Static and Dynamic Properties of Quantum Systems with Many Interacting Particles

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1. Introduction

Everything in nature is made of many microscopic particles, which interact with one another. A single atom may have certain properties, but once several atoms are put together so that they can interact, they may behave differently. Quantum systems with many interacting particles are known as quantum many-body systems, and such systems are the subject of this thesis. Understanding the consequences of these interactions can have significant applications in various areas. A quantum computer, which is a quantum many-body system, is a computer design that uses the principles of quantum mechanics to increase the computational power of computers. Another application is understanding heat transfer at the fundamental level, which is particularly important in an age in which the rate of technological advancements is rapidly increasing and mitigation of local heating in electronic devices is an increasingly significant goal.

In classical physics we have tools that allow us to describe the static properties and predict the dynamics of a system. Using Newton's Laws we have a firm understanding of the interplay between forces, and we can understand how an object's position, velocity, or acceleration may change. These laws are very versatile and correctly describe the behavior of macroscopic objects such as planes, cars, and people. However, many laws of classical physics do not correctly predict the behavior of tiny objects, such as electrons. In order to describe the dynamics of objects that are microscopic in size we must use quantum mechanics, which is an intrinsically probabilistic theory [1].

A wave function $\Psi(x,t)$ is a function of space and time that describes the wave characteristics of a particle or a group of particles[1]. De Broglie hypothesized that like light,

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[1] This is the wave function in one-dimension. $\Psi(r,t)$ is the complete wave function.

matter (electrons, protons, etc.) has characteristics of both particles and waves, and this hypothesis was eventually confirmed experimentally. The Heisenberg uncertainly principle states that one cannot precisely know both the location and the momentum of a particle at the same time. The quantity

$$|\Psi(x,t)|^2 = \Psi(x,t)^*\Psi(x,t)$$

corresponds to the probability of finding the particle at point x at time t if a measurement is done on the system. While Newton's Laws in classical physics can predict the position and velocity of macroscopic objects at a future time, in quantum mechanics the Schrödinger equation governs the probability amplitude, meaning the behavior of the wave function $\Psi(x,t)$. Given initial conditions $\Psi(x,0)$, the Schrödinger equation can determine $\Psi(x,t)$ for all future time. [1, 2]

We use models to describe real systems in nature. When the model can be analytically solved, it is called integrable. In contrast, in classical physics chaotic systems are unpredictable in the long run. Such systems are extremely sensitive to the initial conditions. The trajectories in phase space of two particles with very close initial conditions diverge in time. We can find approximate numerical solutions to them, but we are unable to describe them in the long term. Most systems found in nature are in fact chaotic. Examples include weather, population growth, and the spread of diseases [3].

While on the quantum level it does not make sense to talk about precise trajectories because of the uncertainty principle, some properties of the spectrum of the system indicate whether or not it would be chaotic in the classical domain. Quantum systems showing such signatures of chaos are then referred to as chaotic quantum systems[4].

In this thesis we analyze a model for quantum many body systems known as Heisenberg spin-1/2 systems. Such systems closely model some magnetic compounds such as copper oxides. Some of these real systems have been shown to have a great ability to transport heat, making them very interesting to study [5]. The Heisenberg model is also used as a model for quantum computers in studies of transfer of information in a controllable way.

We begin our studies with an integrable, non-chaotic, system. The static and dynamic properties of this system are studied, and we look at conditions that allow for the excitations in the system to easily move, like in a conductor, and factors that limit their spreading, meaning that the system behaves more like an insulator. We then change the parameters of the model to render it a chaotic system and examine the effects of such changes. Finally, we attach the system to baths of different temperatures in an attempt to understand whether or not the transfer of heat in integrable systems differs from the transfer of heat in chaotic systems.

2. Spin System

2.1 Spin

Electrons, like other elementary and composite particle, possess an intrinsic property that is referred to as spin. In order to explain this, we can draw a comparison between the movement of electrons and the movement of planets. A planet has an orbital angular moment due to the fact that it orbits around the sun, where one orbit takes approximately 365 days, and it has an angular momentum due to the fact that it orbits around its own axis, which causes us to have approximately 24 hours in a day. Electrons orbit around the nucleus of the

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atom, thus possessing an orbital angular momentum. There is an additional "angular momentum" that the electron has, one that could be thought of as having to do with the rotation of an electron around its own axis like the planet, but in fact it is only an intrinsic property and not actually a physical property of electrons. If this angular momentum were to be attributed to the rotation of the electron, the electron would have to be spinning faster than the speed of light, which is not possible. Therefore, this angular momentum, or spin, is simply an inherent property of the electron. The orbital (spin) angular momentum is associated with the orbital (spin) magnetic dipole moment of the particle. [1, 6]

In 1921-22 Otto Stern and Walther Gerlach ran a series of experiments that gave great insight into the behavior of these spins. The experiment began by heating up silver atoms. Silver atoms contain 47 electrons. 46 of these electrons can be thought of as creating a symmetrical electron cloud that has no net angular momentum. This leaves one electron with a spin that is not counteracted by any other electron, thus giving the atom as a whole a spin.

These silver atoms are sent through a magnetic field created by shaped magnets and reach a detector at the other end. This magnetic field is non-uniform, and increases in the positive z-direction. It is expected that the atoms will be deflected as they go through the beam depending on the magnitude and direction of each atom's magnetic moment. This setup is meant to show the z-component of the electron spin because the amount by which each atom is deflected is proportional to the magnitude of the dipole in the z-direction. The atoms are randomly oriented in the oven, and therefore classically we would expect the alignment of the magnetic moments, or the values of the spins, to be a continuous distribution and appear that way on the detector, each being deflected by the magnetic field differently based on their orientation. However, what they found was that the magnetic field seemed to split

the original beam from the oven into two distinct components. This suggests that there are only two different values of the z-component of the magnetic moment, and thus there are only two possible orientations for the spin – up or down. This phenomenon is known as the quantization of the electron spin angular momentum. This occurrence is not only true for the z-direction, but the same phenomenon of the splitting of the beam into two distinct beams was seen, for example, when the magnetic field was non-uniform and increasing in the positive x-direction.

The results became more surprising when Stern and Gerlach placed multiple magnetic fields in a row and sent the beam through the magnetic fields to a detector at the other end. For example, they sent the beam of silver atoms from the oven through a non-uniform magnetic field in the z-direction, and blocked the beam of atoms oriented in the –z direction. They allowed the other beam, composed of atoms oriented in the +z direction, to go through a non-uniform magnetic field in the x-direction, and blocked those atoms oriented in the –x direction. They then allowed the +x beam to go through another non-uniform magnetic field in the z-direction. We may have expected that since we previously blocked the –z beam from continuing, we would only see one beam at the detector at this point, namely those electrons with +z orientation. However, what they found was that two distinct beams emerged, one corresponding to +z and one to –z. This example illustrates that in quantum mechanics we cannot determine both the z-spin and the x-spin simultaneously; once we select one beam by sending it through a non-uniform magnetic field, we destroy any previous information about the spin in another direction. This is a characteristic of quantum mechanics, and not a flaw in the design of the experiment [7].

