Quantum Origins of Irreversibility

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I.   Introduction

If one were to place a collection of atoms in the corner of a box in a vacuum, and then release the atoms, what would happen? The atoms would spread uniformly throughout the box. One would not expect these atoms to then suddenly rearrange themselves back in their original corner, leaving the rest of the box empty. The process of atoms spreading through a box is therefore irreversible. The rearrangement of atoms into one corner of the box would be in conflict with what we know from the Second Law of Thermodynamics, which states that for natural irreversible processes entropy always increases. Entropy, introduced in the 1860s, is a function of the state of a system, in the same way that temperature is a function of state. Another general way to phrase the Second Law of Thermodynamics is that natural processes tend towards greater disorder [1]. Entropy is also called "time's arrow", since it allows us to find which direction time is going (always towards states of greater disorder).

Ludwig Boltzmann [2] clarified the concept of entropy further by applying a statistical approach. He defined the "macrostate" of a system as the macroscopic properties (such as volume and temperature), and the "microstate" as the velocity and position of every particle in the system. Generally, we cannot determine every single microstate in a system; there are far too many particles to allow this. However, we do know that many different microstates can correspond to the same macrostate. In this context, the Second Law reduces to the statement that the processes which occur are the most probable ones. In terms of probability, the second law does not forbid a decrease in entropy. Rather, it says that the probability is extremely low [1]. This statistical approach assumes that each microstate itself has an equal probability to any other microstate. A system in which all accessible microstates are equally probable over a long period of time is said to satisfy the ergodic hypothesis [3]. In an ergodic

system, the particles will move at all speeds and reach all places in space that are allowed by conservation of energy. This type of system is said to be chaotic and can be described by statistical mechanics.

Classical physics explains the behavior of macroscopic systems, such as how fast a rock is falling, or what the heat increase in a given fluid is. But we know that all macroscopic systems are in fact made up of many, many microscopic systems – each individual particle is a microscopic system. Microscopic systems are described by quantum physics – the theory which describes the behavior of very small objects, such as electrons. Thus, we should be able to explain any macroscopic behavior by describing the microscopic behavior of the system's particles. However, to do this, we need to understand what makes a quantum system ergodic. Because of the difference in nature between classical physics and quantum physics, the notion of ergodicity (or chaos) in quantum systems must be defined differently as I explain in Section III.

The goal of my research was to understand ergodicity and chaos at the quantum level in order to connect the concept of irreversibility with microscopic physics. To do so, it was important also to understand some basics of quantum mechanics, and what quantities are important in this field.

II.   What is Quantum Mechanics?

One way to explain the behavior of quantum particles is by contrasting it with the behavior of classical systems which are easier to understand and which are part of our daily lives. We can do this by way of two experiments: the bullet, and the wave. Both experiments involved a metal sheet with two holes in it, which can be covered or uncovered [4].

The bullet experiment

Let us imagine a machine gun which sprays a stream of bullets randomly over a large angular spread. The holes in our metal sheet are just large enough to allow a bullet to go through. Beyond the sheet is a bullet detector. This detector can be moved anywhere along the line behind the sheet and counts the bullets. Thus we can determine what percentage of bullets will land at any particular distance from the center. This enables us to calculate the probability of a bullet landing at that position. We cannot say definitively where the bullet will land, since a bullet which glances off the side of the hole can have its trajectory changed drastically. Bullets always arrive as a whole bullet; they arrive in "lumps".

For this system, the probability distribution for when both holes are open is equal to the probability distributions of each hole added together (see Figure 1). This means that there is no interference. A bullet going through one hole has no effect on a bullet going through the other hole.
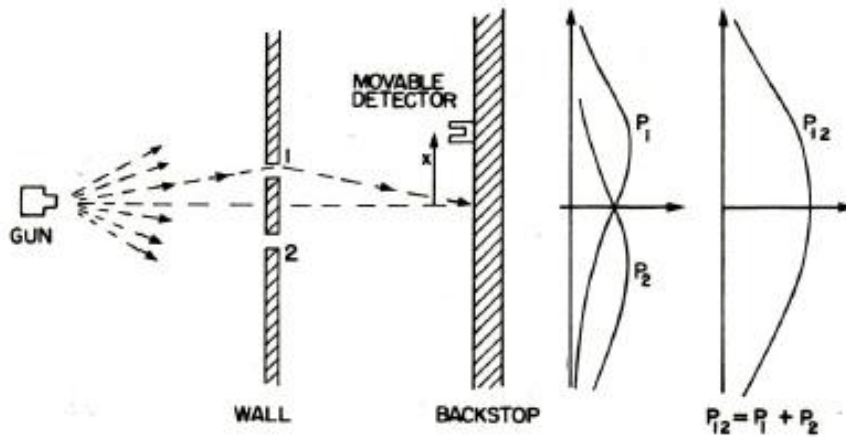

Figure 1: Experiment with bullets (from Ref. [4])

The wave experiment

Let us now imagine the same experiment, but instead of a machine gun, we have circular water waves propagating through the holes in the metal sheet. Our detector detects the intensity of the wave, measured according to the height of the wave. This intensity can have any value; it does not come in lumps as do bullets. We find with waves a different phenomenon than with bullets. Instead of the probability for each position when both holes are open being the sum of the probabilities from each hole, we see an interference pattern.
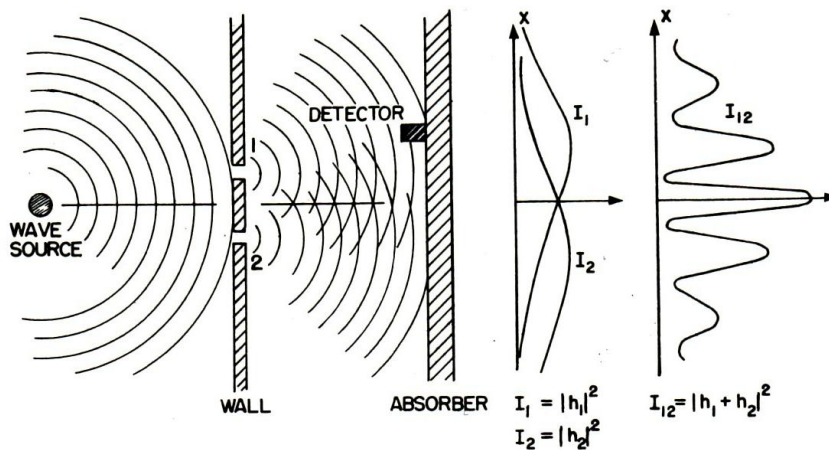

