The Quantum-Classical Transition

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Abstract

Since the days of Galileo Galilei and Isaac Newton, classical mechanics has been used to describe the macroscopic world in which we live. From the projectile acceleration of a baseball to the elliptical orbit of Mars, classical mechanics quite accurately predicts the behavior of most physical phenomena we encounter on a daily basis. However, classical mechanics fails to describe the microscopic, atomic, and sub-atomic domains, where particles have both particle-like and wave-like properties. In this domain, quantum mechanics is needed to accurately describe the system. When the particles behave like waves, they may exist in a coherent quantum superposition of different states and exhibit interference. On the contrary, on the classical level, macroscopic quantum superpositions are very difficult to observe.

My goal in this thesis is to study the transition from the quantum domain to the classical domain. Why, if quantum superpositions are such an integral part of our world on the microscopic level, do they all but disappear in the macroscopic world which we experience? What defines the border between the quantum and the classical?

In the mid-20th century, H. Dieter Zeh pointed out that realistic systems are never isolated and always interact with their environments. Zeh suggested that this interaction could explain the fragility of quantum states and the disappearance of coherent quantum superpositions [1]. Wojiech Zureck advanced this theory, introducing the term "decoherence" to describe the loss of coherence and therefore the quantum-classical transition [2]. In this thesis, I will examine the theory of decoherence, as well as the criticisms it generated.

1. Introduction

The Schrödinger equation,$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle$, describes the dynamics of a quantum system. It is a deterministic equation. It says that given the initial state (wave function), $|\Psi(0)\rangle$, and the Hamiltonian, H, of the system, the state at a future time can always be obtained. This equation is at the core of the formalism of quantum mechanics. Experiments have shown that quantum mechanics provides an extremely accurate description of the behavior of objects at the microscopic scale. However, there is a fundamental question associated with the Schrödinger equation and the formalism of quantum mechanics. When applied to a microscopic or a macroscopic system, the equation evolves the initial state, $|\Psi(0)\rangle$, into a superposition of different states. Nothing in the mathematical formulation of quantum mechanics prevents these superpositions. In microscopic systems, superpositions are indirectly observed through interferences. However, superpositions are very hard to observe in the macroscopic world. Furthermore, when a measurement is performed on a system, the superpositions disappear and we have always a single outcome. This is known as the "collapse of the wave function". Both the rareness of macroscopic superpositions and the measurement process are not described by the Schrödinger equation.

Why is there a discrepancy between what is predicted by the Schrödinger equation and what we observe? The Copenhagen interpretation, suggested by Niels Bohr and others, asserts that there exists a distinct, yet mobile, boundary between the quantum and the classical. According to Bohr, the quantum-classical boundary exists separately from the formalism of quantum mechanics, so that quantum calculations cannot incorporate a classical measuring apparatus or any classical object, in general. It is therefore impossible that the wave function collapse will emerge from the mathematical formalism of quantum mechanics or that macroscopic superpositions will be observed [3].

Experimental advances since Bohr challenge the existence of a defined limit between quantum and classical. Whereas we usually associate quantum with microscopic, the cryogenic version of the Weber bar, which is a gravity-wave detector cooled to 10^{-3} K and of a couple of meters long, must be considered as a quantum harmonic oscillator because it deals with tiny oscillations [4]. Within the category of superconducting quantum interference devices (SQUIDs), which are devices based on superconducting Josephson junctions and used to measure extremely weak signals, a macroscopic superposition of two magnetic-flux states - one corresponding to a few microamperes of current flowing clockwise, the other corresponding to the same amount of current flowing anticlockwise - was observed one decade ago [5]. At the present, much more advanced research is expanding the frontiers of the quantum-classical boundary [6].

Is there a defined physical quantum-classical boundary? And, if superpositions exist throughout the universe, why are they not easily observed? Though the superpositions exist, the process of measurement somehow selects, or at least appears to select, a single outcome. Why does one state become observed over the other possibilities? The decoherence approach, initiated by Zeh [1] and further developed by Zurek [2], attempts to solve the problem of infrequent macroscopic superpositions by suggesting that macroscopic systems are never completely isolated from their environments. Schrödinger's equation describes a closed system that cannot exist in our universe. According to the decoherence program, the loss of quantum coherence from the system to its surroundings leads to the emergence of classical properties [1,2,6]. It is important to note, however, that contrary to its original goal, the decoherence approach was not able to solve the measurement problem. The description of the collapse of the wave function remains a main topic of debate in foundations of quantum mechanics [6,7,8]. In short, the decoherence approach provides a good description of the effects of the interaction of a system with its surroundings, it justifies the rareness of macroscopic superpositions, it has been tested experimentally, but it does not explain the collapse of the wave function.

2. Wave-particle duality and Quantum Superpositions

Particles / Double-slit experiment: On the macroscopic level, it is simple to predict what will occur when two cars crash, when a baseball is thrown, or even how long it will take for an explosion that originates on the Sun to be seen on Earth. In classical mechanics, objects are taken to act as particles, and as such, the physical properties of an object can be described accurately with nearly complete certainty.

Newtonian mechanics deals with the behavior of the particle. The double-slit experiment is often used to illustrate the parameters of the particle-like nature of matter and to compare them with those that define the wave-like nature of matter and quantum behavior [9]. The experiment is set up by placing a moving gun some distance away from a wall with two slits. Behind the wall, there is a backstop and a movable detector which collects the bullets where they hit the backstop (See Figure 1). The experiment measures the probability of arrival of each (indestructible) bullet.

In this (somewhat idealized) experiment, the bullets are shot at a slow rate, so that exactly one bullet arrives at the detector at a given moment in time. Each bullet that reaches the detector is found to have passed through either slit 1 or slit 2. When hole 2 is covered, the bullets can only pass through hole 1, and we get curve P_1. When hole 1 is covered, we get curve P_2. When both holes are open, the probability that a bullet will pass through either of the slits is the sum of the probability that it will pass through slit 1 and the probability that it will pass through slit 2, and can be modeled using the curve P_{12} in Figure 1 [9].

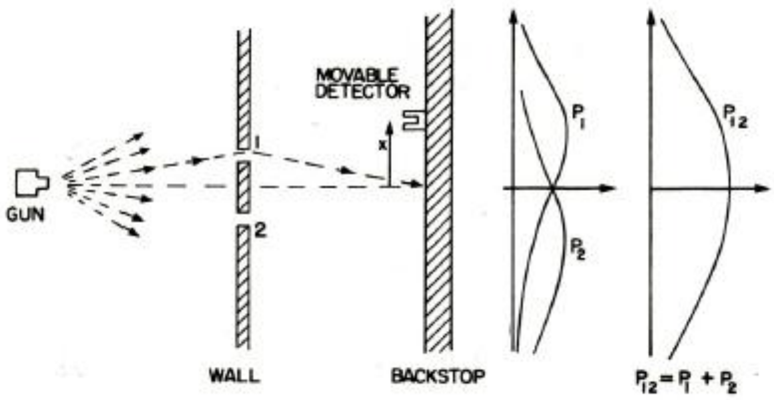

Figure 1 [9]: Interference experiment with bullets

Waves / Double-slit experiment: According to classical mechanics, water, light, and sound behave like waves. The wave-like nature of matter is shown by performing the double-slit experiment using water waves. The experiment is set up in the same way, except that gun shooting bullets is replaced by a wave source and the entire system is placed in a shallow pool of water.

The experiment is performed by a motor, which gently moves the wave source up and down to form a circle of waves around the source (See Figure 2). The detector is set to measure the intensity of the waves, a property which is proportional to the square of the amplitude of the waves, and directly proportional to the energy transmitted by the waves.

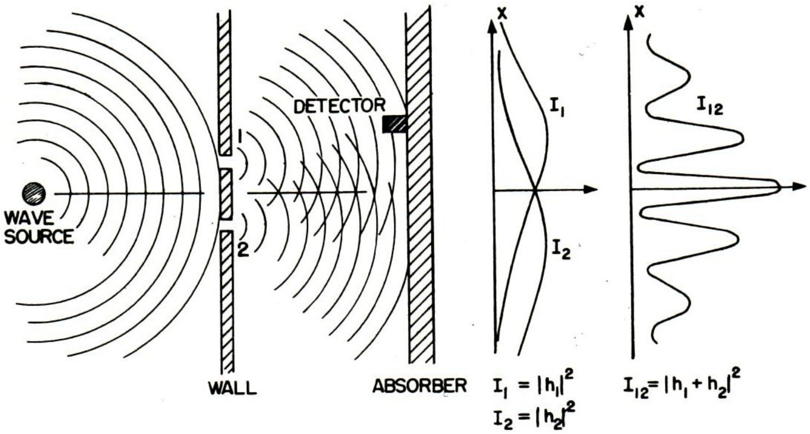

Figure 2 [9]: Interference experiment with water waves.