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2.2 Spin-1/2 Chain

The system being studied is a one-dimensional system (chain) of many interacting spin-1/2 particles described by the Heisenberg model. Each site on the chain, numbered 1 through L, contains one spin-1/2 particle. When a static magnetic field acts on spin-1/2 particles and the interaction among them is negligible, these particles each point either parallel or antiparallel to the direction of the magnetic field, as was seen in the Stern-Gerlach experiment. In our case a magnetic field in the z-direction is applied to the system, so we refer to the two possible orientations of the spin as pointing down or up.

We study systems with open boundary conditions as well as systems with periodic boundary conditions. For open boundary conditions, the first site and the last site are not linked. When the first and last site can communicate and the sites form a ring, this is referred to as a closed chain with periodic boundary conditions.

Particles having a net spin-1/2 include protons, neutrons, electrons, neutrinos, and quarks. An up-spin can be denoted by $|\uparrow\rangle = |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Similarly, a down-spin can be denoted by $|\downarrow\rangle = |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The vector form is useful for when applying a spin operator, such as the Pauli matrices, to the spin.

3. Static Properties of the System

3.1 Hamiltonian

The Hamiltonian is an operator that describes the energy of the system. We are working with the Heisenberg spin-1/2 model, where the Hamiltonian is given by

$$H = \sum_{n=1}^{L-1}\left[J\Delta S_n^z S_{n+1}^z + J\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right)\right], \tag{1}$$

where

$$S^{x,y,z} = \hbar\frac{\sigma^{x,y,z}}{2}$$

are spin operators, and

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli spin matrices. In our work we set $\hbar$ equal to 1.

To better understand how these spin operators work we will show some examples:
When the σ^x spin operator is applied to a spin, it flips the orientation of that spin.

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

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

Similarly, when the σ^y operator is applied to the spin, it flips the orientation of that spin, but there is an additional coefficient depending on the orientation of the original spin.

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

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

The σ^z operator maintains the orientation of the spin, but there is a coefficient of +1 if the spin is oriented up and a coefficient of -1 if the spin is oriented down.

$$\sigma^z |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle$$

$$\sigma^z |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -|0\rangle$$

For this reason we refer to an up-spin as the excitation.

The two coupling terms involved in this Hamiltonian are the Ising interaction and the flip-flop term. We first focus on cases with only nearest neighbor coupling, meaning that each spin interacts only with the spins that are directly next to it. Under open boundary conditions, most of the sites on the chain interact with two different sites, one on each side, while the two sites on the edges of the chain only interact with one site each. This will be significant in later discussions of border effects.

J is the strength of the flip-flop term, $S_n^x S_{n+1}^x + S_n^y S_{n+1}^y$, and J$\Delta$ is the strength of the Ising interaction, $S_n^z S_{n+1}^z$. In our analysis, J, which sets the energy of the system, is chosen to be 1. The ratio of the strength of the Ising interaction to the strength of the flip-flop term is the anisotropy parameter, Δ. When Δ is equal to1 and the strength of the two terms is equal it is an isotropic model, known as the XXX model. We are working with the anisotropic XXZ model, where Δ is not equal to 1. When Δ is very large the Ising interaction dominates the Hamiltonian, and when Δ is very small, the flip-flop term dominates the Hamiltonian. When the value of Δ is varied, there are significant effects on the dynamics of the system, as we will see later on.

When there is only nearest neighbor coupling, the value of the Ising interaction term depends on the orientation of one spin in relation to its neighboring spin. Two adjacent spins that are oriented in the same direction have an energy of JΔ/4. If the two adjacent spins are oriented in opposite directions, they have an energy of -JΔ/4. Therefore, if JΔ is positive, the

state with lowest energy (ground state) is the one with the most antiparallel pairs, known as an antiferromagnetic configuration.

The flip-flop term takes adjacent spins that are antiparallel and flips the orientation of both of the spins. The flip-flop term is like the kinetic energy of the system, moving the excitation along the chain.

It is significant to note that neither of the terms included in the Hamiltonian create or remove excitations from the system. If the system begins with a certain number of excitations, that number will be fixed throughout the evolution of the system. In other words, there is a conservation of total spin in the z-direction.

3.2 Hamiltonian in the Form of a Matrix

To represent that Hamiltonian in the form of a matrix, we need to choose a basis in which to create the matrix. The entire Hamiltonian matrix, with dimension 2^L, can be split into blocks called subspaces, with each subspace corresponding to configurations containing the same number of up-spins. The states from one subspace do not interact with states from another subspace, and therefore we were able to create a matrix of one subspace at a time. In order to create these matrices we consider what is called the site-basis. To create this basis, we determine how many sites our chain will have and how many excitations there will be. As was previously mentioned, the Hamiltonian conserves the number of excitations, and therefore that number will remain constant assuming no new magnetic fields or sources of energy are introduced. Once we know the number of sites and the number of excitations, we find the total number of possible distinct configurations of these up-spins and down-spins along the chain, keeping in mind that all up-spins are identical to one another and all down-

spins are identical to one another. The total number of distinct permutations possible is equal

to $\frac{L!}{(N!)(L-N)!}$, where N is the number of excitations in the system. This can be written in

shorter form using the binomial coefficient $\binom{L}{N}$. This value is also the dimension of our

matrix. Based on the various configurations of the spins along the chain we can create the

basis used for the Hamiltonian matrix, the site-basis.

For example, in a case where there are 4 sites and 2 excitations, there are six possible

distinct configurations. These six configurations are:

$$|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle. \qquad (2)$$

These configurations can also be represented as vectors, with (100000) representing the first

configuration, (010000) representing the second, and so on, with these vectors making up the

basis for our matrix. Because there are six distinct configurations, our matrix would have a

dimension of 6, with 6 rows and 6 columns.

Using this site-basis we can fill in the elements of the matrix. The Ising term fills in

values for the diagonal elements of the matrix, and the flip flop term fills in the off-diagonal

elements. For the Ising term, to compute the value of the element H_{11} in the matrix for a

closed system with 4 sites and 2 up-spins we look at how many pairs of parallel spins and

how many pairs of antiparallel spins there are in the associated configuration of the spins. We

will look at the first configuration $|1100\rangle$, since that is the configuration corresponding to

element H_{11} of the matrix. For $|1100\rangle$, the spins in sites 1 and 2 are parallel, so we add $J\Delta/4$.

The spins in sites 2 and 3 are antiparallel so $J\Delta/4$ is subtracted. The spins in sites 3 and 4 are

parallel, adding another $J\Delta/4$. Finally, since it is a closed chain the first and last sites must be

compared, and since those spins are antiparallel to one another, an additional $J\Delta/4$ is

subtracted. Therefore, element H_{11} of the matrix is $\frac{J\Delta}{4} - \frac{J\Delta}{4} + \frac{J\Delta}{4} - \frac{J\Delta}{4} = 0$. The same calculations are done for elements $H_{22,}$ $H_{33...,}$ H_{66}.

