathematical object that gives information about the possible measurements on an object and their outcomes. The probability density function is the modulus of the probability amplitude squared. (If you remember from the complex numbers unity, a "modulus" of a complex number is the absolute vale of that complex number.) Just like the probability density functions in statistics, the probability density function of a quantum object is a graph of the likely hood of a certain outcome happening - of finding the object in a certain place/state when measuring. See an example of a probability density function below!

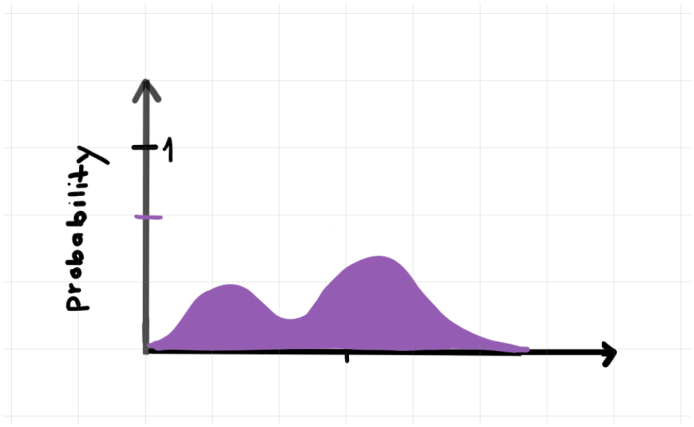

Figure 8: Probability Density Function

The Heisenberg Uncertainty Principle

Another counter-intuitive quantum principle is the Heisenberg Uncertainty Principle. In classical physics, the position and momentum (acceleration times mass - where the mass is moving) can both be measured and known. However, in quantum mechanics, there is a limit to the degree of certainty the values of

acceleration and momentum can be determined from initial conditions. German physicist Werner Heisenberg was the first to introduce the idea, claiming that there is a trade off between position and momentum - for example, if the position of a particle is fairly certain, the momentum of that particle will be fairly uncertain. This idea is highlighted by the equation below ($o_x o_p \geq \frac{h}{4\pi}$). The equation shows that uncertainty in position of the object (o_x) times the uncertainty in momentum of the object (o_p) must be greater than Planck's constant (just a constant - h) over 4π - essentially, the uncertainty must be greater than this constant value; if the uncertainty in position of an object is very small (it is very certain where the object is), than the uncertainty of momentum must be very high so the product of the two is still greater than the constant.

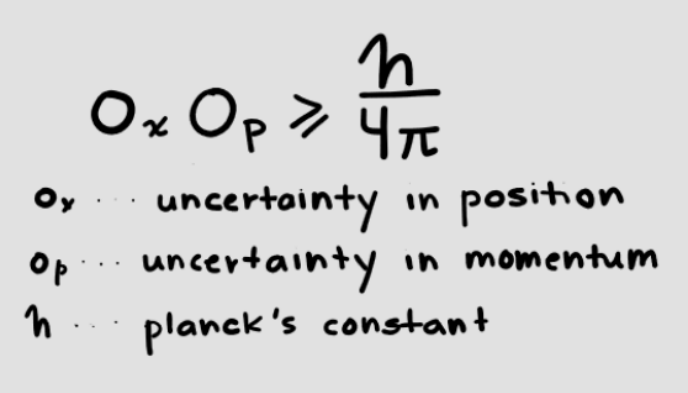

Figure 9: The Heisenberg Uncertainly Principle Formula

1.4 Postulate 1 of Quantum Mechanics

"Associated with any particle moving in a conservative field of force is a wave function which determines everything that can be known about the system."

Each quantum object has a set of physical qualities attached to it - such as position, momentum, spin and polarization. The collection of all of this physical information is called the "state" of the system. The first postulate of quantum mechanics says that all of this information, the state, can be described by the 'wavefunction' of that particle, $\psi(r,t)$ The wavefunction can also serve to describe the probability of the quantum object being found in a certain volume of space. $\psi*(r,t)\psi(r,t)d\tau$: the conjugate of the wavefunction (sort of like the complex conjugate) times the wavefunction times the volume at location r and time t. If you've worked with integrals before, you'll recognize

$$\int_{-\infty}^{\infty} \psi*(r,t)\psi(r,t)\,d\tau$$

which must be equal to 1, as the quantum object is located somewhere in $d\tau$. Wavefunctions that are tied to probability must also be single-valued, continuous and finite.

1.5 Linear Algebra in Quantum Mechanics

Quantum Objects as Vectors

Since quantum objects are in multiple states (places) at once due to superposition, and it is often impossible to predict exactly where they are, the "state" of a quantum object cannot be described as simply in a certain place or not (0 or 1). Instead, as the wavefunction demonstrates, a quantum object has a probability of being in a certain place or not. Thus, it has a chance between 0 and 1 of being in a certain place.

If we think of the states '0' and '1' as vectors, with 0 pointing straight up along the z axis and 1 pointing straight down along the z axis (both of length 1), then the 'state' of an qubit can be written as a linear combination of the two vectors, which would reflect the probabilities of that qubit being in a certain state.

Quantum Computing

Classical computing uses things called "bits" to store information. "Bits" can either be in the state 0 or 1, but not both at once. Binary, a number system just using 0 and 1 is used to describe data at the most fundamental level of classical computing. However, quantum computing uses "quantum bits" or "qubits" to express information. Qubits are similar to classical bits in the sense that they also store information and have states 0 and 1. Unlike classical bits though, qubits can be *both* 0 and 1, due to superposition.

In both classical and quantum computing, the data stored by (qu)bits needs to be dynamic. In order for a computer to function properly, it needs to be able to change data by performing operations on it, and thus the values of both qubits and bits need to be able to change. Bits can be flipped from 0 to 1, or kept constant, but it's a little bit more difficult with qubits. Since qubits can be expressed as vectors (see section on the Two State System), somehow altering the vector describing a qubit will change the data stored by it. When dealing with altering vectors, matrices are 'transformers', and can alter a vector just as functions do in algebra classes. Thus, to model the alteration of a quibit, we can apply a matrix to it's corresponding vector.

The two most common operator matrices are the X Operator and the H Operator.

X Operator: Flips the state of a qubit. If the qubit is in state 0, it'll be flipped

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

Figure 10: X Operator

to 1, and vice versa.

H Operator: Changes a qubit into a state of superposition. After the operation the qubit has a equal chance of collapsing into 0 or 1.

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

Figure 11: H Operator