Figure 2: Experiment with waves (from Ref. [4])

The electron experiment

We now imagine the same experiment, but with a machine gun spraying electrons. As our detector, we use a Geiger counter, which clicks when an electron hits it. As we spray the electrons, we hear that all clicks are exactly the same. We also hear that the clicks come at seemingly random intervals of time, but that if we listen over a long period of time, the average number of clicks per time period remains about the same. If we had two detectors, they would never click at exactly the same time. Thus, it seems that electrons arrive at the

detector in lumps, and so we first believe that they must either go through hole one or through hole two, but not both at the same time, like waves.

The rate of clicks will change depending on where we place our detector. Strangely, if we consider the rate of clicks as the probability, for the situation in which both holes are open, we obtain a distribution similar to the interference pattern of the water waves. It seems that electrons come in lumps, but also show interference (see Figure 3). It seems that electrons behave partly as particles and partly as waves. Showing interference, though, seems to imply that the electron passes through both holes at once.
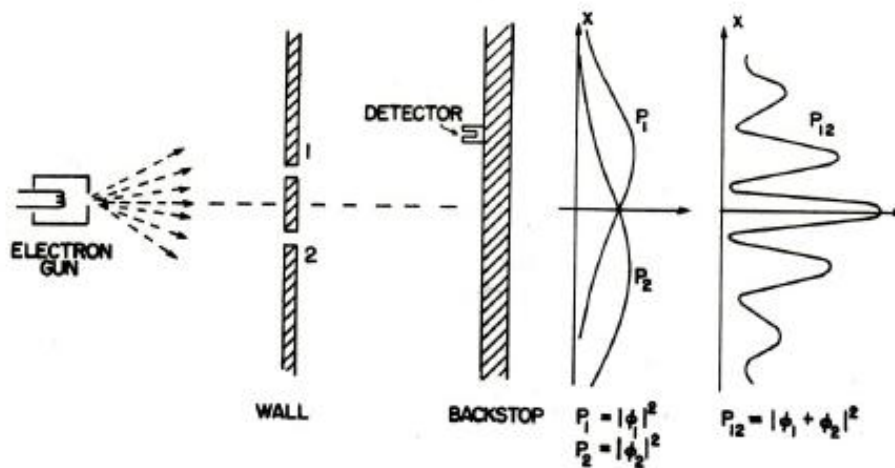

Figure 3: Experiment with electrons (from Ref. [4])

We can test our initial assumption that electrons go through one hole or the other but not both. Let us place a very strong light source directly behind the metal sheet, equidistant from the two holes. Electric charges scatter light, so when an electron passes the light source on its way to the detector, we will see a flash. If the flash is on the side of hole 1, we will know that the electron passed through hole 1, and the same with hole 2. If both sides flash at the same time, the electron can be said to pass through both holes at once.

When we do this experiment, we see that every time we hear a click from our detector, we also see a flash. The flash is always near one hole or the other, never both. It therefore seems that the electron goes through hole 1 or hole 2, but not both at once. But once we perform this experiment, what happens to the probability distribution? Does it still show interference?

To analyze the probability distribution in terms of the holes which the electrons go through, we keep track of where the electrons end up (by listening to the detector) and what hole they came through (by looking at the light flashes). We find that if we look at only the electrons which come through hole 1, we get exactly what we would expect if we blocked off hole 2, and vice versa. But when we look at the total probability, the probability of the electron arriving at the detector via either hole, we get a surprise. We now find the same distribution as by the bullets! We no longer see interference. Yet, when we had no light source, no way of keeping track of which hole the electrons came through, we did see interference. It seems that electrons behave differently if we look at them or not.

Perhaps, we conjecture, the electrons behave differently because just as electrons scatter light to make the flash, the light affects the trajectory of the electrons. Maybe if we make the light source dimmer, the electrons will not scatter as much.

Using a dimmer light source, we try the experiment again. Strangely, we notice that the intensity of the flash given off when the electrons pass by the light source does not vary; the flash is always the same size. We see from here that light also acts as lumps; it always arrives in photons. Changing the intensity of a light source does not change the size of the photons, rather the rate at which they are emitted. We also notice that there are times now when we

hear a click but do not see a flash. The lower density of photons means that some electrons pass without scattering light.

When we attempt to plot their probability distributions, we find an interesting phenomenon. We now have three categories of electrons: those seen near hole 1, those seen near hole 2, and those we don't see at all. We notice that those which we see follow the same distribution as we find when we use a stronger light source, the distribution of bullets. Those which we do not see follow the interference pattern which we saw when we had no light source at all, the distribution of waves.

Lowering the intensity of the light source thus did not help us to avoid scattering electrons significantly. We must attempt to find another way.

Since electrons scatter when a photon hits them, the amount that they scatter should be proportional to the momentum of the photon. A photons momentum is given by $\frac{h}{\lambda}$. So if we increase lambda, which can be done by decreasing frequency ($\nu = \frac{c}{\lambda}$), maybe we can decrease the momentum of the photon to the point that it will not scatter the electrons away from the distribution we know we should get.

