Shrinking the Wavefunction

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Abstract

In quantum mechanics, the collapse of the wavefunction has long been a topic of heated discussion subject to multiple interpretations. We will try to deduce Copenhagen quantum mechanics from strictly unitary quantum mechanics. We do this by compressing a fourdimensional unitary operator composed of a subsystem and a random environment to a two-state space by averaging over and squeezing out the environment. Under certain conditions Copenhagen quantum mechanics might be reconciled with strictly unitary quantum mechanics because our method of reduction, on average, results in non-unitary time evolution operators. These operators allow for the violation of unitarity because the ratios of their eigenvalues can sometimes be much greater than one, resulting in an almost definite state, i.e. the shrinkage or collapse of the wavefunction.

1 Introduction

Quantum systems can be decomposed into a superposition of basis states. These wavefunctions, in turn, represent probability for finding the system in different configurations. These quantum systems evolve by means of a unitary operator, which can be represented, in the finite-dimensional case, as a square matrix. This means that going from one moment of time to the next is accomplished by multiplying by a matrix.

An illustrative example of a simple quantum system is Erwin Schrödinger's Cat Experiment[2]. In this experiment, a cat is placed in a closed steel chamber. Inside the chamber is a radioactive nucleus, a Geiger-counter, and a canister of poison gas. The radioactive nucleus has a 50% chance of decaying. If decay occurs, an alpha particle will be detected by the Geiger-counter, which will in turn set off a hammer that will break open the canister of poison gas, killing the cat. Otherwise no poison is released, and the cat remains alive. The state of the cat while it is in the chamber is described by the quantum principle of superposition. The cat is said to be both dead and alive, with a certain probability. Once the experimenters open the chamber, they will find that the cat is either dead or alive. This is known as the collapse of the wavefunction because once a measurement is made, the cat is no longer in a superposition state; instead it is in a fixed state. Schrödinger's Cat Experiment demonstrates the Copenhagen interpretation of quantum mechanics[3], which states that a system ceases to be a superposition of basis states and "collapses" to a particular basis state when a measurement is taken.

The laws of quantum mechanics do an excellent job of describing a wide range of atomic phenomena and can be applied to creating new technologies such as quantum computers. These computers would have the potential to be exponentially faster than classical computers. Such advances are the motivating factors behind understanding quantum mechanics and solving complex quantum mechanics problems. The objective of this research is to deduce Copenhagen quantum mechanics from strictly unitary quantum mechanics. To determine if the Copenhagen quantum mechanics can be reconciled with the strictly unitary quantum mechanics we consider the environment, which may include a macroscopic measurement apparatus, in which a quantum system is embedded. However, since realistic environments may have a large number of states, they are difficult to describe with deterministic models. To overcome this limitation, we resort to a probabilistic description of the environment, namely Monte-Carlo simulation[1].

The rest of the paper is structured as follows. In Section 2, we present the underlying theory of our research by discussing some background information, presenting an almost collapse hypothesis, and producing some simple tests of our theory. In Section 3, we discuss how to model the environment of a quantum system using Monte-Carlo simulation. We then present and analyze the results of our tests. In the final section, we conclude our research. Appendix A contains the mathematical foundations of quantum mechanics used in this paper, while Appendix B contains the Mathematica routine of the simulation we used to obtain our results.

2 Research

We are trying to deduce Copenhagen quantum mechanics from strictly unitary quantum mechanics. We do this by considering a quantum mechanical system consisting of a subsystem and its environment. If the environment is large and chaotic, we cannot hope to describe it in detail, so we must resort to a probabilistic description. Please refer to Appendix A if further elaboration of a math or notational concept is required.

2.1 Background

Here are four postulates from the Copenhagen version of quantum mechanics[3]:

- 1. Physical systems are completely described by state vectors $|\psi\rangle$ living in a complex vector space.
- 2. Time evolution is generated by a unitary operator: $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$, except during measurement.
- 3. The probability that a measurement will show that $|\psi\rangle$ is in state $|\phi\rangle$ is $|\langle\phi|\psi\rangle|^2$. The probability is known as the absolute square of the amplitude. The amplitude is the scalar product $\langle\phi|\psi\rangle$.
- 4. Immediately after a measurement that shows $|\psi\rangle$ is in state $|\phi\rangle$, $|\psi\rangle = |\phi\rangle$.