If this were an open chain as opposed to a closed chain we would not compare the first and last sites. Element H_{11} of the Hamiltonian matrix for the open chain would be $\frac{J\Delta}{4} - \frac{J\Delta}{4} + \frac{J\Delta}{4} = \frac{J\Delta}{4}$. This is an example of how the geometry of the system would change the spectrum. Another difference between closed and open chains is that closed chains are translationally invariant. This means that translating the sites does not change the energy; $|1000\rangle$ has the same energy as $|0100\rangle$ which is not the case with an open chain.

The calculation of the flip-flop term is slightly more complicated. When two states can couple, the corresponding elements in the matrix will contain J/2. In order to see if two states can couple, we must compare the two states site by site. With nearest neighbor coupling, if the orientation of the spins differ in only two sites, and the two sites are next to each other, then the states are directly coupled. For example, when comparing the first two states, $|1100\rangle$ and $|1010\rangle$, we see that site 1 of each of the states has an up-spin, and site 4 of each of the states has a down-spin. Additionally, we see that the states differ when it comes to the orientation of the spins in sites 2 and 3. Since there are two sites in which they differ, and these two sites are next to each other, this is a case of nearest neighbor coupling. Given that $|1100\rangle$ is the first basis vector and $|1010\rangle$ is the second basis vector, the elements H_{12} and H_{21} will have a value of J/2. The same process is done comparing all of the different states. Since the Hamiltonian matrix is a Hermitian matrix, and therefore symmetrical, we can use this to our advantage and only do the calculations for one triangle of the matrix.

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An example of what this matrix looks like is given below for a closed system with 4 sites and 2 excitations. On the right side are some matrix elements.

$$H=\begin{pmatrix} 0 & J/2 & 0 & 0 & J/2 & 0 \\ J/2 & -J\Delta & J/2 & J/2 & 0 & J/2 \\ 0 & J/2 & 0 & 0 & J/2 & 0 \\ 0 & J/2 & 0 & 0 & J/2 & 0 \\ J/2 & 0 & J/2 & J/2 & -J\Delta & J/2 \\ 0 & J/2 & 0 & 0 & J/2 & 0 \end{pmatrix}$$

$$H_{11} = \langle \uparrow \uparrow \downarrow \downarrow | H | \uparrow \uparrow \downarrow \downarrow \rangle = 0$$
$$H_{12} = \langle \uparrow \uparrow \downarrow \downarrow | H | \uparrow \downarrow \uparrow \downarrow \rangle = \frac{J}{2}$$
$$H_{22} = \langle \uparrow \downarrow \uparrow \downarrow | H | \uparrow \downarrow \uparrow \downarrow \rangle = -J\Delta$$

3.3 Eigenvalues and Eigenvectors

When the Hamiltonian operator acts on special cases of vectors, that will give back that same vector multiplied by a constant. That vector is called an eigenvector, and the corresponding constant is known as an eigenvalue [2]. The eigenvalues describe the possible energies of the system. The set of energies, or the eigenvalues, of the system are known as the spectrum.

Once we have the matrix completed, we can diagonalize the matrix and compute the eigenvectors and the eigenvalues. To find the eigenvalues analytically, we subtract λ from each of the diagonal elements of the matrix. We find the determinant of the new matrix, which will be a polynomial with degree equal to the dimension of the matrix. Setting this polynomial equal to zero allows us to solve for λ, which are the eigenvalues. Once we have the eigenvalues, we can then compute the eigenvectors [1]. However, we deal in this thesis with large and complex matrices, so the diagonalization is done numerically.

We start by analyzing the eigenvalues and eigenvectors to try to predict the dynamics of the system. We later study the dynamics and confirm our predictions.

3.4 Histograms – Predicting Dynamics

The study of the interplay between the Ising interaction and the flip-flop term allows us to make predictions about what to expect from the dynamics of the system. We first analyze the structure of the histograms of the possible energy values of the system. We begin by creating a histogram of only the diagonal elements of the Hamiltonian. In Fig. 1 we show the histograms for systems with L=10, N=5, Δ=0.5. The plot on the left shows results for an open chain, and the plot on the right shows results for a closed chain. We see in both histograms that there are distinct energy values that the states can possess, and there are clear gaps between the different bands of energy.
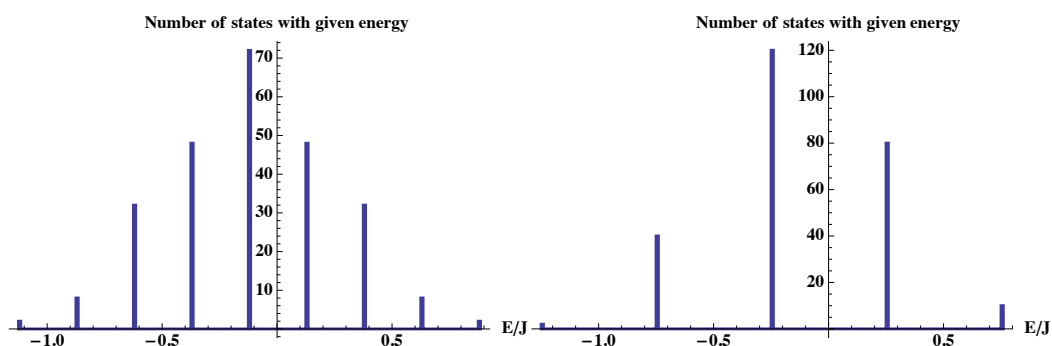
Fig. 1: L=10, N=5, Δ= 0.5. Histograms of the diagonal elements of the Hamiltonian matrix written in the site-basis. Left panel: open chain; right panel: closed chain.

For the histogram of the open chain there are two states in the first band, corresponding to those states with the lowest energy. The difference in energy between one band and the next is $J\Delta/2$, and the general expression for the energy of each band can be given by $[2p - (L - 1)]J\Delta/4$, where p is the total number of pairs of adjacent parallel spins. For a closed chain the energy difference between consecutive bands is $J\Delta$, and the diagonal energies are given by $[2p - L]J\Delta/4$. As can be seen by comparing the two histograms in Fig. 1, the gaps between the bands are larger for a closed chain than an open chain. We also notice that there are fewer bands for a closed system than an open system.

The histogram for an open chain contains *L*-1 bands, and the histogram for a closed chain contains *L*/2 bands. Additionally, it is clear that the middle band for the closed chain is higher than that of the open chain. These differences between closed and opened chains are due to the border effects that are present only in open chains.

For an open chain where N=L/2, the histogram is symmetrical, with the least populated bands always containing two states each, and the band containing the largest number of states in the middle. The bands increase in height until they reach the largest one, and then decrease symmetrically until reaching back to a height of 2. If L is divisible by 4, the three middle bands are of equal height. Otherwise, the center band is the highest.

We then made another histogram of the eigenvalues of the Hamiltonian matrix for the closed system. Depending on the strength of the anisotropy parameter, different results were obtained.

In Fig. 2 we show histograms for systems with L=10, N=5, and periodic boundary conditions. The left column shows results for a system with Δ=0.5, and the right column shows results for a system with Δ=10. The top row displays histograms of the diagonal elements, and the bottom row displays histograms of the eigenvalues.