As we increase our wavelength, nothing seems to happen. We still have hole 1 electrons and hole 2 electrons, and we still do not see interference. So we keep on increasing our wavelength, hoping that it will help.

Eventually, we increase the wavelength until it is longer than the distance between the two holes. At this point, we encounter a problem.

Since light exhibits wavelike properties, once two spots are too close together, they will be unable to be seen as two separate spots. When the wavelength is longer than the distance between the holes, we are no longer able to see the flash as being uniquely near one hole or

the other. There is just one big flash. We no longer know which hole the electron went through. And it is at just this wavelength that the probability distribution again shows some level of interference. To obtain the same level of interference as we had before, the wavelength of the light must be much longer than the space between the holes.

This experiment showed that we cannot have a light source in a way such that we are able to both observe what hole the electron went through and not disturb the probability distribution. This observation leads to the Heisenberg uncertainty principle.

The Heisenberg uncertainty principle

Heisenberg stated his uncertainty principle in the following manner:

When you measure an object and find its momentum's x-component with an uncertainty of Δp, you then cannot determine the x-component of its position with a greater certainty than $\Delta x = h/\Delta p$, where h is Planck's constant $6.63 \times 10^{-34} \, Js$.

Therefore, no matter what we do in our electron experiment, we will never be able to accurately determine the hole it went through and at the same time obtain the desired interference pattern.

Superposition

Our discussion of the experiments above has had to do with probability. The probability P of an event is given as:

$$P = |\phi|^2$$

where ϕ is the probability amplitude, which is a complex number.

With quantum particles we can only ever talk about probabilities. We cannot predict exactly what will happen in any given circumstance. We can never know exactly what state a

quantum system is in at any given time, unless we measure it, which then collapses the system to one particular state.

When the experiment is able to determine precisely which alternative was actually taken, the total probability is the sum of each alternative's probability. There is no longer interference:

$$P = P_1 + P_2 = |\phi_1|^2 + |\phi_2|^2$$

When a particular event can occur in several different ways, then the total probability is the square of sum of the the probability amplitudes of each way in which it can occur. Thus

$$P = |\phi_1 + \phi_2|^2$$

The product between the complex numbers ϕ_1 and ϕ_2 leads to the interference term, responsible for the interference pattern.

Since we do not know what state the system is in, we say that it is in a superposition of states. In the case of the particle going through the slits, it is in a superposition of both states: $\phi = \phi_1 + \phi_2$. As another example, suppose we have a system with four spins-1/2, two spins pointing up and two pointing down. Our description of the system (using 1 as up-spin and 0 as down-spin) would be a linear combination (that is a superposition) of all states possible for that system. By using the notation $|1\rangle$ for spin up and $|0\rangle$ for spin down, we write this state as:

$$|\psi\rangle = a_1|1100\rangle + a_2|1010\rangle + a_3|1001\rangle + a_4|0110\rangle + a_5|0101\rangle + a_6|0011\rangle$$

$|\psi\rangle$ is known as the wavefunction of the system and $a_{1,2,3,4,5,6}$ are the probability amplitudes of each individual state (or basis vector). The wavefunction is normalized, that is, all together, the probabilities will always add up to 1:

$$\sum_{n=1}^{D} |a_n|^2 = 1$$

where D is the total number of available states of the system.

III. What is Quantum Chaos?

Classical chaos is generally characterized by hypersensitivity to initial conditions. This means that if I have two particles which begin with almost identical initial states, their trajectories will diverge exponentially in time. This definition applies only to systems in which we can determine the initial position in phase space with enough certainty to differentiate between the two. Phase space refers to the space in which we consider both the position of a particle, and its momentum. There are therefore six dimensions to phase space: $\{x_1, x_2, x_3\}$ and $\{p_1, p_2, p_3\}$ where 1,2,3 are the directional coordinates. The rate at which separation between trajectories occurs is characterized by the Lyapunov exponent [5]. Another important concept associated with classical chaos is ergodicity. A particle that visits every position in phase space with an equal probability is said to follow an ergodic trajectory.

One way to visualize the notion of classical chaos is to picture a billiards table. This billiard table is a dynamical billiard table; there is no friction, and a ball reflects elastically from the boundaries, which can have any shape. Two balls which begin next to each other and with very close initial velocities (they are moving in the almost same direction with almost the same speed), will reach the wall and bounce off. They will then keep rolling until they bounce off the next wall they hit, and so forth. Eventually, their trajectories will be very different, due to their initial states being only slightly off. This is a visualization of hypersensitivity to initial conditions.

To visualize ergodicity, imagine a large room. Someone (possibly a small child) has let a fly into this room. A non-ergodic fly will buzz around, but perhaps likes to frequent one place more than another (it likes to sit on the potted plant in the corner, for example), or prefers one velocity over another. An ergodic fly will visit every point in the room with equal frequency and fly at every available velocity with equal frequency [6].

However, this definition of chaos will not work with the quantum world. Due to Heisenberg's uncertainty principle, the idea of trajectories in phase space loses meaning. Since we cannot know the position and velocity of a particle at any given time with a large degree of certainty, we can no longer say "their initial states are almost identical" or "it visits every position in phase space with equal frequency." We are limited by the uncertainty involved.

However, since classical systems are but a limit of quantum systems, we should be able to find a quantum signature of any classical phenomena. Chaos should be no different. Quantum chaos refers to the relationship between the quantum world and its rules, and the concept of classical chaos.

IV.   **The System**

To study quantum chaos, we consider a system composed of *L* sites arranged linearly in a chain. This configuration is called "open", since the ends are not attached; if they were as in a ring, it would be called "closed".