Unlike the bullets, which arrive at the detector one-by-one, the height of the waves as they reach the detector varies continuously, and therefore intensities of an infinite number of values within a range of values are measured. When both slits are open and intensity of the waves as they reach the detector is plotted against the distance from the center of the backstop where the waves hit, the resulting plot, I_{12}, shows a pattern of constructive and deconstructive addition of waves, known as interference [9].

Quantum mechanics / Electrons / Double-slit experiment: The conceptual basis of the wave-particle duality which is observed on the quantum scale is exemplified by performing the double-slit experiment with microscopic particles, such as electrons. The experiment is set up by placing an electron gun in front of a wall with two holes. The electron gun consists of a heated tungsten wire at a negative voltage with respect to a surrounding metal box. The box contains a hole through which some of the accelerated electrons from the wire will pass through. The detector in this experiment is an electron multiplier which is placed at the backstop and connected to a loudspeaker, which will identify when an electron hits the screen (See Figure 3).

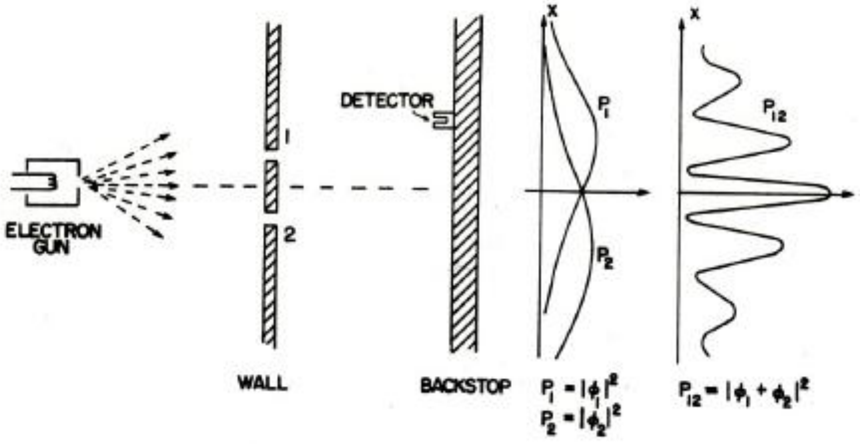

Figure 3 [9]: Interference experiment with electrons.

When the experiment is performed using electrons, only one click is heard at a time, suggesting particulate behavior. Interestingly, however, when both slits are open, the probability of an electron hitting the backstop at a specified distance from the center is visualized by a curve identical to that which the experiment with water waves yielded.

For the probability curves of electrons to yield the same pattern that resulted from the addition of waves, interference must have occurred. And although just one electron is released by the electron gun at a time, and just one electron is detected at the backstop, the interference pattern suggests that the electron must have passed through both slit 1 and slit 2. When propagating, the electron is said to be in a ***quantum superposition*** of both states: passing through slit 1 and passing through slit 2. The electron, which we understand to be a particle when detected clearly has some properties of waves when propagating!

In fact, Richard Feynman envisioned this as an instructive thought experiment [9]. Since then, experimental techniques have advanced greatly, and the experiment has been performed numerous times, using electrons, neutrons, atoms, small molecules, and noble gas clusters. Recently, the boundary of experimental evidence of wave-particle duality expanded as more massive molecules, such as buckyballs (the buckminsterfullerene molecule, C_{60}), were found experimentally to exhibit wave-particle duality [10].

Quantum Superposition: In our macroscopic world, a single bullet is not observed to simultaneously pass through both slit 1 and slit 2. The notion of one object existing in two states at once, that is in a quantum superposition, is one which our minds, entrenched in the world as we experience it, find impossible to comprehend. The most famous application of the conflict between what we know to occur on the microscopic level and what we observe is the paradox of Schrödinger's cat, from Erwin Schrödinger's famous thought experiment [11].

Schrödinger proposed a thought experiment in which the fatality of a cat is coupled to the fate of a single radioactive atom. The cat is placed inside a box with a radioactive atom and a vial of poison. If the atom decays, it causes a hammer to break the vial and kill the cat. However, the laws of quantum mechanics state that the atom is at all times in a superposition of "decayed" and "not decayed." If this superposition is extended to the entire system within the box, the cat is also in a superposition of "dead" and "alive."

Applications in Quantum Computing: The numerous applications of the limitless framework of quantum mechanics are only beginning to be discovered. In the realm of computing, quantum mechanics can be used to build a far more advanced and sophisticated computer than classical mechanics allows for. The classical computer stores information in bits, either 0 or 1, each of which can perform a single operation at a time.

The quantum computer, which is currently under development in laboratories spanning the globe, employs quantum bits, or qubits, to store information and perform computations. Each qubit can have a value of 0, 1, or any of the infinite possible superpositions of 0 and 1, $\alpha|0\rangle + \beta|1\rangle$ (α and β are complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$). Therefore, a quantum computer with n qubits can be in 2^n states at the same time. As opposed to a classical system, which requires an exponentially greater amount of space to perform multiple simultaneous computations, in a quantum system, computational capacity increases exponentially with the number of qubits, so that many operations can be executed in parallel in a single machine.

The main question, however, is how to create and maintain superpositions of several qubits. As we will see below, quantum superpositions of many-particle states are very delicate and are rapidly suppressed by the interaction with the surrounding environment. The disappearance of quantum superpositions, the so-called phenomena of decoherence, is the main subject of this thesis. A clear understanding of the causes of decoherence and how to circumvent it is therefore essential to new technologies which try to make use of the properties of the quantum world.

3. Some Mathematical Tools of Quantum Mechanics

3.1 The wave function and the Schrödinger equation

The Wave Function: All the information about a quantum system, including its dynamics, is given by the wave function, $\Psi(x,t)$ [to simplify the notation, a one-dimensional system is considered]. The wave function is obtained by solving the Schrödinger equation,

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

The wave function is a mathematical tool, it is complex and does not have physical reality. Its absolute square, on the other hand, is real and physical, it corresponds to probability.

Quantum mechanics is intrinsically probabilistic, and the integral, $\int_a^b |\Psi(x,t)|^2 dx$, gives the probability that at a time t, the particle will be found in a position between a and b.

Normalization: Since the absolute square of the wave function gives the probability of finding the particle at position x, at time t, then $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx$, which gives the probability of finding the particle anywhere, at a given time t, must be equal to one. As per the Schrödinger equation, if $\Psi(x,t)$ is a solution, then so too is $A\Psi(x,t)$, where A is a real or complex constant. After solving Schrödinger's equation, the wave function must then be normalized by choosing a value for A whereby $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$. Only normalized wave functions can yield physically solutions to the Schrödinger equation.

To see how the wave function can be applied to a real-life example, we return to our double-slit experiment with electrons. In a general case, the wave function of a superposition of basis states $|\Psi_n\rangle$ can be represented as $|\Psi\rangle = \sum_n c_n |\Psi_n\rangle$. Our specific case is described by the expression

$$|\Psi\rangle = c_1|\Psi_1\rangle + c_2|\Psi_2\rangle \qquad (2),$$

where $|\Psi_1\rangle$ and $|\Psi_2\rangle$ denote the probability amplitude for the particle to pass through slit 1 and slit 2, respectively. Before proceeding, we must ensure that our wave function is normalized. To do so, we place coefficients before $|\Psi_1\rangle$ and $|\Psi_2\rangle$ so that, when squared, their sum is equal to one, that is, $|c_1|^2 + |c_2|^2 = 1$. Additionally, we know experimentally that there is a probability of $\frac{1}{2}$ that the electron will go through slit 1, and there is a probability of $\frac{1}{2}$ that the electron will go through slit 2. Therefore, we can rewrite the normalized wave function as $|\Psi\rangle = \frac{1}{\sqrt{2}}|\Psi_1\rangle + \frac{1}{\sqrt{2}}|\Psi_2\rangle$.

Although the wave function for our experiment describes a superposition of “slit 1” and “slit 2,” we cannot confirm this via measurement, because once we measure which slit the particle is passing through, we effectively collapse the wave function to just $|\Psi_1\rangle$ or $|\Psi_2\rangle$, and we observe pure particle behavior. However, the resultant interference patterns which we saw in our experiment illustrate, that, in fact, the electron was in a superposition of “slit 1” and “slit 2” [9].