Postulates one and two (without the "except during measurement") apply to the theory called "strictly unitary quantum mechanics." As one can see from above, Copenhagen quantum mechanics modifies the second postulate by adding "except during measurement" and also adds postulates three and four to describe measurement. Strictly unitary quantum mechanics fails to explain most measurements because when a measurement is made, the system collapses from a superposition of eigenstates to a single eigenstate of the observed operator, and this collapse violates unitary evolution. Postulates three and four, known as the measurement postulates, were added to patch up quantum mechanics. Even though the measurement postulates seem ad hoc, they accurately describe the results of real experiments.

The challenge is to determine whether Copenhagen quantum mechanics can be reconciled with strictly unitary quantum mechanics. We note that measurement involves the interaction of a quantum mechanical system with a macroscopic measurement apparatus. A macroscopic measurement apparatus should be described by quantum mechanics, if quantum mechanics is to be consistent. Therefore, the quantum system must be enlarged to include not only the original system, but also an environment which may include a macroscopic measurement apparatus. In a closed system, the state vector $|\psi\rangle$ contains all the information about the system. A closed system is a physical system, which cannot be influenced by its environment[4]. Postulates one and two always hold true for closed systems, but not for open systems. An open system is a physical system that can exchange information (energy, momentum, etc.) with its surroundings[4]. In an open system composed of a subsystem and the environment, postulates one and two cannot fully describe the subsystem in isolation; therefore, postulates three and four must be added.

2.2 Almost Collapse

How can measurement be consistent with postulates one and two? If $|\psi\rangle$ is any normalized state, there is no operator \hat{O} such that $\hat{O}|\psi\rangle = |1\rangle$, a definite state. For a two-state system, for example, we can always write:

$$|\psi\rangle = \alpha |1\rangle + \beta |2\rangle$$
 where $|\alpha|^2 + |\beta|^2 = 1$ (1)

then applying an operator, \hat{O} , results in:

$$\hat{O}|\psi\rangle = \alpha \hat{O}|1\rangle + \beta \hat{O}|2\rangle.$$
⁽²⁾

The operator, \hat{O} , is fully described by its action on a complete set of basis states. Suppose $\hat{O}|1\rangle = \lambda|1\rangle$ and $\hat{O}|2\rangle = 0$. Then $\hat{O}|\psi\rangle = \alpha\lambda|1\rangle$. \hat{O} is not unitary unless $|\alpha\lambda| = 1$ for all α , which is impossible.

We would like to explore if there is an operator \hat{O} that has one eigenvalue much larger than the rest. If \hat{O} is Hermitian ($\hat{O} = \hat{O}^{\dagger}$) and has *n* eigenvectors, then any vector $|\psi\rangle$ can be written as a combination of these eigenvectors:

$$|\psi\rangle = \sum_{i=1}^{n} c_i |i\rangle \tag{3}$$

where $|i\rangle$ is an eigenvector of \hat{O} and c_i are some complex numbers. Suppose that one of the eigenvalues of \hat{O} is much larger than the rest and has eigenvector $|big\rangle$. Then

$$|\psi\rangle = c_1 |\text{big}\rangle + \text{remainder}.$$
 (4)

If the eigenvalues and eigenvectors are λ_i and $|i\rangle$, with $\lambda_1 \gg \lambda_i$, then

$$\hat{O}|\psi\rangle = c_1\lambda_1|\text{big}\rangle + \sum_{i=2}^n c_i\lambda_i|i\rangle \approx c_1\lambda_1|\text{big}\rangle.$$
(5)

A time evolution operator, which has one eigenvalue that is much larger than the rest could result in shrinking the wavefunction or the almost collapse of the wavefunction. However, this is impossible for a unitary operator because the eigenvalues of a unitary operator all have modulus equal to one.

For a closed quantum system, unitary time evolution cannot collapse or even almost collapse the wavefunction. For an open system, however, measurement involves interaction with a macroscopic apparatus and/or an environment. It is possible that open systems do not obey unitary evolution, in which case \hat{O} does not have to be unitary. A state vector for a combined system can be represented by:

$$|\psi\rangle = |\text{subsystem}, \text{environment}\rangle = |\text{subsystem}\rangle|\text{environment}\rangle.$$
 (6)

Two state vectors next to each other represent a tensor product. The tensor product of two state vectors is itself a state vector, but resides in a larger vector space called the tensor product space.