Assuming a static magnetic field pointing in the z direction, each site contains either a spin up or a spin down particle. In each site, a spin pointing up will have more energy than a spin pointing down; they will be referred to as "excitations". This energy splitting, caused by

the magnetic field and known as Zeeman splitting, will be denoted by ω_i. The energy on site i with a spin up is $+\frac{\omega_i}{2}$, where the energy on site i with a spin down is $-\frac{\omega_i}{2}$.

We consider systems in which all sites have the same energy splitting ω, except one. This site, d, has a different energy splitting, $\omega + \varepsilon_d$. This site is called the defect, and we can place it anywhere along the chain that we wish. The difference in energy of the defect site is caused by a magnetic field slightly larger than that of the other sites.

The spins in our system can also couple to those next to them. This is described by the Hamiltonian below (the Hamiltonian is a matrix which describes the energy of a given system):

$$H = H_z + H_{NN}$$

where

$$H_z = \sum_{i=1}^{L} \omega_i S_i^z = \left(\sum_{i=1}^{L} \omega S_i^z \right) + \varepsilon_d S_d^z$$

and

$$H_{NN} = H_{xy} + H_{zz} = \sum_{i=1}^{L-1} \left[J_{xy} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z S_i^z S_{i+1}^z \right]$$

Here, we have set $\hbar = 1$. $S_i^{x,y,z} = \sigma_i^{x,y,z}/2$ are the spin operators at site i. $\sigma_i^{x,y,z}/2$ are the Pauli matrices. The Pauli matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can denote spins up and spins down by the vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, respectively. Then the spin operator matrices can act on them by multiplying the spin operator by the spin vector in accordance with linear algebra.

The H_z term gives the Zeeman splitting of each spin i:

$$\frac{\omega_i}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = +\frac{\omega_i}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\frac{\omega_i}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\omega_i}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The H_{NN} term, as shown above, describes the nearest-neighbor interactions in this system. It is made of two terms (H_{xy} and H_{zz}) proportional to J_{xy} and J_z. J_{xy} and J_z are the strength of their associated terms. The J_{xy} term is called the "flip-flop" term. It changes the position of neighboring up and down spins, moving the excitations through the chain. When neighboring spins are identical, nothing happens. But when neighboring spins are anti-parallel, they switch positions.

An example is given for two particles, with in the state $|10\rangle$:

$$\sigma_1^x |1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |0\rangle$$

$$\sigma_2^x |0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle$$

$$\sigma_1^y |1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = i \begin{pmatrix} 0 \\ 1 \end{pmatrix} = i|0\rangle$$

$$\sigma_2^y |0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i|1\rangle$$

When they are added, we obtain:

$$J_{xy}(S_1^x S_2^x + S_1^y S_2^y)|10\rangle = \frac{J_{xy}}{4}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)|10\rangle = \frac{J_{xy}}{4}[|01\rangle + (i)(-i)|01\rangle] = \frac{J_{xy}}{2}|01\rangle$$

The J_z term describes the Ising interaction, and implies that neighboring pairs of parallel spins have higher energy than pairs of antiparallel spins. When neighboring spins are parallel, the energy is $+J_z/4$, and when they are antiparallel, it is $-J_z/4$.

An example using parallel spins is:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Multiplying the coefficients will yield a positive, since they are both positive:

$$J_z S_1^z S_2^z |11\rangle = \frac{J_z}{4} \sigma_1^z \sigma_2^z |11\rangle = \frac{J_z}{4}|11\rangle$$

Using antiparallel spins, we obtain:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Multiplying the coefficients will yield a negative, since they are opposite in sign.

$$J_z S_1^z S_2^z |10\rangle = \frac{J_z}{4} \sigma_1^z \sigma_2^z |10\rangle = -\frac{J_z}{4}|10\rangle$$

We can then fill the Hamiltonian matrix, item by item.

Filling the Hamiltonian, a practical example

We will now demonstrate how the Pauli matrices act on one state in a four-particle, two spins-up system. We choose the state $|1100\rangle$. We also assume that all energies are equal to 2, and $J_{xy} = J_z = 1$ (arbitrary units).

$$H_{zz}|1100\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= (1 + 1 - 1 - 1)|1100\rangle = 0|1100\rangle$$

$$H_{zz}|1100\rangle = (1/4 - 1/4 + 1/4)|1100\rangle = (1/4)|1100\rangle$$

$$H_{xy} = H_{xy_{12}} + H_{xy_{23}} + H_{xy_{34}}$$

$$H_{xy_{12}}|1100\rangle = 0$$

$$H_{xy_{23}}|1100\rangle = \frac{1}{2}|1010\rangle$$

$$H_{xy_{34}}|1100\rangle = 0$$

The Hamiltonian neither creates nor destroys excitations; it can only move them along the chain. For us, this means that it conserves spin in the z-direction.

To find the Hamiltonian, diagonalize it, and find the eigenvalues and eigenstates, we must first choose a basis. The natural choice of basis is referred to as the site basis, and means that we use arrays corresponding to the up and down spins. In this basis, the H_z and

the Ising interaction contribute to the diagonal elements, and the flip-flop term to the off-diagonals.

The importance of the Ising interaction

With no Ising interaction, the excitations are free to move around the chain, even if a defect is present. The eigenvalues and eigenvectors can be found analytically, which means that the system is integrable, or nonchaotic. Adding Ising interaction will eventually lead to quantum chaos, due to the interplay between the Ising interaction and the defect.

To bring the system to chaos, we set $J_{xy} = 1$, $J_z = \varepsilon_d = 0.5$ (arbitrary units) and place the defect on site $\lfloor L/2 \rfloor$. These choices are based on [7]:

1) The strength of the Ising interaction cannot be much larger than J_{xy}, since then basis vectors with different numbers of pairs of parallel spins would have very different energies, thus rending J_{xy} ineffective at coupling them. As a result, the eigenstates would involve only a few of the basis vectors, which means they are localized and thus nonchaotic.