The Schrödinger Equation: The Schrödinger equation [see Eq.(1)] describes how the wave function evolves in time. It is composed of a kinetic energy part, $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, and a potential energy part, V, where $\hbar$ is Planck’s constant and m is the mass of the particle. It may also be denoted as

$$i\hbar\frac{\partial \quad \Psi}{\partial t} = H\Psi \qquad (3),$$

where H is an operator called the Hamiltonian (see Section 5).

The general Schrödinger equation is time-dependent and difficult to solve. However, when the potential of the system remains constant in time, we can apply the method of separation of variables to solve it [12]. We write $\Psi(x,t) = \psi(x)\varphi(t)$, where ψ is a function exclusively of x and φ is a function exclusively of t. We can solve two separated ordinary equations. The first equation, $\frac{i\hbar}{\varphi}\frac{d\varphi}{dt} = E$, is easy to solve, and can be reduced to $\varphi(t) = e^{-iEt}/_{\hbar}$. The second equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\Psi = E\Psi \qquad (4),$$

is known as the time-independent Schrödinger equation. The time-independent Schrödinger equation may also be written as

$$H\psi = E\psi, \quad (5)$$

where H is the Hamiltonian and E represents the total energy of the system. To solve the time-independent Schrödinger equation, we need the potential, V. In the case of a continuous potential, there is an infinite number of solutions to the time-independent Schrödinger equation $(\psi_1(x), \psi_2(x), \psi_3(x), \ldots)$, which are called eigenstates. Each eigenstate has an associated energy value, which is called the eigenvalue.

The general solution to the time-dependent Schrödinger equation, describing a non-stationary state, is any linear combination[1] of specific solutions to the time-independent Schrödinger equation. The general solution is expressed as

$$\Psi(x,t) = \sum_n c_n \Psi_n(x) e^{-{iE_n t}/{\hbar}} \quad (6).$$

The constant, c_n, is chosen so that the wave function corresponds to the initial state at t=0. The general solution denotes a superposition of all eigenstates of $H\psi = E\psi$, and is what we compute for a given Hamiltonian, H, describing our system. The particular Hamiltonian considered in this thesis is described in Section 5.

3.2 Density matrix

Density matrix: The density operator, ρ, is another way to describe the state of a system. Whereas $|\Psi\rangle$ is a vector, ρ, is a matrix, equivalent to

$$\rho \equiv |\Psi\rangle\langle\Psi| \quad (7).$$

For example, in the double-slit experiment, we previously wrote out the wave function in bra-ket notation $|\Psi\rangle = \frac{1}{\sqrt{2}}|\Psi_1\rangle + \frac{1}{\sqrt{2}}|\Psi_2\rangle$. This is a pure state, which contains all possible

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[1] A linear combination of function $f_1(x), f_2(x), \ldots$ is the expression $f(x) = c_1 f_1(x) + c_2 f_2(x) \ldots$, where c_1, c_2 ... are any complex constant [12].

information about the state of the electron. In matrix form, $|\Psi\rangle$ can be represented by the column vector $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$, and its Hermitian conjugate, $\langle\Psi|$, can be represented by the row vector $\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix}$; ρ then becomes

$$\rho = \left(\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}\right)\left(\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix}\right) = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} \quad (8).$$

Trace: In linear algebra, the sum of the diagonal elements of a matrix M is called trace and is denoted by $Tr[M]$. As a consequence of the normalization of the wave function, the sum of the diagonal elements of the density matrix has to be equal to 1. In the case of the double-slit above, the trace operation is defined as $Tr[\rho] = \langle\psi_1|\rho|\psi_1\rangle + \langle\psi_2|\rho|\psi_2\rangle$. More generally, for the matrix M written in the orthonormal basis vector $\{|\psi_i\rangle\}$, the trace can be written as

$$Tr(\mathrm{M}) \equiv \sum_i \langle\psi_i|\mathrm{M}|\psi_i\rangle \quad (9).$$

Pure vs Mixed States: A pure state can be described by a ket vector, or equivalently, by its corresponding density matrix. It may be a single well-defined state or a superposition of different possibilities, as we showed above for the case of an electron in the double-slit experiment.

Mixed states, however, can only be described by density matrices. A mixed state corresponds to an ***ensemble*** of different systems possibly in different states. For example, suppose we have an ensemble with several spins- ½, where half of them are pointing up and half are pointing down. This ensemble cannot be described by a single vector, but it can be described by a density matrix as

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| \quad (10).$$

In the general form of the equation, $\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i| = \sum_i p_i \;\rho_i$, where p_i is a classical probability and $\rho_i = |\psi_i\rangle\langle\psi_i|$ is pure-state density matrix. Notice that Eq. (10) in matrix form is simply $\rho = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. It does not contain off-diagonal elements. In contrast, ρ in Eq. (8), which is a matrix describing a system in a quantum superposition, does contain off-diagonal elements. A mixed state presents probabilistic aspects that we may find also at the classical level; quantum interferences are characteristically nonexistent in the mixed state. The off-diagonal elements, on the other hand, represent the coherent superpositions of different states and correspond to purely quantum mechanical features of the system [2,6]. In this thesis, we will show how the off-diagonal elements of the density matrix describing our system disappear due to the interaction with the surrounding environment.

Purity: A simple criterion for checking whether a density matrix is describing a pure or mixed state is that the trace of ρ^2 is equal to 1 if the state is pure and less than 1 if the state is mixed. Compare the two density matrices above. In the case of the double-slit experiment [Eq.(8)], $Tr[\rho^2] = 1$, but for the ensemble of spins-½ [Eq.(10)], $Tr[\rho^2] = \frac{1}{2}$. In this thesis we will show a simple model where $Tr[\rho^2]$ for a spin system decays from 1 to ½.

Partial trace: The partial trace operation is performed when we do not have access to some parts of the system. For example, in the case of the double-slit, if we could only perform measurements right after slit 1, we could trace out slit 2. The operation corresponds to $\langle\psi_2|\rho|\psi_2\rangle$, which in this case yields simply ½.

In general, the trace is performed over larger systems and what it does is to reduce the density matrix to contain information only about some part of the system we can have access to. In the studies of decoherence, for instance, we trace over the degrees of freedom of the environment, which we do not have access to and focus simply on the reduced density matrix of the system of interest [2,6].

4. Decoherence and the Transition from Quantum to Classical

Von Neumann measurement scheme: Historically, the problem of the disappearance of quantum properties was very disturbing to the founders of quantum mechanics. Many theories were developed to explain how classical properties can emerge from quantum mechanics and why measurement of a quantum system destroys the system's quantum properties. Neils Bohr was aware of the necessity of using a classical language for describing the results of experiments and constructed his interpretation of quantum mechanics based on this [13]. The need for a classical language is imposed, according to him, by the classical nature of observers and experimental apparatuses. Observers and apparatuses are not described by wave functions. According to Bohr, wave functions pertain only to the microscopic world.

The desire to have a single description of the world in quantum terms led von Neumann to address quantum mechanically the system as well as the measuring apparatus [14]. This approach, if successful, would have removed the somewhat arbitrary division between the classical and the quantum world introduced by Bohr. However, in so doing, he had to face the problem of superpositions of macroscopic distinguishable states. To illustrate von Neumann's proposal, consider a system of two spins-½. The system is initially in the pure state $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$, where $|\alpha|^2 + |\beta|^2 = 1$. Taking the measuring device into account and assuming that initially it is in the state , $|d_\downarrow\rangle$, the joint initial state of system and apparatus becomes $|\phi_i\rangle = (\alpha|\uparrow\rangle + \beta|\downarrow\rangle)|d_\downarrow\rangle$. Interaction between the system and the measuring apparatus evolves $|\phi_i\rangle$ into a correlated state,

$$|\phi_c\rangle = \alpha|\uparrow\rangle|d_\uparrow\rangle + \beta|\downarrow\rangle|d_\downarrow\rangle \quad (11),$$

or equivalently in the form of a density matrix,

$\rho_c = |\phi_c\rangle\langle\phi_c| =$

$= |\alpha|^2|\uparrow\rangle\langle\uparrow||d_\uparrow\rangle\langle d_\uparrow| + \alpha\beta^*|\uparrow\rangle\langle\downarrow||d_\uparrow\rangle\langle d_\downarrow| + \alpha^*\beta|\downarrow\rangle\langle\uparrow||d_\downarrow\rangle\langle d_\uparrow| + |\beta|^2|\downarrow\rangle\langle\downarrow||d_\downarrow\rangle\langle d_\downarrow|.$

von Neumann managed to move the quantum/classical cut away from the system/apparatus boundary, but at the price of leaving the joint system in a coherent superposition of states which is not observed. No matter how many apparatuses are included, the superpositions will remain. At this stage von Neumann distinguished two types of processes in quantum mechanics: the one described above, leading to undesirable macroscopic superpositions as a consequence of the reversible unitary evolution of Schrödinger’s equation and the other one, corresponding to our knowledge of the result of the measurement, which is irreversible.