A physical example of an open system is a pair of two state systems. The first particle, an electron, has spin that can point up (\uparrow) or down (\downarrow). The subsystem is the one that is being measured. The basis states for the subsystem are $|\uparrow\rangle$ and $|\downarrow\rangle$. The second particle, representing the environment, can go through door number one or door number two. Its basis states are $|1\rangle$ and $|2\rangle$. The combination of the subsystem and the environment results in a tensor product space with four total basis states:

$$\{|\uparrow\rangle|1\rangle, |\uparrow\rangle|2\rangle, |\downarrow\rangle|1\rangle, |\downarrow\rangle|2\rangle\}.$$
(7)

A one-to-one correspondence is required between state vectors and the column vectors we are using to represent them. The orthonormal basis for this state space are:

$$|\uparrow\rangle|1\rangle \leftrightarrow \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} \quad |\uparrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix} \quad |\downarrow\rangle|1\rangle \leftrightarrow \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} \quad |\downarrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} 0\\0\\0\\1\\0 \end{pmatrix} \quad . \tag{8}$$

We can represent the pair of two-state systems with two basis states,

$$|a\rangle = a_1|\uparrow\rangle|1\rangle + a_2|\uparrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} a_1\\ a_2\\ 0\\ 0\\ 0 \end{pmatrix} \quad |b\rangle = b_1|\downarrow\rangle|1\rangle + b_2|\downarrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} 0\\ 0\\ b_1\\ b_2 \end{pmatrix}.$$
(9)

The state $|a\rangle$ describes subsystem up, $|\uparrow\rangle$, and environment in a superposition state. The state $|b\rangle$ describes subsystem down, $|\downarrow\rangle$, and environment in a superposition state. $|a\rangle$ and $|b\rangle$ are definite quantum states. The scalars a_1 , a_2 , b_1 , and b_2 are complex numbers known

as complex amplitudes. Normalization requires that:

$$|a_1|^2 + |a_2|^2 = |b_1|^2 + |b_2|^2 = 1.$$
(10)

We write the complex amplitudes a_1 , a_2 , b_1 , and b_2 using the modulus and phase, e.g. $a_1 = ae^{i\theta_1}$.

$$|a\rangle = ae^{i\theta_{1}}|\uparrow\rangle|1\rangle + \sqrt{1 - a^{2}}e^{i\theta_{2}}|\uparrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} ae^{i\theta_{1}} \\ \sqrt{1 - a^{2}}e^{i\theta_{2}} \\ 0 \\ 0 \end{pmatrix}$$
(11)
$$|b\rangle = be^{i\theta_{3}}|\downarrow\rangle|1\rangle + \sqrt{1 - b^{2}}e^{i\theta_{4}}|\downarrow\rangle|2\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ be^{i\theta_{3}} \\ \sqrt{1 - b^{2}}e^{i\theta_{4}} \end{pmatrix}$$
(12)

Now that we have the basis states, we need a unitary operator giving the time evolution of the full four-dimensional system, \hat{U} . Once we have a four-dimensional unitary operator, we can reduce the state space so as to eliminate the environment. We can compress the fourstate space to a two-state space by only using two basis states that describe the subsystem, instead of four basis states that describe both the subsystem and the environment. This effectively squeezes out the environment. The matrix elements of the resulting matrix Ware evaluated using two basis states $\{|a\rangle, |b\rangle\}$:

$$W \leftrightarrow \begin{pmatrix} \langle a|\hat{U}|a \rangle & \langle a|\hat{U}|b \rangle \\ \langle b|\hat{U}|a \rangle & \langle b|\hat{U}|b \rangle \end{pmatrix}.$$
(13)

2.3 Tests

To test our ideas, we created the following two unitary matrices.

$$\hat{U}_1 \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 & 0 \\ 0 & 0 & 1 & i \\ 0 & 0 & i & 1 \\ 1 & -i & 0 & 0 \end{pmatrix} \qquad \hat{U}_2 \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ -i & 0 & 0 & -i \\ 0 & -i & i & 0 \end{pmatrix}$$

The eigenvalues for matrix \hat{U}_1 are:

-.042 + 0.999i, -.991 - .136i, .913 + .407i, .826 - .563i

The eigenvalues for matrix \hat{U}_2 are:

$$-1, 1, \frac{1+i}{\sqrt{2}}, \frac{1-i}{\sqrt{2}}$$

All these eigenvalues are complex roots of unity. Now we apply the procedure of equation (13) for reducing a four-by-four unitary matrix, \hat{U}_1 , to a two-by-two matrix, W_1 . When we use $a = \frac{1}{2}$ and $b = \frac{1}{2}$ for the complex amplitudes of the basis states $|a\rangle$ and $|b\rangle$, with $\theta_1 = \theta_2 = \theta_3 = \theta_4 = 0$, we obtain the eigenvalues of W_1 and their ratio r_1 :

 $\lambda_1 = .854 + .235i$ and $\lambda_2 = -.371 + .248i$

$$r = |\lambda_1/\lambda_2| = |(.854 + .235i)/(-.371 + .248i)| = 1.98$$

Now that we have separated the subsystem and the environment, we have shown that the subsystem alone can violate unitary evolution since $r \neq 1$ and λ_1 and λ_2 are not complex roots of unity.