2) The defect cannot be placed on the edges of the chain, since in this case an analytical solution still exists, which means the system is integrable.

3) ε_d cannot be much larger than J_{xy}, because this would effectively break the chain in two; an excitation on one side of the defect would not have enough energy to overcome the defect and reach the other side of the chain. We would thus be effectively dealing with two smaller, independent chains, each of which is integrable.

V.   Level Spacing Distribution

We determine when a system becomes chaotic by observing the level spacing distributions. Quantum systems have a discrete energy spectrum. This means that there are

certain energies which are allowed, and some which are not. The distribution (that is, the histogram) of the spacings between these levels indicates whether a system is chaotic or not.

In an integrable system, the energy levels are uncorrelated and are allowed to cross. The distribution $P(s)$ is Poissonian, given by

$$P(s) = e^{-s}$$

In chaotic systems, however, the eigenvalues are correlated and crossings are prohibited. This is called level repulsion, and the distribution of the spacings is given by the Wigner-Dyson distribution. The form of the Wigner-Dyson distribution depends on the symmetry properties of the Hamiltonian. For real and symmetric matrices,

$$P_{WD}(s) = \frac{\pi s}{2} e^{-\pi s^2/4}$$

To obtain a Wigner-Dyson distribution, we need to separate the eigenvalues according to their symmetry sectors, since eigenvalues from different symmetry sectors are independent, and thus uncorrelated and do not repel each other. Since our Hamiltonian conserves spin in the z direction, the matrix is made of uncoupled blocks. These blocks correspond to subspaces with a fixed number of up spins. We use the subspace with $L/3$ spins up. This means that the block of the Hamiltonian that we are considering has a dimension of

$$D = \frac{L!}{\left(L/3\right)! \left(L - L/3\right)!}$$

We also need to unfold the spectrum. This means that we need to rescale the energies so that we can compare the spectrum from this system with spectra from other systems.

We employed a very common method, which is to order the spectrum in increasing values of energy, then separate it into smaller sets of eigenvalues. We then divide each

eigenvalue by the mean spacing of its particular set. Thus, the mean level spacing of the new set is 1.

Once we have the unfolded spectrum, we can compute a histogram and compare the distribution with the theoretical curves. Figure 4 below shows the level spacing distribution when the defect is placed on site 1 and on site $\lfloor L/2 \rfloor$. The first case follows the Poisonnian distribution, and is therefore integrable, where the second case follows the Wigner-Dyson distribution so is chaotic [7].
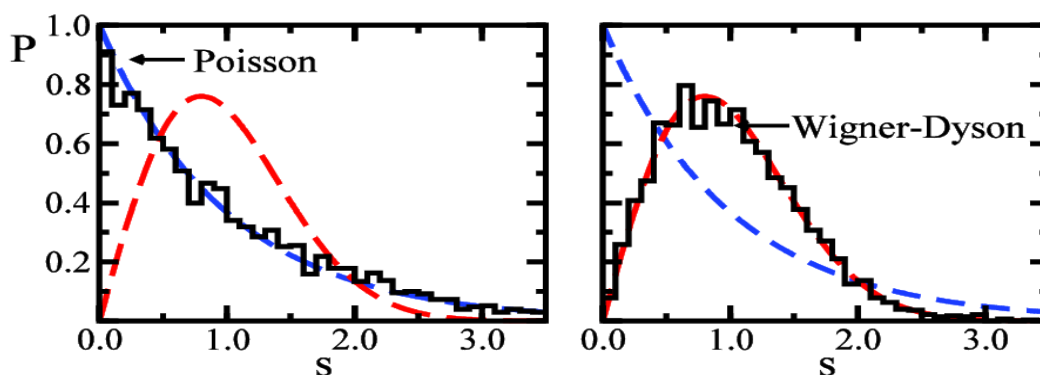
Figure 4: Level spacing distributions, L=15, 5 spins up, J_{xy}=1, J_z =.5, ε =.5, ω=0 (arbitrary units)

VI.   Number of Principal Components

The transition from a Poisson to a Wigner-Dyson distribution affects the structure of the eigenstates of the system, in particular their delocalization.

To determine the delocalization of an eigenstate, we consider its components. Let us look at an eigenstate $|\psi_i\rangle$, written in the basis vectors $|\xi_k\rangle$ as $\psi_i = \sum_{k=1}^{D} c_{ik}|\xi_k\rangle$. If it has only a few basis vectors significantly contributing to it, it is considered localized. If it has many, it is considered delocalized.

To analyze this, we use the coefficients of the basis vectors. We cannot use the coefficients themselves, since they are complex numbers. We call the linear combination of states which describe the system its wave function. The coefficients of each available state

are complex numbers. The sum of the squares of the coefficients is 1, which is called normalization.

We would then consider using the coefficients squared, $|c_{ik}|^2$, but since normalization implies unity, $\sum_{k=1}^{D}|c_{ik}|^2 = 1$ in all cases. We therefore define the number of principal components (NPC) of the eigenstate i as

$$n_i = \frac{1}{\sum_{k=1}^{D}|c_{ik}|^4}$$

Since the basis vectors are of utmost importance here, our choice of basis makes a large difference in our NPC values. We consider two bases: site basis, and mean-field basis.

The site basis has been explained above, and is appropriate to use when analyzing the spatial delocalization of the system. The mean-field basis is more appropriate when analyzing the regular or chaotic behavior of a system. It consists of the eigenstates of the integrable limit of our system, which corresponds to $J_{xy} \neq 0$, $\varepsilon_d \neq 0$, and $J_z = 0$.