von Neumann formalized the irreversibility in quantum mechanics by postulating a non-unitary evolution, the so-called “process 1”, which leads ρ_c into a mixed state. The density matrix of the pure correlated state ρ_c becomes a reduced density matrix,

$$\rho_r = |\alpha|^2|\uparrow\rangle\langle\uparrow||d_\uparrow\rangle\langle d_\uparrow| + |\beta|^2|\downarrow\rangle\langle\downarrow||d_\downarrow\rangle\langle d_\downarrow| \quad (12).$$

Both outcomes are still present in the reduced density matrix, however in the reduced density matrix, the probabilities are ***classical probabilities*** of an unknown state. The system and detector may either be in the state $|\uparrow\rangle\langle\uparrow||d_\uparrow\rangle\langle d_\uparrow|$ ***or*** in the state $|\downarrow\rangle\langle\downarrow||d_\downarrow\rangle\langle d_\downarrow|$.

To avoid imposing the postulate without any physical justification, von Neumann introduced the observer and his/her subjective perception becomes essential. Needless to say, this interpretation is thereby weakened and open to severe criticisms. The goal of the decoherence approach has been to provide a justification to process 1 through the inevitable interaction between the joint system and its environment.

The idea of the environment-induced decoherence is the following. Following von Neumann's tradition, system, apparatus and environment are treated quantum mechanically. Assuming the environment is initially in the state , $|\varepsilon_0\rangle$, we have,

$$|\Psi\rangle \quad = |\phi_c\rangle|\varepsilon_0\rangle = (\alpha|\uparrow\rangle|d_\uparrow\rangle + \beta|\downarrow\rangle|d_\downarrow\rangle)|\varepsilon_0\rangle \qquad (13),$$

which after some time, because of the interaction, becomes an enormous superposition of macroscopically different states,

$$|\Psi\rangle \quad = \alpha|\uparrow\rangle|d_\uparrow\rangle|\varepsilon_0\rangle + \beta|\downarrow\rangle|d_\downarrow\rangle|\varepsilon_0\rangle = |\Psi\rangle \qquad (14).$$

As the environment has a large number of degrees of freedom, the observer has no access to them and therefore, they must be traced over, ignored. The desired reduced density matrix of the detector-system, after the degrees of freedom of the environment have been traced over, $\rho_{\mathcal{SD}} = Tr_\varepsilon|\Psi\rangle\langle\Psi| = \sum_i \langle\varepsilon_i|\Psi\rangle\langle\Psi|\varepsilon_i\rangle = \rho_r$, is obtained if the states of the environment, $|\varepsilon_i\rangle$, are orthogonal. The system is now in a mixed state given by Eq.(12); interactions between the system and environment have destroyed coherent superpositions [1,2,6].

Time scale of decoherence: The time scale for the disappearance of the off-diagonal elements, or quantum coherences, will depend on the system and its environment. In a simple model of a particle interacting with a scalar field and in the limit of high temperature, it is possible to show that the decoherence time τ_D is [Ref.[2] and references therein]

$$\tau_D \cong \tau_R \frac{\hbar^2}{2mk_BT(\Delta x)^2} = \gamma^{-1}\left(\frac{\lambda_T}{\Delta x}\right)^2 \qquad (15),$$

where $\lambda_T = \frac{\hbar^2}{\sqrt{2mk_BT}}$ is the thermal de Broglie wavelength[2], m is the mass of the particle, k_B is Boltzmann constant, T is the temperature and τ_R is the relaxation time. The mass in the denominator indicates that the decoherence time is very fast in macroscopic systems and also at large temperatures.

In the case of the Weber bar, the large mass is offset by very small cryogenic temperature values, making the decoherence time longer. However, for an electron, the very small mass in the denominator significantly increases the decoherence time, so that superpositions persist for longer.

Reversibility: Another feature of quantum mechanics which is remarkably absent from our world is reversibility. On the quantum level, the arrow of time shows no preference. When we move into the macroscopic domain the arrow of time becomes unidirectional, and the second law of thermodynamics states that the universe progresses toward a state of maximum entropy. In the decoherence approach, irreversibility arises from statistical causes: the environment has a very large number of degrees of freedom and we have no access to information that is lost through it. Accessing information about the system that is dissipated to the environment would be as difficult as keeping track of the trajectories of the particles in the Maxwell-Boltzmann gas.

5. System Model: one spin-1/2 in a bath of spins-1/2

The system we analyze consists of one spin-½ and its surrounding environment (bath) is composed of 7 spins-½. Particles with spin-1/2 are very common in nature; the basic constituents of matter - electrons, protons and neutrons – have spin ½. The state of a spin-½

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[2] The thermal de Broglie wavelength is the wavelength of matter waves at a specified temperature.

is described by a vector with two components and its corresponding operators are the Pauli matrices:

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The Hamiltonian describing our whole system is

$$H = \sum_{n=2}^{7} (J_x \sigma_1^x \, \sigma_n^x + J_y \sigma_1^y \sigma_n^y + J_z \sigma_1^z \sigma_n^z). \quad (16)$$

Above we set $\hbar = 1$, n refers to the spins of the environment, 1 is the system spin, and $J_{x,y,z}$ are the coupling strengths. Because the total system is too small and far from mimicking a real environment with many degrees of freedom, recurrences in time might occur. To prevent recurrences, the coupling strengths were taken as random real numbers between 0 and 1 for couplings in all directions and with all environment spins. A term in the Hamiltonian, such as the coupling between the system spin 1 and the environment spin 4, $\sigma_1^y \sigma_4^y$, corresponds, in fact, to

$$\sigma_1^y \otimes I_2 \otimes I_3 \otimes \sigma_4^y \otimes I_5 \otimes I_6 \otimes I_7 \otimes I_8,$$

where $I_n \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ is the identity matrix for spin n and $\otimes$ stands for the Kronecker product between matrices.

6. Computer Code

We used the software *Mathematica* to write the Hamiltonian (16) in a matrix form, diagonalize it, and then evolve a certain initial state in time. By tracing out the environment, we were able to simulate numerically the decoherence process. The entire program is shown in the Appendix. The main steps for writing the code were the following ones.

First step: In order to write the matrix elements of the Hamiltonian, we need to choose a basis $|i\rangle$. Our choice corresponds to the two possible states of each spin in the z-direction: up $|\uparrow\rangle$ or down $|\downarrow\rangle$, so that our basis vectors span all the $2^8 = 256$ possible configurations, from $|\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\rangle$ to $|\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$. Each matrix element H_{ij} is obtained by calculating $\langle i|H|j\rangle$.

Second step: The second step is to obtain all eigenvalues, $E_1, E_2, \dots E_{256}$, and eigenstates $\psi_1, \psi_2, \dots \psi_{256}$, by diagonalizing the Hamiltonian [which is equivalent to saying, by solving Eq.(5)]. This is done with specific commands from *Mathematica*.

Third step: We choose as initial state for the system + environment, $\rho_{S+E}(0) = \rho_S \otimes \rho_E$, one in which the system spin is in a superposition, $\rho_s = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, and the environment is in a complete mixed state given by the identity matrix of dimension $2^7 = 128$.

Fourth step: We propagate the total initial state in time and then trace over the spins of the environment to focus only on the evolution of the system.

Using Eq.(3) and a time-independent Hamiltonian, the evolution of the wave function is given by

$$|\psi\rangle = exp\left(-\frac{iHt}{\hbar}\right)|\psi(0)\rangle = U(t)|\psi(0)\rangle \qquad (17),$$

where $U(t)$ is the propagator. From the equation above and Eq.(7), our total system is then evolved according to

$$\rho_{S+E}(t) = U(t)\rho_{S+E}(0)U^{\dagger}(t)$$

The method to perform the partial trace over the environment was obtained from the Wolfram Library Archive [15].