We apply the same procedure to \hat{U}_2 , and subsequently obtain the eigenvalues of W_2 and their ratio r_2 :

$$\lambda_1 = .744 - .165i$$
 and $\lambda_2 = -.037 + .165i$
 $r_2 = |\lambda_1/\lambda_2| = |(.744 - .165i)/(-.037 + .165i)| = 4.50$

This is an even better result because r_2 is bigger. Unlike the eigenvalues for the unitary matrices above, the eigenvalues for both reduced matrices are not complex roots of unity.

3 Probabilistic Unitary Quantum Mechanics

In general, the environment is large and chaotic, so we cannot represent it accurately. Throwing dice is a good case in point because if we knew all the initial conditions, namely the velocity and the spin of the dice, the material properties of the dice and the surface the dice are thrown on, and the properties of the air the dice fly through, then we could accurately predict how they would fall. Since we do not keep track of complete information about the dice the result seems random. We say that there is a $\frac{1}{6}$ chance for each outcome of a single die roll. By analogy, we will let the environment be random. We will then be able to describe many possible environments using the laws of probability. While there is no probability in strictly unitary quantum mechanics, we explicitly introduce probability to describe the interaction of an open system and its environment.

We are going to use the following three properties of probability theory.

- The set of all possible outcomes of a random process is called the probability space. For example, the probability space for a coin toss is {H, T}, which is a discrete and finite set. The probability space for a continuous roulette wheel is {θ ∈ ℝ : 0 ≤ θ < 2π}, which is a continuous and infinite set.
- 2. A random variable is an element of the probability space.

3. For a continuous probability space $\{\theta\}$, the probability that the random process yields $\theta_1 \leq \theta \leq \theta_1 + d\theta$ is $f(\theta_1)d\theta$, where $d\theta$ is a differential, $f(\theta) \geq 0$ is called the probability density (frequency function), and $\int f(\theta) d\theta = 1$.

In the present case, we take the phase angles $(\theta_1, \theta_2, \theta_3, \theta_4)$ to be independent random variables each with a uniform probability density in the range $[0, 2\pi]$:

$$f(\theta) = \frac{1}{2\pi}$$
 for $0 \le \theta < 2\pi$ and $f(\theta) = 0$ otherwise

To create a random environment we use random values for θ_1 , θ_2 , θ_3 , and θ_4 . Generating and using random numbers is known as Monte-Carlo Simulation[1], which will hopefully give us an approximate representation of real physical systems. We use predetermined numbers for the complex amplitudes a and b. After each different test, we obtain one sample of two eigenvalues (λ_1, λ_2) . Using this sample we calculate $|\lambda_1/\lambda_2| = r$. We want to know whether $r \gg 1$ is typical. If r is very big, then we would have succeeded in shrinking or almost collapsing the wavefunction. In our Monte-Carlo simulations, we used seven different combinations of values for a and b, for both of our unitary matrices. For each test, we ran 10,000 trials and produced histograms of r and $\ln r$. Table1 summarizes our results.

From Table 1, one can see certain trends for \hat{U}_1 and \hat{U}_2 . When the complex amplitudes a and b are the same, for \hat{U}_1 , r approaches one as a and b get closer to either zero or one. In contrast, when a and b are the same, for \hat{U}_2 , r increases as a and b get closer to either zero or one. When a and b are different, for both \hat{U}_1 and \hat{U}_2 , r gets larger as a and b get farther apart from each other. Using both matrices with a = 1 and b = 0 and vice-versa, results in infinite values of r. Using a = 1 and b = 1 or a = 0 and b = 0, with \hat{U}_1 , always results in r = 1, which means that our reduced 2-by-2 matrix W is unitary. In contrast, using the same values for a and b with \hat{U}_2 results in infinite values of r.