To utilize the mean-field basis, we start by writing the site basis. We will refer to the site basis vectors as $|\phi_j\rangle$. When there is no Ising interaction, the diagonalization of the Hamiltonian leads to the mean-field basis vectors. They are given by $|\xi_k\rangle = \sum_{j=1}^{D} b_{jk}|\phi_j\rangle$. When we diagonalize the Hamiltonian which includes Ising interaction, we get the eigenstates in the site basis $|\psi_i\rangle = \sum_{j=1}^{D} a_{ij}|\phi_j\rangle$. Using the relation between $|\phi_j\rangle$ and $|\xi_k\rangle$, we can write the eigenstates of the total Hamiltonian in the mean-field basis as

$$|\psi_i\rangle = \sum_{k=1}^{D}\left(\sum_{j=1}^{D} a_{ij}b_{kj}^*\right)|\xi_k\rangle = \sum_{k=1}^{D} c_{ik}|\xi_k\rangle$$

Figure 5 below shows the number of principal components for both the integrable and the chaotic case, in each basis. We observe that the level of delocalization increases significantly when the system becomes chaotic, but the large values are concentrated in the middle of the spectrum. We also see that in the regular system, the number of principal components shows large fluctuations; for similar energy levels, the NPC may be very different. However, in the chaotic case, the number of principal components approaches a smooth function of energy. This indicates that chaotic states close in energy have very similar structures. This may be used as a signature of chaos based on its eigenstates, as opposed to its eigenvalues, as the level spacing distribution [7].
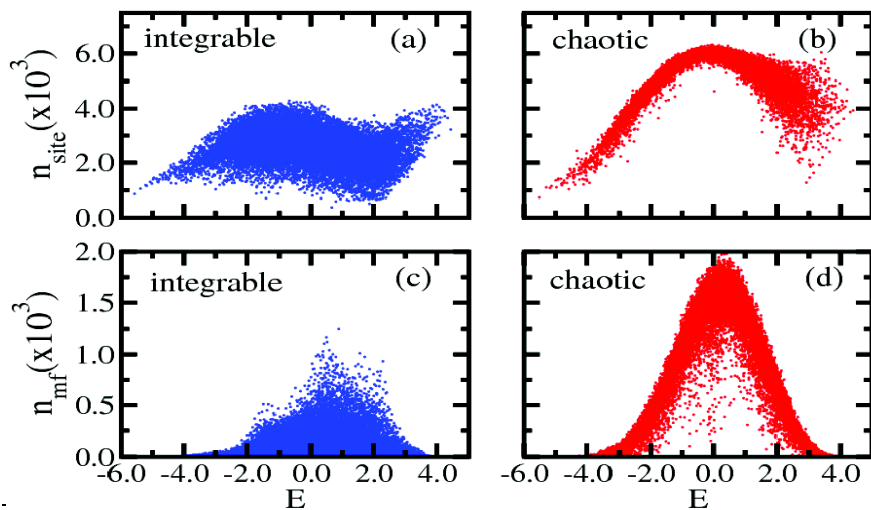

Figure 5: NPC values, L = 18, 6 spins up, $\omega = 0$, $\varepsilon = 0.5$, $J_{xy} = 1$, $J_z = 0.5$ (arbitrary units)

VII.   Symmetries

The presence of a defect breaks the symmetries of the system. A system with no defect, $\varepsilon_d = 0$, is integrable even in the presence of Ising interaction, unlike a system with a defect. In order to drive such a system into the chaotic domain, we add more couplings. We no longer consider only nearest neighbor couplings, but also next nearest neighbor couplings. The Hamiltonian then becomes

$$H = H_{NN} + \alpha H_{NNN}$$

where

$$H_{NNN} = \sum_{n=1}^{L-2} \left[J'_{xy}\left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y\right) + J'_z S_n^z S_{n+2}^z \right]$$

For sufficiently large α, when H_{NN} and H_{NNN} become comparable there are various ways in which chaos can develop. These include the absence of Ising interactions ($J_z = J'_z = 0$), the absence of the next-nearest-neighbor flip-flop term ($J'_{xy} = 0$), the absence of next-nearest-neighbor Ising interaction ($J'_z = 0$), or the presence of all four terms.

However, we may not obtain a Wigner-Dyson distribution even in cases which are chaotic if we neglect to take into account all symmetries of the system. Such symmetries include parity, spin reversal, and total spin.

Parity

Parity can be understood by imagining a mirror in one edge of the chain. For eigenstates written in the site basis, the probability of each basis vector is equal to that of its reflection. For example, if we have four sites and one excitation, the eigenstates are given by $|\psi_i\rangle = a_{i1}|\uparrow\downarrow\downarrow\downarrow\rangle + a_{i2}|\downarrow\uparrow\downarrow\downarrow\rangle + a_{i3}|\downarrow\downarrow\uparrow\downarrow\rangle + a_{i4}|\downarrow\downarrow\downarrow\uparrow\rangle$. For even parity, the amplitudes are $a_{i1} = a_{i4}$ and $a_{i2} = a_{i3}$, whereas for odd parity they are $a_{i1} = -a_{i4}$ and $a_{i2} = -a_{i3}$. (Note that in odd parity, the probabilities of each basis vector are still equal, since probabilities are related to the amplitude squared.)

Spin reversal

If the chain has an even number of sites and $L/2$ spins up, vectors are equivalent to those which become equal if we rotate all spins from one vector by $180°$. For instance $|\downarrow\uparrow\uparrow\downarrow\rangle$ pairs with $|\uparrow\downarrow\downarrow\uparrow\rangle$.