7. Numerical Results

In the figure below, $Tr(\rho^2)$ decays from 1, defining a pure state, to a value of less than 1, indicating a mixed state. Here, ρ is the ***reduced*** density matrix of the system after tracing out the spins of the bath. This decay is caused by the interaction of the system with the bath. Information about the superposition contained in the initial state is lost to the various degrees of freedom of the bath. Thus decay into a mixed state reflects the loss of coherent superpositions, that is, decoherence.

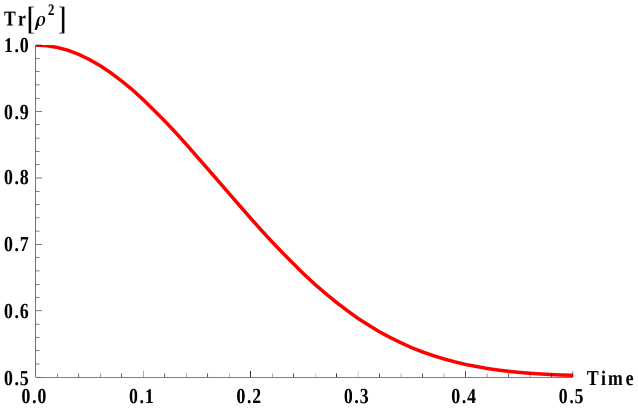
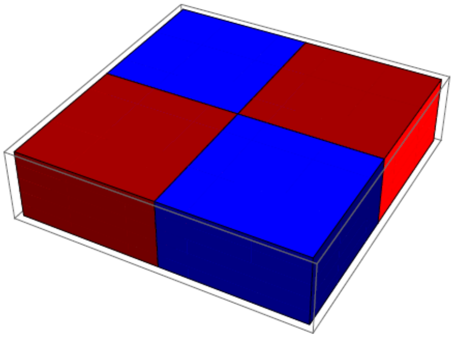


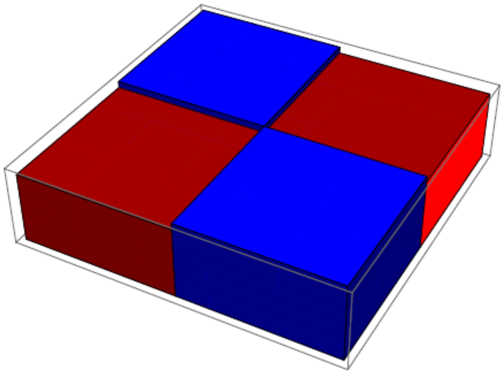
Figure 4: Loss of coherence of the system spin.

Another nice illustration is shown below: The diagonal elements (blue) of the reduced density matrix of the system remain, but the off-diagonal elements (red) decay because of the interaction with the bath. Superpositions, and therefore the quantum aspect of the system, disappear in time [J in the figures below sets the time scale].

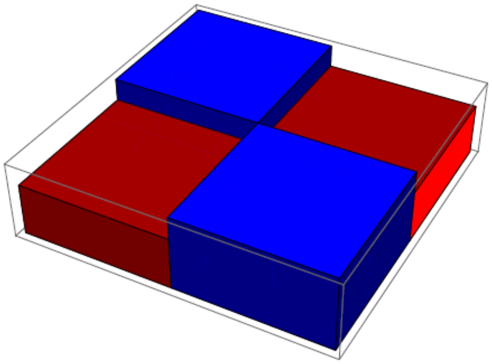
At time=0



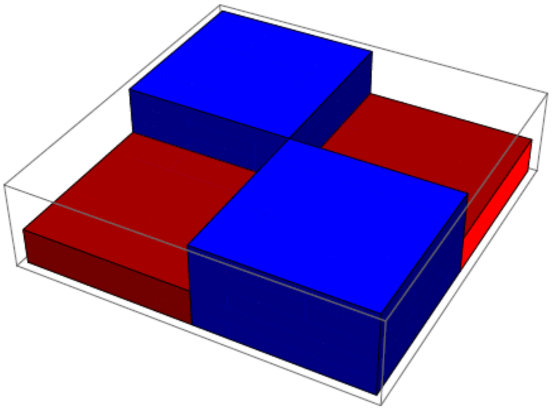
At time=0.1 J



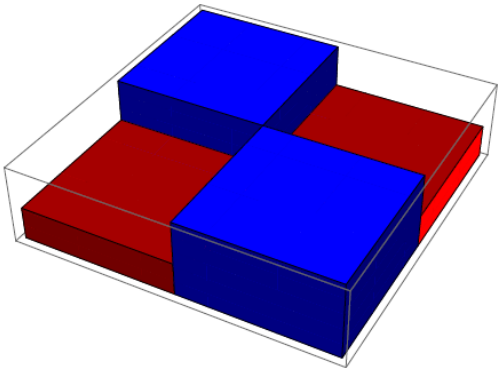
At time=0.2 J



At time=0.3 J



At time=0.4 J



8. Conclusions

Is wave function collapse a subjectivist or objectivist process? Von Neumann subscribed to the subjectivist view, which holds that the human conscious is to blame for the loss of observable superpositions. It is interesting and rather unusual that he does, because physicists prefer their subject to be self-contained; according to the subjectivists, the physical model itself is incomplete, and must be intertwined with psychology to craft a comprehensive quantum theory. Yet, as research advanced, the predominant position held by physicists became the objectivist view that the measurement problem exists apart from the psyche of the human observer. Objectivists refuse to accept the notion of a “black-box” process by which measurement collapses the wave function, and assume that wave function collapse must be an intrinsic part of the quantum theory and its formalism.

While nobody denies the effects of the interaction with surrounding environments and the contributions to the subject added from the studies about decoherence, decoherence has not fulfilled its original purpose, which was to solve the measurement problem. In its formalism, quantum mechanics still lacks a mathematical description for the infamous collapse of the wave function, the instantaneous disappearance of superpositions once a measurement is performed. Decoherence does not explain this fact. Decoherence deals with density matrices and therefore with an ensemble interpretation. It is incapable of describing the collapse of a ***single*** wave function. The partial trace in the decoherence approach is not the same as the projection operation [7,8].

To solve the measurement problem, decoherence needs to be associated with an interpretation, be it the many-world interpretation, Bohm-de Broglie interpretation, the many-minds interpretation, or other interpretations. Surprisingly enough, Zeh himself is a proponent of the many-minds theory, and Zurek accepts the many-worlds interpretation. The principle belief behind the many-worlds interpretation is that many universes exist apart from the one which we observe. Within the many-worlds interpretation, decoherence explains, statistically, the existence of the preferred basis. According to the many-minds interpretation, there are an infinite number of mental states; in this view, the mental state of the observer, which is probabilistic and deterministic by nature, determines the preferred basis [6].

9. Acknowledgements

I would like to thank Dean Bacon, Dr. Wachtell, and the S. Daniel Abraham Honors Program at Stern College for Women for all the wonderful educational opportunities offered to me. Special thanks to Dr. Santos for all the time and energy invested in advising me on this project above and beyond the call of duty.

REFERENCES

[1] Zeh, H. D. 1970, “On the interpretation of measurement in quantum theory”, *Found. Phys.* **1**, 69-76.

[2] Zurek, W. H. 1991, “Decoherence and the Transition from Quantum to Classical”, *Phys. Today* **44**, 36-44.

[3] Bell J. S. 1987, *Speakable and Unspeakable in Quantum Mechanics*, (Cambridge University Press, Cambridge).

[4] Braginsky V. B. and Khalili F.Ya 1992, *Quantum measurement*, (Cambridge University Press, Cambridge).

[5] Friedman J. R., Patel V., Chen W., Tolpygo S. K., and Lukens J. E. 2000, "Quantum superposition of distinct macroscopic states", *Nature* **406**, 43-46.

[6] Schlosshauer, M. 2007, *Decoherence and the Quantum-to-Classical Transition*. (Springer, Berlin).

[7] Pessoa, O. 1998, "Can the Decoherence Approach Help to Solve the Measurement Problem?", *Synthese* **113**, 323-346.

[8] Bacciagaluppi, Guido, "The Role of Decoherence in Quantum Mechanics", The Stanford Encyclopedia of Philosophy (Fall 2008 Edition), Edward N. Zalta (ed.), URL = <http://plato.stanford.edu/archives/fall2008/entries/qm-decoherence/>.

[9] Feynman, R., Leighton R., and Sands M.2006, *The Feynman Lectures on Physics*. Volume 3. (Pearson/Addison-Wesley), pp. 1-11.