Below is one of the typical results we obtained. To present the results we scaled them

	Amplitude	Minimum	Median	Maximum
\hat{U}_1	$a = \sqrt{1/2}, \ b = \sqrt{1/2}$	1	1.52	581.82
	$a = 1/2, \ b = 1/2$	1	1.41	9.97
	$a = 1, \ b = 1$	1	1	1
	$a = 0, \ b = 0$	1	1	1
	$a = \sqrt{999/1000}, \ b = 0$	30.67	31.87	32.67
	a=1, b=0	∞	∞	∞
	$a = 0, \ b = 1$	∞	∞	∞
\hat{U}_2	$a = \sqrt{1/2}, \ b = \sqrt{1/2}$	1	1.07	17429.7
	$a = 1/2, \ b = 1/2$	1	1.42	1258.77
	$a = 1, \ b = 1$	∞	∞	∞
	$a = 0, \ b = 0$	∞	∞	∞
	$a = \sqrt{999/1000}, \ b = 0$	29.61	31.72	33.61
	$a = 1, \ b = 0$	∞	∞	∞
	$a = 0, \ b = 1$	∞	∞	∞

Table 1: Monte-Carlo Simulation r-value Results

using $\ln r$ instead of r. In this histogram, $a = b = \sqrt{1/2}$, using \hat{U}_2 . Figure 1 shows a positively skewed distribution. Most of the values of $\ln r$ are between 0 and 3.5. Approximately 69% of the values are between 0 and 0.5, which means that most of the reduced matrices produced during this specific Monte-Carlo simulation were either unitary or very close to being unitary. In this simulation, we have made some progress in shrinking the wavefunction because we have some very large values, the maximum $\ln r$ being 9.77, or if one refers to Table 1, r = 17429.7. Since this simulation describes our characteristic results, we have shown that there is usually some slight shrinkage of the wavefunction.

Another very interesting test resulted in r values equal to infinity. We obtained this result for \hat{U}_1 when a = 1, b = 0 and vice-versa. We also obtained this result for \hat{U}_2 when a = 1, b = 0 and vice-versa, as well as a = b = 1 and a = b = 0. The data can be found in Table 1. Before we ran our tests, we stated that ideally we would want a very large r value. The infinite result is evidence that our method works as we intended for certain values for a and b. In these particular tests, we successfully collapsed the wavefunction. This result is



Figure 1: Logarithmic Distribution of r, using \hat{U}_1 , and $a = b = \frac{1}{\sqrt{2}}$

analyzed below using a = 1 and b = 0 with \hat{U}_1 . In this case,

$$|a\rangle \leftrightarrow \begin{pmatrix} e^{i\theta_1} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |b\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{i\theta_4} \end{pmatrix}, \quad |c\rangle \leftrightarrow \begin{pmatrix} 0 \\ e^{i\theta_2} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \text{and} \quad |d\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ e^{i\theta_3} \\ 0 \\ 0 \end{pmatrix}.$$

We then apply our unitary operator, \hat{U}_1 , to the two states, $|a\rangle$ and $|b\rangle$, which we use to reduce the state space. Then we find what linear combination of state vectors describes $\hat{U}_1|a\rangle$ and $\hat{U}_1|b\rangle$.

$$\hat{U}_1|a\rangle \leftrightarrow \frac{e^{i\theta_1}}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\1 \end{pmatrix} \leftrightarrow \frac{1}{\sqrt{2}} \left(|a\rangle + e^{i(\theta_1 - \theta_4)}|b\rangle\right)$$

$$\hat{U}_1|b\rangle \leftrightarrow \frac{e^{i\theta_4}}{\sqrt{2}} \begin{pmatrix} 0\\i\\1\\0 \end{pmatrix} \leftrightarrow \frac{1}{\sqrt{2}} \left(e^{i(\theta_4 - \theta_2 + \frac{\pi}{2})}|c\rangle + e^{i(\theta_4 - \theta_3)}|d\rangle \right)$$

In our Monte-Carlo simulations, we use random values for the phase values θ_i . Thus we can use statistical methods to deal with our model.

$$\overline{e^{i\theta}} = \overline{\cos\theta} + i\overline{\sin\theta} = 0 + i0 = 0$$

The bar over the terms above represents the statistical average. Random phase results in an average of zero because the sine and cosine are periodic functions that are equally likely to be above zero as they are to be below zero. This means that the average of the terms of the states with phase factors is zero and can therefore be removed, yielding

$$\hat{U}_1|a
angle = rac{1}{\sqrt{2}}|a
angle$$
, while $\hat{U}_1|b
angle = 0$.

On average the operator collapses the wavefunction, i.e. leads to a definite state. \hat{U} transforms an initial state $|\psi_0\rangle$ to a final state $|\psi\rangle$. Assume

$$|\psi_0\rangle = \alpha |a\rangle + \beta |b\rangle \,.$$

Therefore,

$$|\psi\rangle = \alpha \hat{U}|a\rangle + \beta \hat{U}|b\rangle$$
.