When the anisotropy parameter was smaller than 1, meaning the Ising term was weak in comparison to the flip-flop term, the histogram of the eigenvalues did not display the gap structure that was seen in the histogram of the diagonal elements (Fig. 2, left). The comparative strength of the flip-flop term, which encourages movement of the excitations along the chain, causes a collapse of the band structure, thus suggesting that a state can evolve from its initial state into several other states. We expect that most basis vectors will

play a role in the evolution of the system because there are no energy gaps stopping a state from effectively coupling with another.
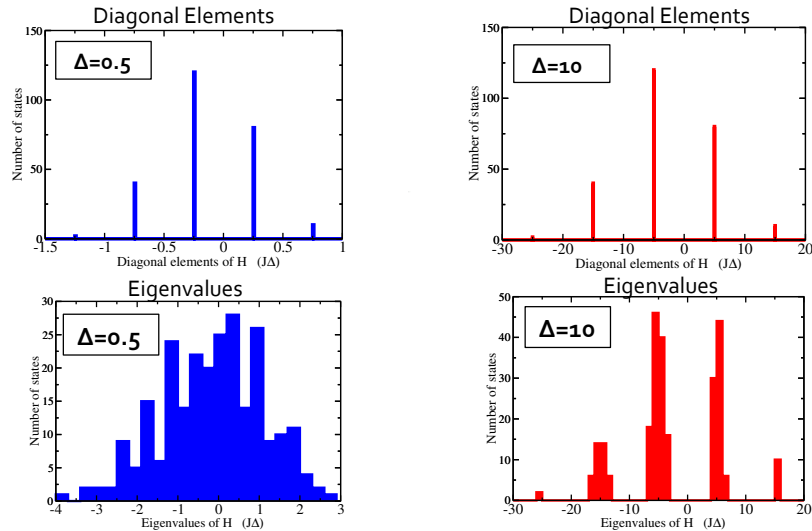

Fig. 2: L=10, N=5, closed chain. Top row: histograms of diagonal elements. Bottom row: histograms of eigenvalues of the Hamiltonian matrix. Left column: Δ =0.5. Right column: Δ =10.

Changing the value of the anisotropy parameter so that the Ising interaction is strong when compared to the flip-flop term reveals very different results. In the histogram of the diagonal terms of the system with Δ=10 (Fig. 2, top, right), we again see a clear band structure with gaps between the energy bands. In the two histograms of the diagonal elements the bands are separated from one another by a value of $J\Delta$ since it is a closed chain. Therefore, when Δ is larger, there is a larger difference in energy between adjacent bands. In contrast with the case of Δ=0.5, the plot on the bottom right (where Δ=10) shows that the flip flop term is not strong enough to overpower the Ising interaction. The histogram of the eigenvalues of this system retains some of its gap structure and there are still clear gaps between different values of energies. This suggests that under such conditions an initial state whose energy belongs in one of the bands would not be able to evolve into another configuration whose energy belongs to a different energy band. In other words, beginning

with an initial state in one band, only the states belonging to the same band can play a role in the evolution of the system.

3.5 IPR

This competition between the Ising interaction and the flip-flop term can also be seen in the structure of the eigenvectors, Ψ_j. Each eigenvector is a linear combination of the basis vectors. For example, with our system of 4 sites and 2 up-spins, each eigenvector is a vector with 6 elements: $a_1|1100> + a_2|1010> + a_3 |1001> + a_4|0110> + a_5|0101> + a_6|0011>$, where a_1, a_2, a_3, a_4, a_5, a_6 are the probability amplitudes associated with each of the basis vectors. When we measure the system to try to find where the excitations are, the wave function collapses to one of the basis vectors. These normalized coefficients tell us about the probability of getting each state after the wave function collapses. $|a_1|^2$ is the probability of getting the corresponding state $|1100>$.

Using these coefficients we can compute the inverse participation ratio (IPR), which provides another way to see the competition between the Ising interaction and the flip-flop term at the level of eigenvectors. In order to compute the IPR we take the sum $|a_1|^4 + |a_2|^4 + |a_3|^4 + |a_4|^4 + |a_5|^4 + |a_6|^4$ for each eigenvector, and compute the inverse of this sum. In other words,

$$IPR^{(j)} = \frac{1}{\sum_{k=1}^{D} |a_k^{(j)}|^4} , \qquad (3)$$

where a_k are the elements of the j-th eigenvector, and D is the dimension of the eigenvector.

This number allows us to determine how much the eigenvectors are spread across the specific basis vectors. When the value of the IPR is very large, the eigenvectors are spread out and delocalized in that basis. When IPR is smaller, this tells us that the eigenvectors are

more localized in that basis and only a few of the basis vectors contribute to the eigenvector. IPR is maximum when all of the probability amplitudes are equal to each other. IPR is minimum when the value of one of the coefficients is 1 and the rest are 0.

We created plots of IPR versus energy. Each dot on the plot corresponds to the value of the IPR for one eigenvector. In Fig. 3 we show this IPR vs. energy plot for an open boundary system with L=10, N=5. In the plot on the left Δ=0.5, in which case the Ising interaction is weak in comparison to the flip-flop term. In the plot on the right Δ=5, and the Ising interaction is strong compared to the flip-flop term.
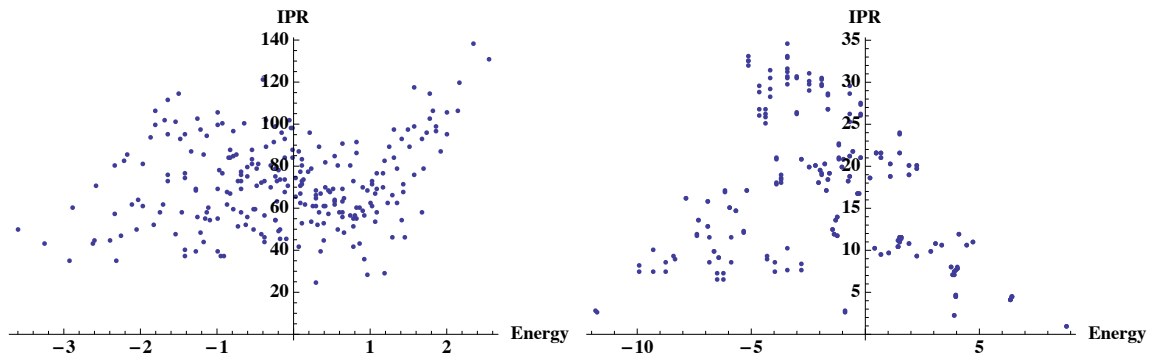

Fig. 3. L=10, N=5, open chain. Left panel Δ=0.5; right panel Δ=5.