[10] Arndt, M., Nairz, O., Vos-Andreae, J., Keller, C., van der Zouw, G., Zeilinger, A. 1999, "Wave-particle Duality of C_{60} Molecules", *Nature* **401**, 680-682.

[11] Schrödinger E. 1935 "Die gegenwärtige Situation in der Quantenmechanik", *Naturwissenschaften* **23,** 807-812, 823-828, 844-849.

[Translation in the book by J. A. Wheeler and W. H. Zurek 1983, *Quantum Theory and Measurement* (Princeton University Press, New Jersey).]

[12] Griffiths, D. J. 2005, *Introduction to Quantum Mechanics*. (Pearson Prentice Hall , New Jersey, 2nd edition).

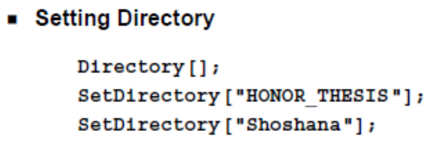
[13] Bohr, N. 1937, *The Causality Problem in Modern Physics, in New Theories in Physics,* (Polish Society for Intellectual Cooperation and International Union of Physics, Warsaw).

[14] von Neumann, J. 1955, *Mathematical Foundations of Quantum Mechanics,* (Princeton University Press, Princeton).

[15] http://library.wolfram.com/infocenter/MathSource/5571/

A. Appendix: The program developed for the analysis of the decoherence process

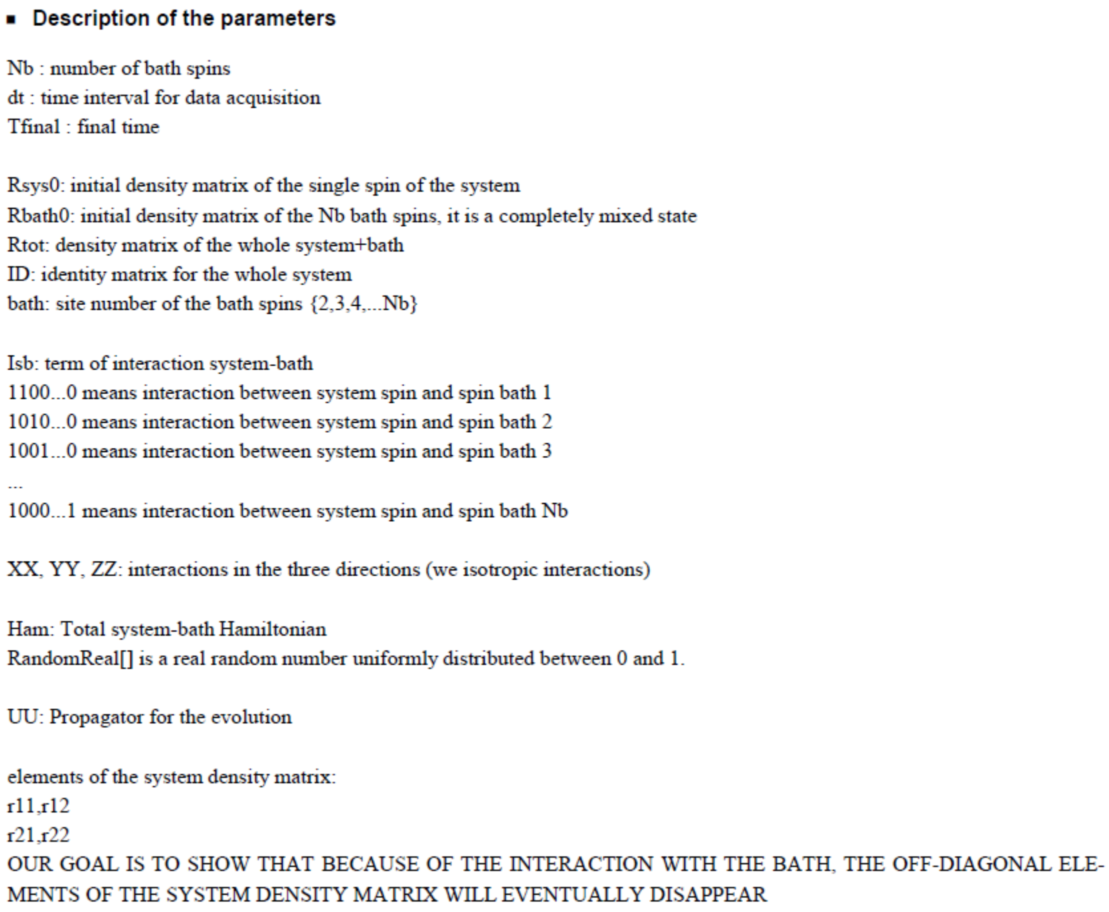
A.1 In *Mathematica*, first we need to let the computer know where (which folder) to dump our results and where to get input data from.



- **Setting Directory**

```
Directory[];
SetDirectory["HONOR_THESIS"];
SetDirectory["Shoshana"];
```

A.2 The description of the parameters that appear in the code is the following.



- **Description of the parameters**

Nb : number of bath spins
dt : time interval for data acquisition
Tfinal : final time

Rsys0: initial density matrix of the single spin of the system
Rbath0: initial density matrix of the Nb bath spins, it is a completely mixed state
Rtot: density matrix of the whole system+bath
ID: identity matrix for the whole system
bath: site number of the bath spins {2,3,4,...Nb}

Isb: term of interaction system-bath
1100...0 means interaction between system spin and spin bath 1
1010...0 means interaction between system spin and spin bath 2
1001...0 means interaction between system spin and spin bath 3
...
1000...1 means interaction between system spin and spin bath Nb

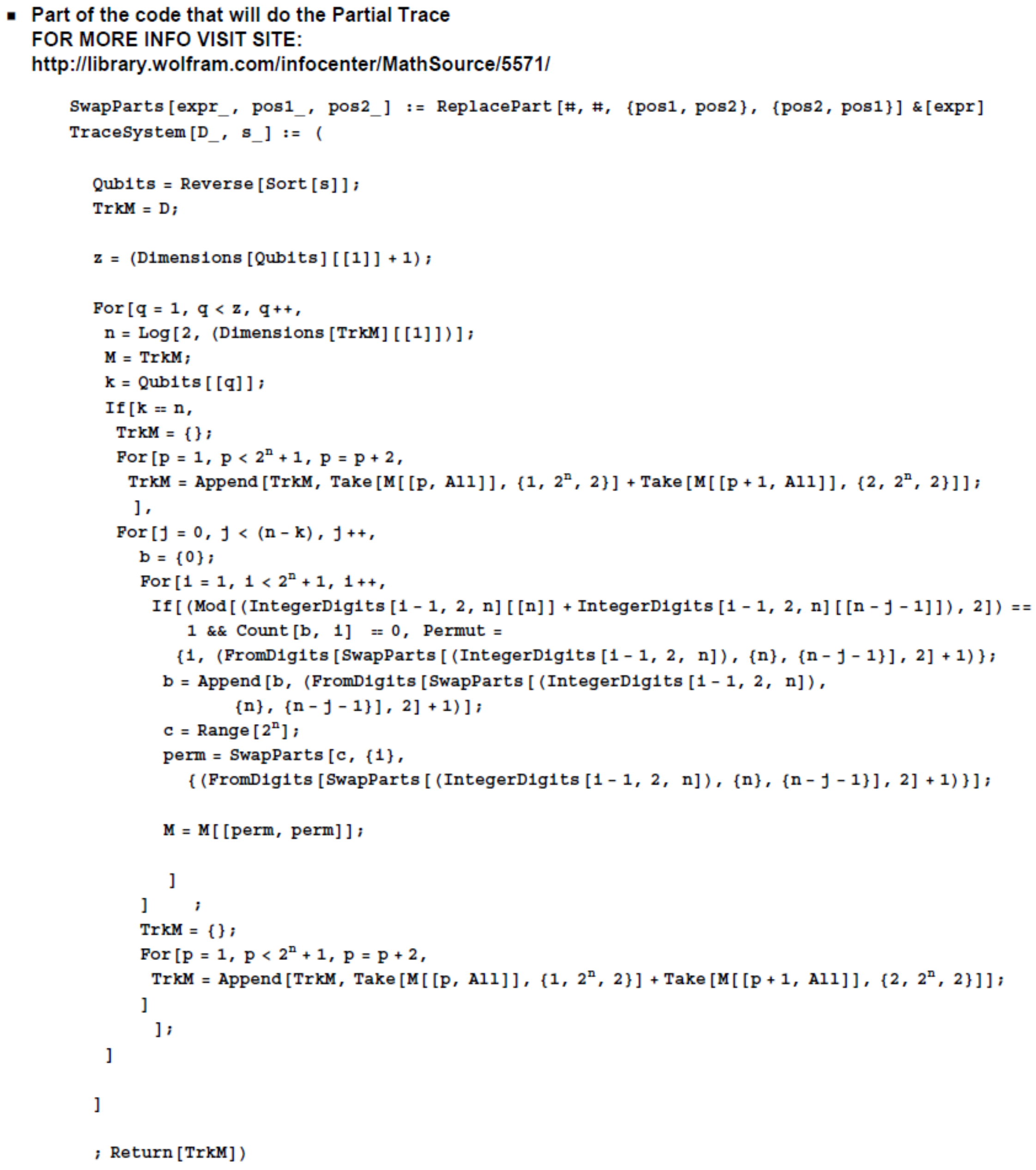
XX, YY, ZZ: interactions in the three directions (we isotropic interactions)

Ham: Total system-bath Hamiltonian
RandomReal[] is a real random number uniformly distributed between 0 and 1.