Total spin

If $J_{xy} = J_z$, and $J'_{xy} = J'_z$, the system is said to be isotropic. Total spin $S^2 = (\sum_{n=1}^{L} \overrightarrow{S_n})^2$ is conserved.

Figure 6 below shows the level spacing distributions for the chaotic systems described above. Panel (a) was obtained for $L = 14$, 7 spins up, $J_{xy} = J_z = J'_{xy} = J'_z = 1$ considering all eigenvalues. All four interactions are present. For all other panels, $L = 15$, 5 spins up, $J_{xy} = 1$. In panel (b), $J'_{xy} = 1, J_z = J'_z = 0.5$. All four interactions are present. In panel (c), $J'_{xy} = 1, J_z = J'_z = 0$. Ising interaction is absent. In panel (d), $J'_{xy} = 0, J_z = J'_z = 0.5$. In panel (e), $J'_{xy} = 1, J_z = 0.5, J'_z = 0$. The parameters are given in arbitrary units.
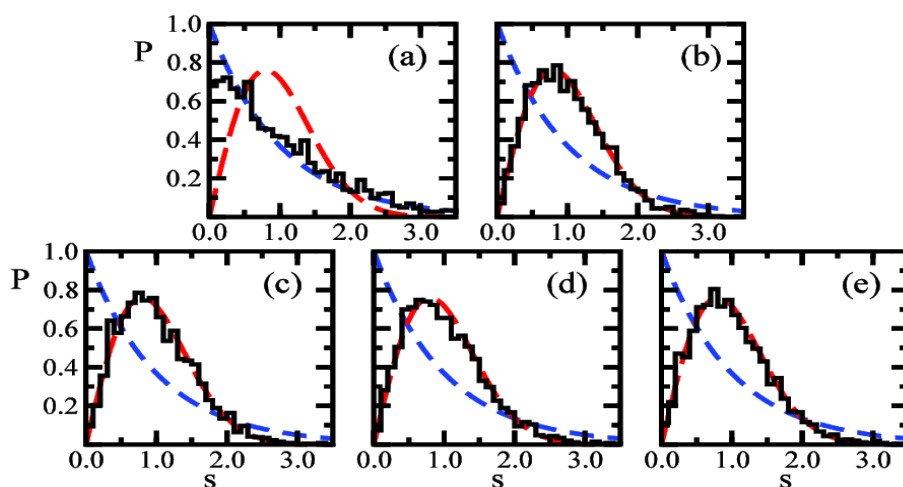

Figure 6: Level spacing distributions for the Hamiltonian with nearest and next-nearest-neighbor terms, $\alpha = 0.5$. All panels show results for chaotic systems, but symmetries were not taken into account in panel (a) [see text for details and parameter values].

All panels show a Wigner-Dyson distribution, except panel (a). In panels (b)-(e), the only symmetry present is parity and we take it into account by averaging the values of the two parity sectors. In panel (a), all three symmetries, parity, spin reversal and total spin, are present, but we neglect to account for them. This explains why we get a Poisson distribution, even though the system is chaotic.

VIII. Observables

As stated above, one of the differences between a classical system and a quantum system is that the latter may be in a superposition of states. In the classical domain, a system has a definite state at any given time. Quantum systems, however, have the property that they only acquire a definite state after being measured. Before the measurement, they may be in a quantum superposition of states; it is as if the system would have more than one state at the same time, with each state associated with a particular probability. For instance, I can say that a particle is in the state $\alpha|x_1\rangle + \beta|x_2\rangle$, which means that before I measure its position, I have $|\alpha|^2$ probability to find it at position x_1, and $|\beta|^2$ probability to find it at position x_2. Here, the quantity I am measuring, i.e. the observable, is position. When I measure it, the particle's state collapses into the position that I measure, but before measurement, all I can say is that its *average* position ($\langle x \rangle$) is given by $\langle x \rangle = \alpha^2|x_1\rangle + \beta^2|x_2\rangle$.

I studied one observable of the system: its interaction energy. Since quantum systems have discrete energy spectra, I was able to compute the average interaction energy for each possible discrete energy of the system. The interaction energy is a part of the system's total energy, it corresponds to the H_{zz} term, which in principle can be measured experimentally. The other part is the kinetic energy, corresponding to the H_{xy} term.

In Figure 7 below, I show the average interaction energies vs the energies of the system for an integrable (non-chaotic) model and a chaotic model. We have only nearest-neighbor couplings, $L = 15$, 5 spins up, $J_{xy} = 1, J_z = 0.5$ (arbitrary units) and in the case of the chaotic system a defect in the middle of the chain with $\varepsilon = 0.5$ (arbitrary units). Each panel contains 3003 points. As seen from the figures, the results for the integrable case show much larger fluctuations. As a consequence, as I discuss next, the agreement between this model and the predictions from statistical mechanics should be worse than for the chaotic model.
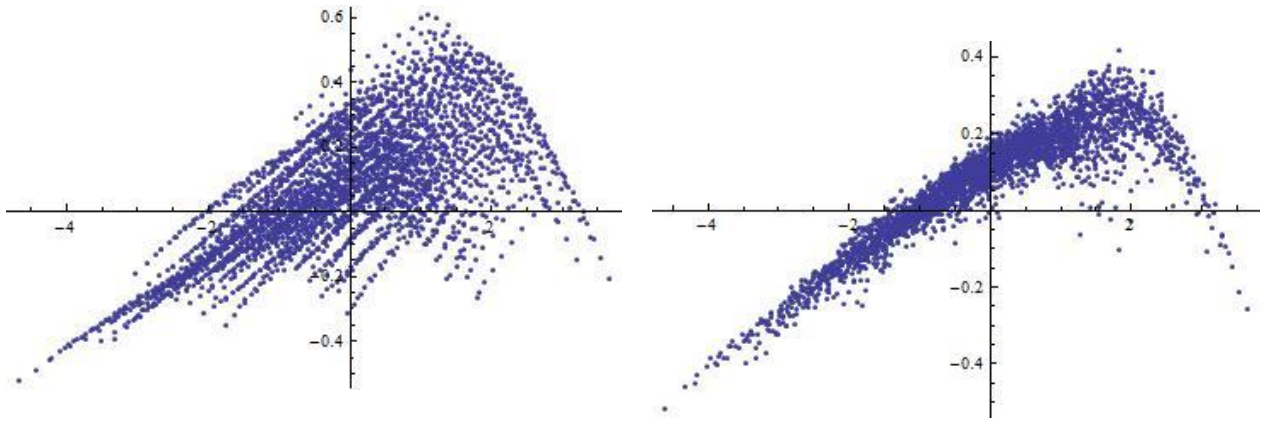