We can see that the values of the IPR are lower in the plot in the right, when the value of Δ is higher, indicating more localized states. In order to show this phenomenon of the localization of the eigenvectors more clearly, we graphed the value of the average IPR as Δ increased from 0 to 20 (Fig. 4).
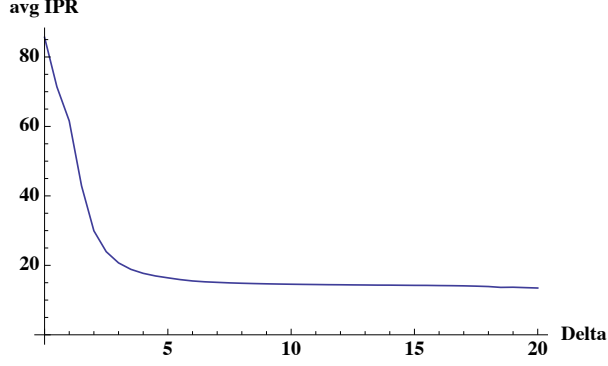
Fig. 4: IPR averaged over all eigenvectors vs. Δ, , L=10, N=5, open chain

In Fig. 4 we see that the maximum delocalization occurs when Δ=0. From there, as Δ increases, the value of the average IPR decreases until it approaches a constant value of about 14. As the strength of the Ising term increases, the average IPR decreases, meaning that fewer members of the basis contribute to the eigenvector. In other words, as the Ising interaction increases and overpowers the role of the flip-flop term, the eigenvectors in the site-basis become less spread. When the plot levels out, at this point the energy bands do not overlap one another and the system is highly localized.

4. Dynamics

4.1 Probability and Magnetization

The histograms and the IPR plots provide us with information about what to expect from the dynamics of the system over time. Next we study what actually happens as the system evolves over time. We begin with an initial state, $\Psi(0)$, which corresponds to one of the site-basis vectors, and the state evolves in accordance with Schrödinger's equation,

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi .$$
(4)

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The initial state couples with other states, transforming the initial state into a superposition of the site-basis vectors. From the histograms and IPR plots we expect that when the Ising term is weak in comparison to the flip-flop term (when $\Delta < 1$) the initial state will spread over several basis vectors. When $\Delta > 1$ and the Ising is stronger than the flip-flop term we expect to see that only states belonging to the same energy band as the initial state will be involved in the dynamics. In order to confirm these predictions we study two different observables, magnetization and probability.

First we need to understand how the system evolves in time. For simplicity, this will be explained for a system with 3 sites and one up-spin. For this system, the basis vectors in the site basis are:

$$\phi_1 = |100\rangle$$

$$\phi_2 = |010\rangle$$

$$\phi_3 = |001\rangle$$

As explained earlier, the eigenvectors are a linear superposition of these basis vectors. For example, $\psi_1 = a_{11}\phi_1 + a_{12}\phi_2 + a_{13}\phi_3$, and similarly for eigenvectors ψ_2 and ψ_3.

In order to evolve the system in time we must put the initial state, with normalized coefficients, in terms of the eigenvectors. To do so we project the vector corresponding to the initial state in the site basis onto the eigenvectors.

Assuming our initial state is given as

$$\Psi(0) = A\psi_1 + B\psi_2 + C\psi_3,$$

to evolve this state in time we add in the time dependence and have the equation

$$\Psi(t) = A\psi_1 e^{-iE_1 t} + B\psi_2 e^{-iE_2 t} + C\psi_3 e^{-iE_3 t},$$

where the constants A, B, C depend on the initial state. In more general terms this equation can be written as

$$\Psi(t) = \sum_{j=1}^{D} a_j \psi_j e^{-iE_j t}. \tag{5}$$

Both probability and magnetization can be used to analyze the dynamics of the system. Magnetization of each site refers to the orientation of the spin on each individual site. A magnetization of +0.5 refers to a spin oriented directly upward, and a magnetization of -0.5 refers to a spin oriented directly downward. As we mentioned earlier, the total spin in the z-direction of the system is conserved. Therefore, since here we are working with an isolated system, the total magnetization is constant throughout the dynamics. To find the magnetization of a site we use

$$M_n(t) = \left\langle \Psi(t) \left| \frac{\sigma_n^z}{2} \right| \Psi(t) \right\rangle,$$

where σ_n^z operates only on site n.

An example of a plot of the magnetization is displayed below in Fig. 5 and clearly shows the movement of a single excitation along a chain. The plot shows results for a chain with open boundary conditions with 6 sites and one excitation initially placed on site number 1. As the system evolves, the excitation moves from one site to the next. The single excitation starts on site 1, so the magnetization on site 1 is +0.5, and the magnetization on the rest of the sites, containing down-spins, is -0.5. As time proceeds, the excitation moves from the first site to the second site, and as this happens the magnetization on site 1 decreases, and the magnetization on site 2 increases. This pattern continues as the excitation moves along the chain. When the spin reaches site 6, the edge of the chain, we see that the magnetization again becomes relatively large. This is an example of a border effect, which does not exist

with a closed chain. This plot allows us to clearly see the excitation being moved from one site to the next along the chain.
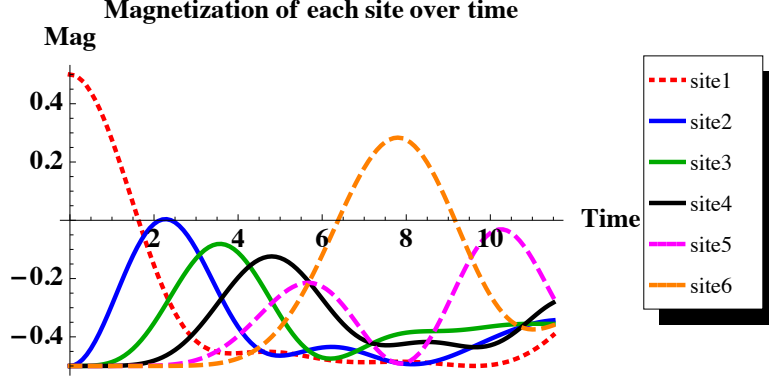
Magnetization of each site over time

Fig. 5: Magnetization over time for an open chain with L=6, N=1, Δ=0.5, Ψ(0)= $|100000\rangle$

When a measurement is done on the system, the system collapses to one of the basis vectors. Probability is the odds of measuring a basis vector ϕ_l at time t. The maximum value, as with all probabilities, is 1, and the minimum value is 0. To calculate the probability we use

$$P_l(t) = \left| \sum_{j=1}^{D} a_k^{(j)} a_l^{(j)} e^{-iE_j t} \right|^2.$$

This expression is obtained by writing Eq. (5) in terms of the basis vectors. We take advantage of the fact that the eigenvectors of a symmetric real Hamiltonian matrix are all real. Since there are no imaginary numbers involved we don't need to include any complex conjugates.