UU: Propagator for the evolution

elements of the system density matrix:
r11,r12
r21,r22
OUR GOAL IS TO SHOW THAT BECAUSE OF THE INTERACTION WITH THE BATH, THE OFF-DIAGONAL ELEMENTS OF THE SYSTEM DENSITY MATRIX WILL EVENTUALLY DISAPPEAR

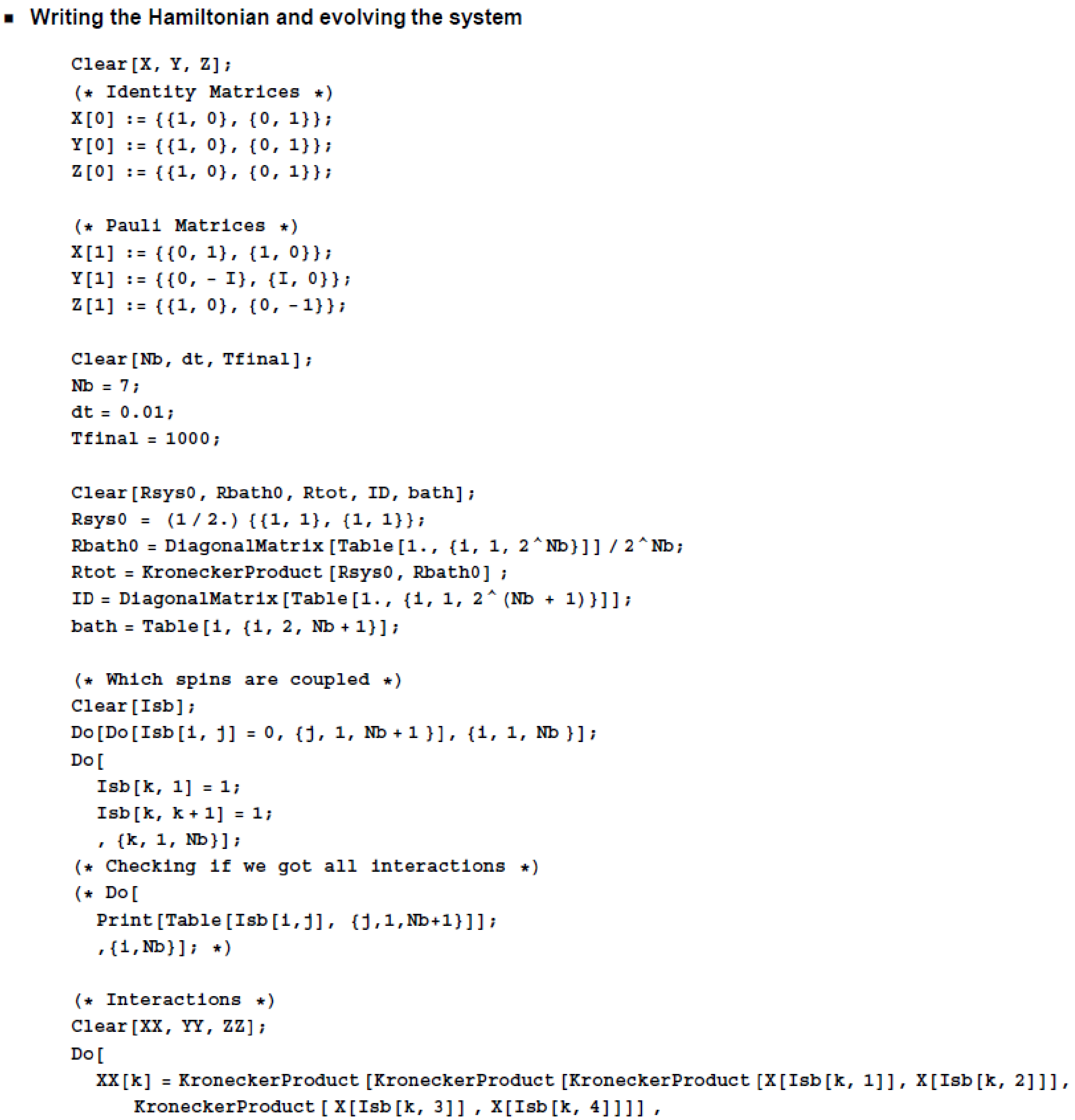
A.3 The part below, copied from the “Wolfram Library Archive”[15] ,computes the partial trace of a given matrix. In the main code, we use the notation “TraceSystem[M, {n1,n2,n3,…}]”, where M is the density matrix of the whole system+bath and {n1, n2, n3,…} are the spins that belong to the bath, which need to be traced out.



- **Part of the code that will do the Partial Trace**
  FOR MORE INFO VISIT SITE:
  http://library.wolfram.com/infocenter/MathSource/5571/

```
SwapParts[expr_, pos1_, pos2_] := ReplacePart[#, #, {pos1, pos2}, {pos2, pos1}] &[expr]
TraceSystem[D_, s_] := (

  Qubits = Reverse[Sort[s]];
  TrkM = D;

  z = (Dimensions[Qubits][[1]] + 1);

  For[q = 1, q < z, q++,
   n = Log[2, (Dimensions[TrkM][[1]])];
   M = TrkM;
   k = Qubits[[q]];
   If[k == n,
    TrkM = {};
    For[p = 1, p < 2^n + 1, p = p + 2,
     TrkM = Append[TrkM, Take[M[[p, All]], {1, 2^n, 2}] + Take[M[[p + 1, All]], {2, 2^n, 2}]];
     ],
    For[j = 0, j < (n - k), j++,
      b = {0};
      For[i = 1, i < 2^n + 1, i++,
       If[(Mod[(IntegerDigits[i - 1, 2, n][[n]] + IntegerDigits[i - 1, 2, n][[n - j - 1]]), 2]) ==
          1 && Count[b, i]  == 0, Permut =
         {i, (FromDigits[SwapParts[(IntegerDigits[i - 1, 2, n]), {n}, {n - j - 1}], 2] + 1)};
        b = Append[b, (FromDigits[SwapParts[(IntegerDigits[i - 1, 2, n]),
              {n}, {n - j - 1}], 2] + 1)];
        c = Range[2^n];
        perm = SwapParts[c, {i},
          {(FromDigits[SwapParts[(IntegerDigits[i - 1, 2, n]), {n}, {n - j - 1}], 2] + 1)}];

        M = M[[perm, perm]];

         ]
      ]    ;
      TrkM = {};
      For[p = 1, p < 2^n + 1, p = p + 2,
       TrkM = Append[TrkM, Take[M[[p, All]], {1, 2^n, 2}] + Take[M[[p + 1, All]], {2, 2^n, 2}]];
      ]
       ];
   ]

  ]

  ; Return[TrkM])
```

A.4 The main code for the system spin-1/2 interactiong with 7 bath spins-1/2.