Figure 7: Interaction energy vs. energy. Integrable system on left, chaotic system on right

To compute the interaction energy according to statistical mechanics, one would simply average the values I obtained above in a small window of energy. This is the procedure used when the system is completely isolated from any other system, technically we say that we deal with a microcanonical ensemble. One would do this for various values of J_z, which determines the transition between non-chaoticity and chaoticity. The expectation is that less fluctuations, and therefore chaos, leads to a better agreement with the statistical (microcanonical) averages [8].

The results for the interaction energies may then be used to explain the onset of irreversibility. Statistical mechanics tells us that each macrostate can have many microstates

associated with it. The macrostate of a system is associated with its macroscopic properties, such as temperature and volume, of the system as a whole, whereas the microstate is the velocity and position of each individual particle in the system. Due to the large number of particles in any given macroscopic system, we are unable to determine every single microstate. Statistical mechanics assumes that each microstate has an equal probability as any other microstate. Therefore, the macrostate with the highest probability of occurrence is the one with the largest number of associated microstates. Irreversibility simply means that once a system is in a highly probable macrostate, it is very unlikely (though not impossible), for it to spontaneously evolve into a less probable one. By showing a correlation between quantum chaos and statistical mechanics, one would be able to suggest that quantum chaos is at the origin of irreversibility in the classical domain.

IX.   Dynamics

I also studied the time evolution of the magnetization of a one-dimensional chain of particles, with and without a defect in the middle of the chain. As I have shown above, the first is an integrable model and the second, chaotic. The magnetization is +1 if the spin points up and -1 if it points down, while a spin in an equally distributed superposition of state up and down will have magnetization zero. I computed the total magnetization M of the first half of the chain and I considered a very particular initial state, where all the spins in the first half of the chain point up and in the other half they point down. Thus, the initial magnetization of the first half of the chain is large. The magnetization values alert us to the presence of symmetries in the chain. Where there are many symmetries, as in the integrable system without defect, the magnetization should oscillate, taking a very long time to decay. However when a defect exists, we expect to find that the magnetization decays very quickly.

In this last scenario, a very large number of states become accessible to the system extremely fast and recurrences of initial states or very particular states of the sort become very unlikely. The magnetization approaches zero rapidly. This behavior suggests an arrow of time, in which a system with few symmetries (as is typical of chaotic systems) tends to evolve towards states of maximum mixing, where almost all accessible states are equally likely. Below in Figure 8 are the plots of the magnetization values versus time for the integrable system (left) and the chaotic system (right), for a chain with ten sites and five excitations. Notice how the plot of the integrable system oscillates, while that of the chaotic system quickly approaches zero.
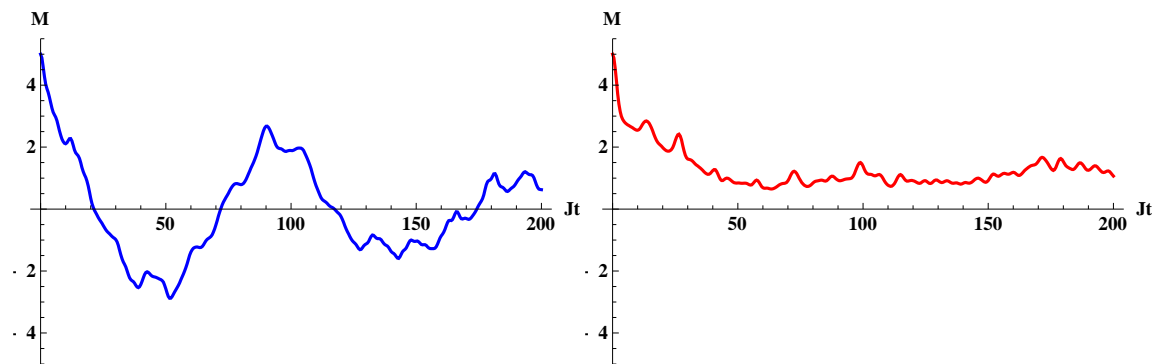

Figure 8: Magnetization of the first half of the chain vs time. Integrable system on left, chaotic system on right

X.   Conclusions

I now know what the important quantities are when analyzing quantum chaos. I have shown that not only eigenvalues, but also the eigenvectors can be used to detect the crossover from integrability to chaos. I also discussed how important it is to take into account the symmetries of the system. If we do not, we may achieve the conclusion that the system is integrable even when it is in fact chaotic. I have obtained data which could be used to further connect quantum chaos with statistical mechanics. My results indicate that statistical

mechanics can describe well chaotic systems, but not integrable ones. Therefore irreversibility seems to be a consequence of the onset of chaos. I have also studied how magnetization behaves in accordance with the chaoticity of the system. My results suggest that for complex systems, where few symmetries are present, the system relaxes to equilibrium rapidly. It is only after relaxing to equilibrium that a system may be described by statistical mechanics.

Acknowledgements

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