Now, applying this to our situation, we find that:

$$\overline{|\psi(t)\rangle} = \frac{\alpha}{\sqrt{2}}|a\rangle.$$

4 Conclusion

If we take the average wavefunction to be a realistic approximation of the actual wavefunction, then we have made a significant step towards reconciling strictly unitary quantum mechanics with Copenhagen quantum mechanics. We did this by adding probability theory to strictly unitary quantum mechanics, i.e. describing the environment by a statistical ensemble of environments. By restricting a unitary operator to a subspace, non-unitary operators resulted quite often. We compressed a four-dimensional unitary operator composed of a subsystem and an environment to a two-state space by averaging over and squeezing out the environment. Since the ratios of the eigenvalues of this reduced state space were often much greater than one, we proved that we could violate unitary evolution and collapse a state from a superposition of basis states to an eigenstate of an observable, or more generally shrink the wavefunction to more closely approximate an eigenstate.

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Appendix A The Mathematics of Quantum Mechanics

The following are explanations of the mathematical foundations of quantum mechanics that are used in this paper.

In quantum mechanics, physical systems are completely described by state vectors $|\psi\rangle$ living in a complex vector space. $|\psi\rangle$ can be put into a one-to-one correspondence with a column vector, for example in a two-dimensional space:

$$|\psi\rangle \leftrightarrow \left(\begin{array}{c} a\\ b\end{array}\right)$$
.

The \leftrightarrow stands for "is represented by". $\langle \phi |$ is known as a covector, which can be put into a one-to-one correspondence with a row vector, for example in a two-dimensional space:

$$\langle \phi | \leftrightarrow (c \ d).$$

Any quantum state can completely represented by a sum of basis states. For example, the basis states for a two-dimensional system could be represented by $|1\rangle$ and $|2\rangle$. These two basis states can be used to construct any state living in a two-dimensional space using c_1 and c_2 as scalars in front of the basis states. In quantum mechanics these scalars are complex numbers.

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle$$

These two basis states could be put into a one-to-one correspondence with column vectors in the following way:

$$|1\rangle \leftrightarrow \begin{pmatrix} 1\\ 0 \end{pmatrix}$$
 and $|2\rangle \leftrightarrow \begin{pmatrix} 0\\ 1 \end{pmatrix}$.

Therefore,

$$|\psi\rangle = \left(\begin{array}{c} c_1\\ c_2\end{array}\right) \,.$$

A linear transformation from one state to another is represented by a linear operator, denoted by a symbol with a caret, for example:

$$|\psi
angle=\hat{O}|\phi
angle$$
 .

Operators can be put into a one-to-one correspondence with a square matrix. For a twodimensional state space we have:

$$\hat{O} \leftrightarrow \left(\begin{array}{cc} e & f \\ g & h \end{array} \right)$$
 .

It is important to note that column vectors and state vectors are two different notions, as are row vectors and state covectors, as are matrices and operators. They are, however, related in that they can be put into a one-to-one correspondence, as we have demonstrated for each case.

Matrix multiplication requires that the number of the columns of the first matrix, A, is equal to the number of rows of the second matrix, B. Then the product AB is the matrix whose ij-entry is obtained by multiplying the *i*th row of A by the *j*th row of B. For example,

$$\left(\begin{array}{cc} a & b \\ c & d \end{array}\right) \cdot \left(\begin{array}{cc} e & f \\ g & h \end{array}\right) = \left(\begin{array}{cc} ae + bg & af + bh \\ ce + dg & cf + dh \end{array}\right)$$

Matrix multiplication can also be represented by [5]:

$$(AB)_{ij} = \sum_{k} a_{ik} b_{kj} \,.$$

Since complex numbers are integral to quantum mechanics, conjugation is also very important. To conjugate a number, one changes the sign of its imaginary part. This means, that for real numbers nothing changes, however, for complex numbers the sign of the imaginary part is switched. The symbol for conjugation is *, for example

$$(a+bi)^* = (a-bi)$$
 and $(re^{i\theta})^* = re^{-i\theta}$.