We use probability plots for a closed chain with 4 sites and 2 excitations to confirm our predictions for the effects of changing the anisotropy parameter Δ on the evolution of the system. In Fig. 6 we show the histogram of the diagonal elements of this system. As we can see there are two distinct bands in this plot, separated by an energy of JΔ. Next to each energy band on the plot there is a list of the states contained in that band. With 4 sites and 2

excitations there are 6 possible configurations. One band, of energy –JΔ, contains 2 of these states. The other band, of energy 0, contains the remaining 4 states.
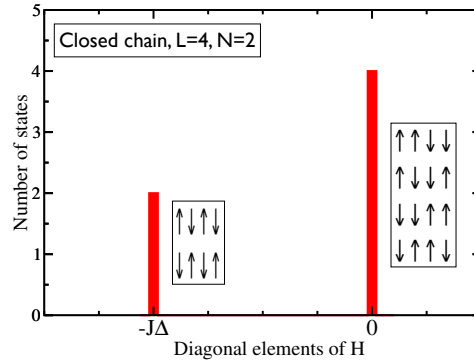

Fig. 6: Histogram of diagonal elements of Hamiltonian matrix for closed chain with L=4, N=2

We do not start the system with an initial state that is an eigenvector of the system because then the system will not evolve. Rather, in this case the system begins with the initial state $|\uparrow\downarrow\uparrow\downarrow\rangle$, which is one of the two states in the first energy band. As Fig. 7 shows, when Δ=0.5, when the system evolves all 6 basis vectors play a role in the evolution. $|\uparrow\downarrow\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\downarrow\uparrow\rangle$ play the greatest role in the evolution, but the other four states also contribute to the dynamics. When Δ=0.5, the energy difference between the two bands is 0.5. Therefore, the flip-flop term is strong enough to collapse this band structure and all the states are involved in the evolution. In contrast, when Δ=10, fewer states play a role in the evolution. The difference in energy between the two bands is 10, and therefore the Ising term overpowers the flip-flop term and the band structure is retained. Beginning again with the state $|\uparrow\downarrow\uparrow\downarrow\rangle$, the only state that plays a role in the evolution is the other state contained in the same energy band, namely $|\downarrow\uparrow\downarrow\uparrow\rangle$. The other 4 states have a probability of practically 0 throughout the evolution because they play no role at all in the dynamics of this system. Additionally, the evolution of the system from one state to another takes much longer when Δ is larger. When

Δ=10, the system must go through several virtual states in order to evolve from $|\uparrow\downarrow\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\downarrow\uparrow\rangle$, and going through those virtual states requires more time.
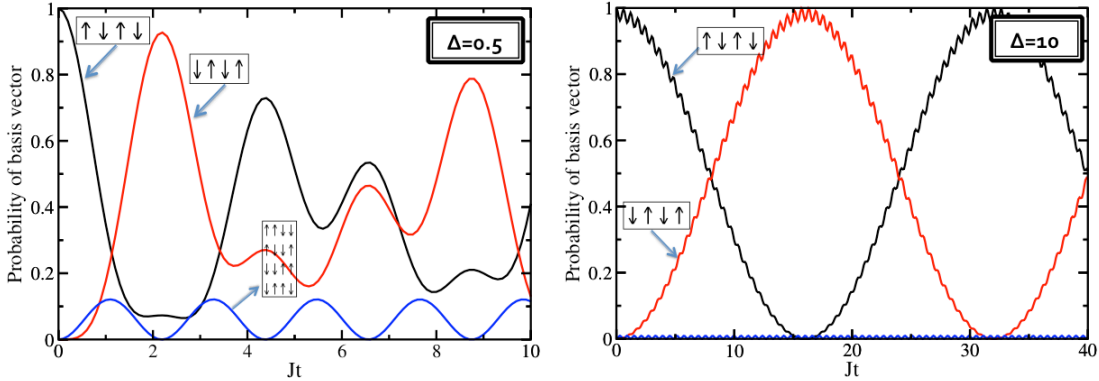

Fig. 7: Probability in time to find a specific basis vector, closed chain, L=4, N=2. Left plot: Δ=0.5. Right plot: Δ=10.

The study of the dynamics using the observables magnetism and probability confirmed the expectations from the histograms and from the analysis of the IPR. As the strength of the Ising interaction increases and overpowers the flip-flop term, fewer of the basis vectors play a role in the evolution of the system, and the evolution from one state to another requires more time.

4.2 Symmetries

As we saw through the study of the dynamics of the system, the relative strengths of the Ising interaction and the flip-flop term can limit the dynamics of the system. There are additional factors that can limit the dynamics of the systems, such as symmetries. If the Hamiltonian is invariant under a symmetry operation that means there is a conserved quantity. In other words, if an operator commutes with the Hamiltonian, it is a sign that some quantity is conserved. One such conserved quantity that we already mentioned is the total spin the z-direction. Total spin in the z-direction commutes with the Hamiltonian, or in other

words $[S_{total}^z, H] = 0.$ This conservation is what led to the creation of subspaces in the complete Hamiltonian matrix. As confirmation, we saw through the dynamics that the total number of excitations, and hence the total magnetization in the z-direction, is conserved. If the initial state has only 1 excitation, the only other states that have a potential to play a role in the dynamics of the system are those states with only 1 excitation. Symmetries limit the number of states that can play a role in the dynamics.

Another type of symmetry that our system may have is parity, $\hat{\pi}$. The initial state of our system is a linear combination of our basis vectors. If there is a combination such as $\left(|\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle \right) / \sqrt{2}$, where the two basis vectors involved are a mirror image of one another, this is referred to as even parity, $\pi = +1$. If one of these basis vectors is subtracted from the other, it has odd parity, $\pi = -1$. An example of a state with odd parity is $\left(|\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\rangle \right) / \sqrt{2}$.

In order to create the probability and magnetization plots that would provide us with information about parity we need to use a different basis. A basis that works is the eigenvectors of the Hamiltonian with only the off-diagonal elements considered, and the diagonal elements being set to zero. This is known as the XX basis.

We again begin with a normalized vector in the site-basis corresponding to the initial state of the system, and project this vector onto the basis of the XXZ eigenvectors. This new vector then evolves in time the same way as was done previously for the dynamics. This new vector is then projected onto the basis of eigenvectors of the XX basis. Using these values to find the probability of measuring a certain XX basis vector at time t permits us to see the effects of beginning with a state with such a symmetry. What we find is that only those basis

vectors that have the same parity as the initial state will play a role in the evolution of the system.

For example, for an open system with 4 sites and 2 excitations, the eigenvectors of the XX Hamiltonian are:

{-0.223607, -0.5, -0.447214, -0.447214, -0.5, -0.223607},

{-0.223607, 0.5, -0.447214, -0.447214, 0.5, -0.223607},

{-0.5, -0.5, 0, 0, 0.5, 0.5},

{-0.5, 0.5, 0, 0, -0.5, 0.5},

{0.632456, 0, -0.316228, -0.316228, 0, 0.632456},

{0, 0, -0.707107, 0.707107, 0, 0}.

In each of these vectors, each element corresponds to the probability amplitude of the basis vectors listed above in Eq. (2), namely the six possible distinct configurations of spins in decreasing numerical order, starting with $|1100\rangle$ and ending with $|0011\rangle$.