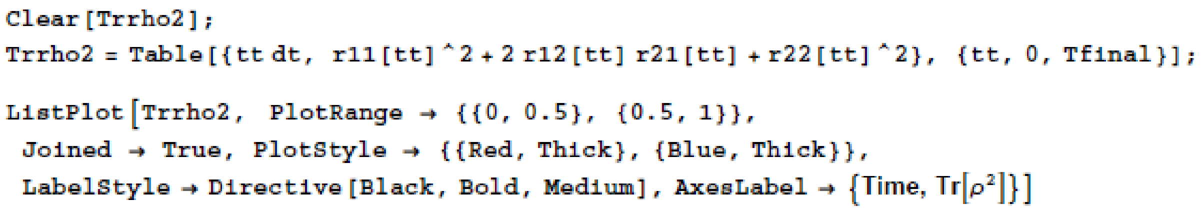
- **Writing the Hamiltonian and evolving the system**

```
Clear[X, Y, Z];
(* Identity Matrices *)
X[0] := {{1, 0}, {0, 1}};
Y[0] := {{1, 0}, {0, 1}};
Z[0] := {{1, 0}, {0, 1}};

(* Pauli Matrices *)
X[1] := {{0, 1}, {1, 0}};
Y[1] := {{0, - I}, {I, 0}};
Z[1] := {{1, 0}, {0, -1}};

Clear[Nb, dt, Tfinal];
Nb = 7;
dt = 0.01;
Tfinal = 1000;

Clear[Rsys0, Rbath0, Rtot, ID, bath];
Rsys0 = (1 / 2.) {{1, 1}, {1, 1}};
Rbath0 = DiagonalMatrix[Table[1., {i, 1, 2^Nb}]] / 2^Nb;
Rtot = KroneckerProduct[Rsys0, Rbath0] ;
ID = DiagonalMatrix[Table[1., {i, 1, 2^(Nb + 1)}]];
bath = Table[i, {i, 2, Nb + 1}];

(* Which spins are coupled *)
Clear[Isb];
Do[Do[Isb[i, j] = 0, {j, 1, Nb + 1 }], {i, 1, Nb }];
Do[
  Isb[k, 1] = 1;
  Isb[k, k + 1] = 1;
  , {k, 1, Nb}];
(* Checking if we got all interactions *)
(* Do[
  Print[Table[Isb[i,j], {j,1,Nb+1}]];
  ,{i,Nb}]; *)

(* Interactions *)
Clear[XX, YY, ZZ];
Do[
  XX[k] = KroneckerProduct[KroneckerProduct[KroneckerProduct[X[Isb[k, 1]], X[Isb[k, 2]]],
     KroneckerProduct[ X[Isb[k, 3]] , X[Isb[k, 4]]]] ,
```

```
    KroneckerProduct[KroneckerProduct[X[Isb[k, 5]], X[Isb[k, 6]]],
     KroneckerProduct[ X[Isb[k, 7]], X[Isb[k, 8]]]] ] ;
  YY[k] = KroneckerProduct[KroneckerProduct[KroneckerProduct[Y[Isb[k, 1]], Y[Isb[k, 2]]],
     KroneckerProduct[ Y[Isb[k, 3]] , Y[Isb[k, 4]]]] ,
    KroneckerProduct[KroneckerProduct[Y[Isb[k, 5]], Y[Isb[k, 6]]],
     KroneckerProduct[ Y[Isb[k, 7]], Y[Isb[k, 8]]]] ]  ;
  ZZ[k] = KroneckerProduct[KroneckerProduct[KroneckerProduct[Z[Isb[k, 1]], Z[Isb[k, 2]]],
     KroneckerProduct[ Z[Isb[k, 3]] , Z[Isb[k, 4]]]] ,
    KroneckerProduct[KroneckerProduct[Z[Isb[k, 5]], Z[Isb[k, 6]]],
     KroneckerProduct[ Z[Isb[k, 7]], Z[Isb[k, 8]]]] ]  ;
  , {k, 1, Nb}];

(* Total Hamiltonian *)
Clear[Ham];
Ham = Sum[RandomReal[] XX[jj] + RandomReal[] YY[jj] + RandomReal[] ZZ[jj],  {jj, 1, Nb}];

(* Propagator for the Time Evolution *)
Clear[UU, Rsys, r11, r12, r21, r22];
UU = ID;
Rsys  = TraceSystem[UU.Rtot.Conjugate[Transpose[UU]], bath];
r11[0]  = Abs[Rsys[[1, 1]]];
r12[0]  = Abs[Rsys[[1, 2]]];
r21[0]  = Abs[Rsys[[2, 1]]];
r22[0]  = Abs[Rsys[[2, 2]]];

(* Time Evolution *)
Do[
  UU  = MatrixExp[-I Ham dt].UU;
  Rsys  = TraceSystem[UU.Rtot.Conjugate[Transpose[UU]], bath];
  r11[tt]  = Abs[Rsys[[1, 1]]];
  r12[tt]  = Abs[Rsys[[1, 2]]];
  r21[tt]  = Abs[Rsys[[2, 1]]];
  r22[tt]  = Abs[Rsys[[2, 2]]];
  If[Mod[tt, 100]  == 0, Print[tt]];
  , {tt, 1, Tfinal}];

diag1  = Table[{tt dt, r11[tt]},  {tt, 0, Tfinal}];
diag2  = Table[{tt dt,  r22[tt]},  {tt, 0, Tfinal}];
off1  = Table[{tt dt,  r12[tt]},  {tt, 0, Tfinal}];
off2  = Table[{tt dt,  r21[tt]},  {tt, 0, Tfinal}];
```

Above, diag1 and diag2 give the results for the diagonal elements and off1 and off2 correspond to the off-diagonal elements.

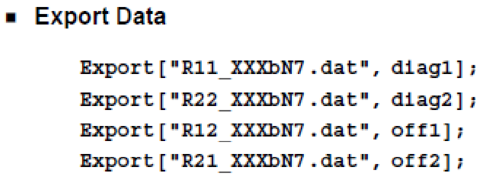
A.5 We use r11, r12, r21, and r22 above to compute $Tr(\rho^2)$ and make the plot



```
Clear[Trrho2];
Trrho2 = Table[{tt dt, r11[tt]^2 + 2 r12[tt] r21[tt] + r22[tt]^2}, {tt, 0, Tfinal}];

ListPlot[Trrho2, PlotRange → {{0, 0.5}, {0.5, 1}},
 Joined → True, PlotStyle → {{Red, Thick}, {Blue, Thick}},
 LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {Time, Tr[ρ^2]}]
```

A.6 Exporting and importing data, and making plots.

To export data in a specific file:



- **Export Data**

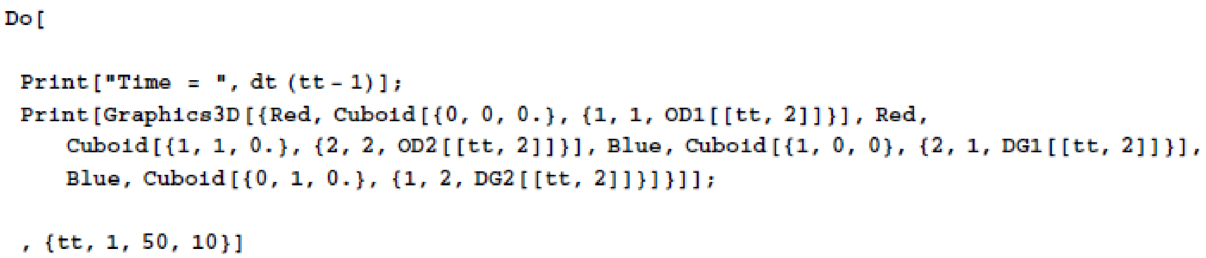
```
Export["R11_XXXbN7.dat", diag1];
Export["R22_XXXbN7.dat", diag2];
Export["R12_XXXbN7.dat", off1];
Export["R21_XXXbN7.dat", off2];
```

To import the date, we write:

- **Import Data and Ilustrations**

```
Clear[DG1, DG2, OD1, OD2];
DG1 = Import["R11_XXXbN7.dat", "Table"];
DG2 = Import["R22_XXXbN7.dat", "Table"];
OD1 = Import["R12_XXXbN7.dat", "Table"];
OD2 = Import["R21_XXXbN7.dat", "Table"];
```

The panels in Section 7 were obtained with the commands:



```
Do[

 Print["Time = ", dt (tt - 1)];
 Print[Graphics3D[{Red, Cuboid[{0, 0, 0.}, {1, 1, OD1[[tt, 2]]}], Red,
    Cuboid[{1, 1, 0.}, {2, 2, OD2[[tt, 2]]}], Blue, Cuboid[{1, 0, 0}, {2, 1, DG1[[tt, 2]]}],
    Blue, Cuboid[{0, 1, 0.}, {1, 2, DG2[[tt, 2]]}]}]];

 , {tt, 1, 50, 10}]
```