The transpose of a matrix A, is the matrix formed by flipping A over the diagonal line from the upper left corner. Taking the transpose is the same as making the columns of the matrix the rows of the new matrix. This can be represented by [5]:

$$(A_{ij})^T = A_{ji} \, .$$

However, in quantum mechanics the transpose is never used by itself. Instead the adjoint, which is the conjugate transpose, represented by the the dagger symbol, †, is used.

$$\left(\begin{array}{cc}a&b\\c&d\end{array}\right)^{\dagger} = \left(\begin{array}{cc}a^{*}&c^{*}\\b^{*}&d^{*}\end{array}\right)$$

A matrix is considered unitary if $A^{\dagger}A = AA^{\dagger} = I$. *I* is the identity matrix, which has ones on the diagonal starting at the top left and ending at the bottom right and zeros everywhere else. For example,

$$I = \left(\begin{array}{cc} 1 & 0\\ 0 & 1 \end{array}\right) \,.$$

The adjoint operation converts a state vector to a state covector.

$$(a|A\rangle + b|B\rangle)^{\dagger} = a^{*}\langle A| + b^{*}\langle B|$$

If $|A\rangle \leftrightarrow \begin{pmatrix} 1\\0 \end{pmatrix}$ and $|B\rangle \leftrightarrow \begin{pmatrix} 0\\1 \end{pmatrix}$, then
$$\begin{bmatrix} a\begin{pmatrix}1\\0 \end{pmatrix} + b\begin{pmatrix}0\\1 \end{bmatrix} \end{bmatrix}^{\dagger} = \begin{pmatrix} a\\b \end{pmatrix}^{\dagger} = (a^{*}b^{*})$$

Unitary matrices have orthonormal rows and columns. This means that the inner product of two of the same rows/columns will be equal to one, while the inner product of two different rows/columns will be equal to 0. For example in a two-dimensional space, if the unitary matrix, $\hat{U} \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, then:

•

$$(1 \quad 0) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 = (0 \quad 1) \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and

$$(1 \quad 0) \cdot \left(\begin{array}{c} 0\\ 1 \end{array}\right) = 0 = (0 \quad 1) \cdot \left(\begin{array}{c} 1\\ 0 \end{array}\right).$$

In quantum mechanics notation with arbitrary state vectors $|\psi\rangle$ and $|\phi\rangle$, orthonormality can

be represented by:

$$\langle \psi | \psi \rangle = 1 = \langle \phi | \phi \rangle$$

and

$$\langle \psi | \phi \rangle = 0 = \langle \phi | \psi \rangle$$
.

A unitary operator can be put into a one-to-one correspondence with a square matrix that fulfills the condition $A^{\dagger}A = AA^{\dagger} = I$:

$$\hat{U} \leftrightarrow \begin{pmatrix} w & x \\ y & z \end{pmatrix} \quad \text{where } |w|^2 + |y|^2 = |x|^2 + |z|^2 = 1 \text{ and } w^*x + y^*z = 0.$$

A unitary operator is one for which if $|\psi\rangle$ is a normalized state, so is $\hat{U}|\psi\rangle.$

Next, we introduce the notions of eigenvectors and eigenvalues. Let A be an n-dimensional square matrix. A scalar λ is called an eigenvalue of A if there exists a nonzero vector, v, for which[6]

$$Av = \lambda v$$

Every vector satisfying this relation is then called an eigenvector of A belonging to the eigenvalue λ . The set E_{λ} of all eigenvectors belonging to λ is called the eigenspace of $\lambda[5]$. For example, let $A = \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix}$ and let $v_1 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$ and $v_2 = \begin{pmatrix} -1 \\ 3 \end{pmatrix}$, then

$$Av_1 = \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 10 \\ 5 \end{pmatrix} = 5 \begin{pmatrix} 2 \\ 1 \end{pmatrix} = 5v_1$$

and

$$Av_2 = \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix} \begin{pmatrix} -1 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ -6 \end{pmatrix} = -2 \begin{pmatrix} -1 \\ 3 \end{pmatrix} = -2v_2.$$

Therefore v_1 and v_2 are eigenvectors of A belonging, respectively, to the eigenvalues $\lambda_1 = 5$ and $\lambda_2 = -2$ of A.

An *n*-dimensional square matrix has *n* eigenvalues. To find the eigenvalues and eigenvectors of a matrix we must find the characteristic polynomial $\Delta(\lambda)$ of *A*. We then find the roots of $\Delta(\lambda)$ to obtain the eigenvalues of *A*. The characteristic polynomial $\Delta(\lambda)$ of *A* is the determinant[6]

$$\Delta(\lambda) = |\lambda I - A|.$$

Let $A = (A_{ij})$ be a square matrix. The determinant of A is written either as det(A) or |A|. If A is a one-by-one matrix, then

$$|A| = A_{11}$$
.