If an eigenvector has even parity, then the elements of the eigenvector will be symmetric with the same signs. If it has odd parity, the elements will be symmetric with opposite signs. In this example, only eigenvectors 1, 2, and 5 have even parity. When we begin with an initial state with even parity, $\left(|\uparrow\uparrow\downarrow\downarrow\rangle+|\downarrow\downarrow\uparrow\uparrow\rangle\right)/\sqrt{2}$, and allow the XXZ system with $\Delta=0.5$ to evolve with time, Fig. 8 shows that only the eigenvectors 1, 2, and 5 play a role in the dynamics. The other eigenvectors have a probability of 0 throughout the evolution.
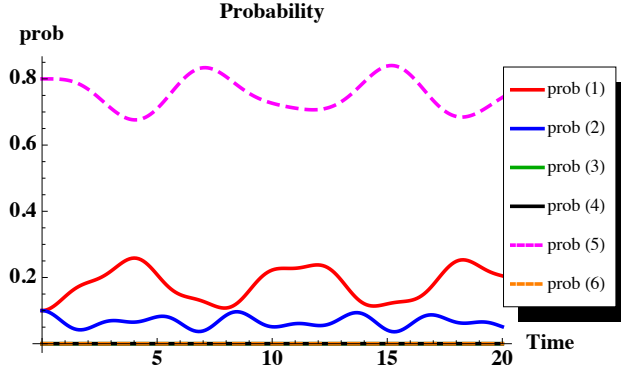
Fig. 8: Probability plot for initial state with even parity. Open chain, L=4, N=2, Δ=0.5

If we were to begin with an initial state with odd parity we would expect that any eigenvectors that play a role in the dynamics would have odd parity. In fact, beginning with the state $(|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle)/\sqrt{2}$, which has odd parity, the probability plot (Fig. 9) shows exactly as we would expect.
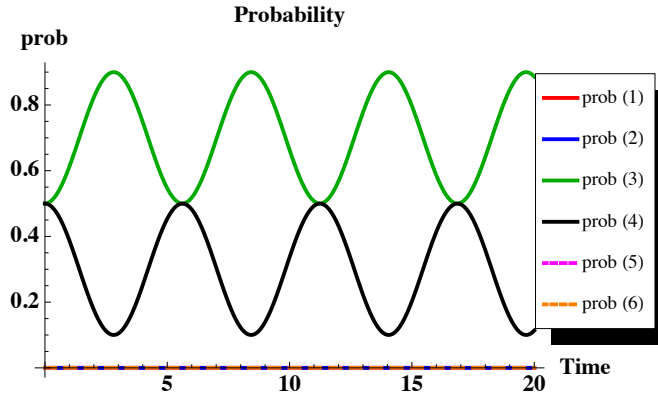

Fig. 9: Probability plot for initial state with odd parity. Open chain, L=4, N=2, Δ=0.5

The two eigenvectors that play a role in the evolution of the system are the third and fourth, or {-0.5, -0.5, 0, 0, 0.5, 0.5} and {-0.5, 0.5, 0, 0, -0.5, 0.5} respectively, which both have odd parity.

In addition to parity there is another symmetry that our system may have, and that is 180° rotation around the x-axis, $\hat{R}^x_{180°}$. This refers to a state in which the orientation of each spin is rotated by 180° around the x-axis. For example,

$$\hat{R}_{180°}^x \left(|\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle \right) / \sqrt{2} = (+1)$$

while

$$\hat{R}_{180°}^x \left(|\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle \right) / \sqrt{2} = (-1).$$

Just as with the parity symmetry, if the initial state has a certain eigenvalue of $\hat{R}_{180°}^x$, only those XX eigenvectors that have the same eigenvalue will appear on the plots as playing a role in the evolution of the system. We see this in Fig. 9 with the absence of the sixth state in the evolution. The sixth state has even parity like the initial state, but this state does not participate in the evolution because it has an eigenvalue of $R_{180°}^x = -1$, while the initial state has $R_{180°}^x = +1$.

As we have seen, symmetries limit the eigenvectors that can contribute to the dynamics of the system. The more symmetries the initial state has, the fewer eigenvectors there are with those same symmetries that can play a role in the dynamics.

To further study the effects of these symmetries on the dynamics we consider four different initial states:

$$\begin{aligned}
|\Psi_A(0)\rangle &= \left(|\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\rangle \right) / \sqrt{2} \\
|\Psi_B(0)\rangle &= \left(|\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\rangle \right) / \sqrt{2} \\
|\Psi_C(0)\rangle &= \left(|\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\rangle \right) / \sqrt{2} \\
|\Psi_D(0)\rangle &= \left(|\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle \right) / 2
\end{aligned}$$

where $|\Psi_A(0)\rangle$ has even parity, $|\Psi_B(0)\rangle$ has odd parity, $|\Psi_C(0)\rangle$ is an eigenvector of the operator $\hat{R}_{180°}^x$ with eigenvalue of $+1$, and $|\Psi_D(0)\rangle$ is an eigenvector of $\hat{\pi}$ with eigenvalue -1 and is also an eigenvector of $\hat{R}_{180°}^x$ with eigenvalue $+1$. In Table 1 each initial state is shown as a linear combination of the eigenvectors of the system in order to see which eigenvectors can play a role in the evolution. The left side of the chart lists the eigenvectors and their

corresponding eigenvalues for the eigenvectors $\hat{\pi}$ and $\hat{R}^x_{180°}$ respectively. The top three rows of the table display the initial states and the corresponding eigenvalues of $\hat{\pi}$ and $\hat{R}^x_{180°}$. The remaining contents of the table show the values of the probability amplitudes of the eigenvectors for each of the four initial states. The table clearly shows that only the eigenvectors that have the same symmetries as the initial state will contribute to the evolution of that initial state [5].

Table 1:

			$\lvert\Psi_A(0)\rangle$	$\lvert\Psi_B(0)\rangle$	$\lvert\Psi_C(0)\rangle$	$\lvert\Psi_D(0)\rangle$
			$\Pi = +1$	$\Pi = -1$	$\Pi = \varnothing$	$\Pi = -1$
			$R^z_\pi = \varnothing$	$R^z_\pi = \varnothing$	$R^z_\pi = +1$	$R^z_\pi = +1$
	Π	R^z_π	$c_A^{(j)}$	$c_B^{(j)}$	$c_C^{(j)}$	$c_D^{(j)}$
$\psi^{(1)}$	−	−	0	−0.16	0	0
$\psi^{(2)}$	+	+	−0.19	0	−0.19	0
$\psi^{(3)}$	−	+	0	0.33	0.33	0.46
$\psi^{(4)}$	−	−	0	−0.07	0	0
$\psi^{(5)}$	+	+	0.19	0	0.19	0
$\psi^{(6)}$	+	−	−0.48	0	0	0
$\psi^{(7)}$	+	+	−0.05	0	−0.05	0
$\psi^{(8)}$	−	+	0	−0.28	−0.28	−0.40
$\psi^{(9)}$	−	−	0	0.33	0	0
$\psi^{(10)}$	−	−	0	0.42	0	0
$\psi^{(11)}$	+	+	−0.50	0	−0.50	0
$\psi^{(12)}$	+	−	−0.15	0	0	0
$\psi^{(13)}$	+	+	−0.34	0	−0.34	0
$\psi^{(14)}$	−	−	0	0.11	0	0
$\psi^{(15)}$	−	−	0	−0.30	0	0
$\psi^{(16)}$	−	+	0	−0.56	−0.56	−0.79
$\psi^{(17)}$	+	−	0.50	0	0	0
$\psi^{(18)}$	+	+	0.04	0	0.04	0
$\psi^{(19)}$	−	−	0	−0.28	0	0
$\psi^{(20)}$	+	+	−0.24	0	−0.24	0