If A is a two-by-two matrix, then

$$|A| = A_{11}A_{22} - A_{21}A_{12}.$$

If $A = \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix}$, then the determinant of A, |A| = 4(-1) - 3(2) = -4 - 6 = -10. Let us apply this to the characteristic polynomial and verify that it yields the same eigenvalues

and eigenvectors we found before.

$$\Delta(\lambda) = |\lambda I - A| = \left| \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix} \right| = \left| \begin{pmatrix} \lambda - 4 & -2 \\ -3 & \lambda + 1 \end{pmatrix} \right| = \lambda^2 - 3\lambda - 10 = (\lambda - 5)(\lambda + 2)$$

Then we set $\Delta(\lambda) = (\lambda - 5)(\lambda + 2) = 0$. The roots $\lambda_1 = 5$ and $\lambda_2 = -2$ are the eigenvalues of A.

Once we have the eigenvalues we can find the eigenvectors of A. To do this we have to

solve[6]

$$(\lambda I - A)v = 0.$$

For the eigenvalue $\lambda_1 = 5$ the corresponding eigenvector v_1 would be found by solving $(\lambda I - A)v = 0.$

$$\begin{bmatrix} 5\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix} \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 & -2 \\ -3 & 6 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

This results in

$$x - 2y = 0$$

and

$$-3x + 6y = 0$$

This system has infinitely many solutions, x = 2a and y = a for any real number a. Thus we give the normalized eigenvector because there is only one. The normalized vector, represented by \hat{v} , is found by dividing the vector by its norm. The norm (length) of a vector, v is written as |v|. Let $v^T = (v_1 \ v_2 \ \dots \ v_n)$, then

$$|v| = \sqrt{v^T v} = \sqrt{v_1^2 + v_2^2 + \ldots + v_n^2}.$$

Therefore, taking one possible unnormalized eigenvector $v_1^T = (2 \ 1)$ we can find the norm and then the normalized eigenvector:

$$|v_1| = \sqrt{2^2 + 1^2} = \sqrt{5}$$
.

Thus $v_1^T = \begin{pmatrix} \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix}$ is the normalized eigenvector for the eigenvalue $\lambda_1 = 5$. The same procedure would be used to find the normalized eigenvector v_2 of A belonging to the eigenvalue

 $\lambda_2 = -2.$

In quantum mechanics notation, $|\psi\rangle$ is an eigenstate of the operator \hat{O} if and only if

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle$$

for some eigenvalue λ . In general, if $|\psi\rangle$ is a state vector in a *n*-dimensional vector space, \hat{O} has *n* eigenstates and *n* eigenvalues. It is very important to note that the eigenvalues of a unitary operator or matrix are complex roots of unity with modulus one. That is, $\lambda = e^{i\theta}$, where θ is a real number.

Appendix B Mathematica Routine

The generic Mathematica routine we used for our Monte-Carlo tests can be found on the next page.

```
 \mathbf{v} = \begin{pmatrix} 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \end{pmatrix}  Unitary Operator
 a = 0 < x < 1
b = 0 < y < 1
 array = \{ \}_i
 array2 = \{ \};
 For[i = 0, i < 10000, i++,</pre>
  phase1 = Random[];
  phase2 = Random[];
  phase3 = Random[];
  phase4 = Random[];
  al = a e<sup>12 x *phase1</sup>;
  a2 = \sqrt{1 - a^2} e^{I2x + phase2};
  b1 = b e<sup>12 x * phase3</sup>;
  b2 = \sqrt{1 - b^2} e^{i 2 \pi \cdot p hase4};
 basisA = (a1) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} + (a2) \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix};
  basisB = (b1) \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} + (b2) \begin{pmatrix} 0\\0\\0\\0\\1 \end{pmatrix}; Waa = Conjugate[Transpose[basisA]].V.basisA;
  Wab = Conjugate[Transpose[basisA]].V.basisB;
  Wba = Conjugate[Transpose[basisB]].V.basisA;
  Wbb = Conjugate[Transpose[basisB]].V.basisB;
  W = ( Waa[[1]][[1]] Wab[[1]][[1]] );
Wba[[1]][[1]] Wbb[[1]][[1]] );
  eigen = N[Bigenvalues[W]]; x = eigen[[1]]; y = eigen[[2]];
  r = Abs[(x) / (y)]; If[r < 1, r = 1 / r, r];
  array = Flatten[ {r, array }];
  r = Log[r];
  array2 = Flatten[ {r, array2 }]]
 Save["2Unitary4", array]
 Save["2UnitaryLn4", array2]
 << Graphics 'Graphics'
 Histogram[array]
 Min[array]
 Max[array]
 Mean[array]
 Median[array]
 Histogram[array2]
 Min[array2]
 Max[array2]
 Mean[array2]
 Median[array2]
```