5. Chaotic Systems

The clean integrable systems studied above were all non-chaotic systems. We now look at chaotic systems and compare the behavior of these systems with that of the non-chaotic systems. Specifically, we analyze the effects of introducing an impurity, ε, to the middle of the chain, and separately the effects of including next nearest neighbor (NNN) coupling in addition to nearest neighbor (NN) coupling [8]. The impurity is created with a magnetic field acting on site $(L/2)+1$ that is slightly different from the field acting on the other sites. With next nearest neighbor coupling, a spin on one site no longer communicates only with the spins immediately next to it, but also with the spins two sites away. With NNN coupling, as opposed to with only NN coupling, $|\uparrow\uparrow\downarrow\downarrow\rangle$ can successfully couple with $|\uparrow\downarrow\downarrow\uparrow\rangle$.

An impurity in the middle of the chain and next nearest neighbor coupling individually render the system as being chaotic. In both of these cases the system can no longer be solved analytically, and must be solved numerically.

In classical physics, the time evolution of non-chaotic systems are predictable, while chaotic systems diverge and are not predictable. As we mentioned above, if the system starts with the same initial conditions, a chaotic system will diverge and behave differently each time. Quantum systems showing signatures of chaos are referred to as chaotic quantum systems. Integrable systems flow ballistically, which means they flow easily and don't encounter obstacles, and can provide for transport of things such as energy or magnetization. In contrast, chaotic systems are diffusive and encounter obstacles.

Now that we have slightly changed the system, the Hamiltonian is

$$H = H_Z + H_{NN} + \alpha H_{NNN}, \tag{6}$$

where

$$H_Z = \varepsilon_{L/2+1} S^z_{L/2+1},$$

$$H_{NN} = \sum_{n=1}^{L-1} J\left[\left(S^x_n S^x_{n+1} + S^y_n S^y_{n+1}\right) + \Delta S^z_n S^z_{n+1}\right],$$

and

$$H_{NNN} = \sum_{n=1}^{L-2} J\left[\left(S^x_n S^x_{n+2} + S^y_n S^y_{n+2}\right) + \Delta S^z_n S^z_{n+2}\right],$$

This H_{NNN} is the Hamiltonian for next nearest neighbor coupling, corresponding to the couplings between a spin and those two sites away, and the ratio between NNN and NN is α.

The observable we use to study the time evolution of these systems is local magnetization, which is the sum of the magnetization of the sites of the first half of the chain. An excitation on one site contributes +0.5 to the local magnetization, while a down-spin contributes -0.5 to the local magnetization. Our initial state has L/2 spins pointing up, so the dynamics is confined to the subspace with $S^z_{total} = 0$. We begin with a domain wall state, in which all of the up-spins are on the left of the chain and all of the down-spins are on the right side of the chain [8]. Using a chain with open boundary conditions containing 12 sites and 6 up-spins, the local magnetization begins at a value of 3 and decreases as the system evolves in time and the excitations move to the right. Below, in Fig. 10, we have a plot showing the decay of the local magnetization over time for three different clean systems with NN couplings that differ only in the values of the anisotropy parameter. The values of Δ for the systems being analyzed include Δ=0, 0.5, and 1.

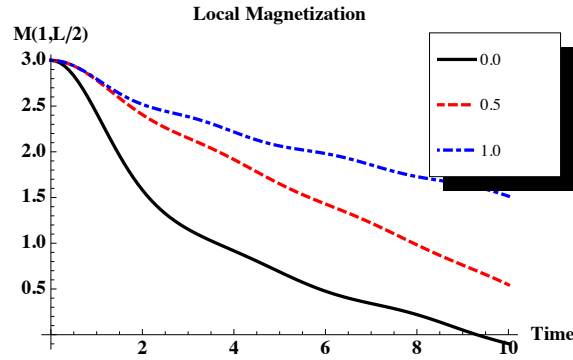Fig. 10: Clean, integrable system. Black: Δ=0; Red: Δ=0.5; Blue: Δ=1. L=12, N=6, open chain

From the plot it seems that for the clean integrable system the magnetization of the system decays the fastest when Δ=0. As expected based on the analysis above, as the strength of the Ising interaction increases, the excitations move more slowly, and therefore the local magnetization decreases more slowly.

Similar plots were created showing the decay in magnetization for the system with an impurity and the system with next nearest neighbor coupling respectively. The system with the impurity behaved similarly to the clean integrable system (figure not shown). The rate of decay of the magnetization decreased as the value of the anisotropy parameter increased. However, the system with NNN coupling showed strange behavior. As Fig. 11 shows, the conditions under which the system decayed most rapidly was when Δ=0.5. This is different than the expected results where the decay of the local magnetization is greatest when Δ=0.

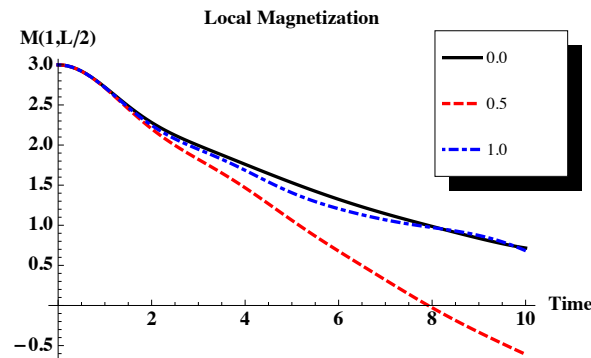Fig. 11: NNN coupling. Black: Δ=0; Red: Δ=0.5; Blue: Δ=1. L=12, N=6, open chain

We took several approaches to try to understand the cause of this strange behavior. First we looked at plots for a chain with periodic boundary conditions and found that the same phenomenon was seen. Namely, with the NNN coupling the local magnetization of the system with $\Delta=0.5$ decayed most rapidly, and not the system with $\Delta=0$. Since the strange phenomenon was seen in a system with periodic boundary conditions, we can remove boundary effects as a possible reason for this anomalous behavior.

We also compared the energy of the initial state to the spectrum of the whole system, expecting to find some distinguishing feature for the system with NNN coupling and $\Delta=0.5$, such as perhaps having the initial state with energy too close to the middle of the spectrum, where the density of states is larger. We created histograms of the eigenvalues, corresponding to the allowed energies of the system. The vertical red line denotes the energy of the initial state. The percentage shows where in the range of possible values the energy of the initial state lies. As Fig. 12 shows, as the Ising interaction increases in strength, the energy of the initial state increases and moves more towards the maximum eigenvalue. When an impurity or NNN coupling is introduced to the system, the movement of the initial energy towards the maximum eigenvalue is slightly less drastic. However, based on the histograms below we concluded that this strange behavior of the system with NNN coupling does not find a justification from this analysis.
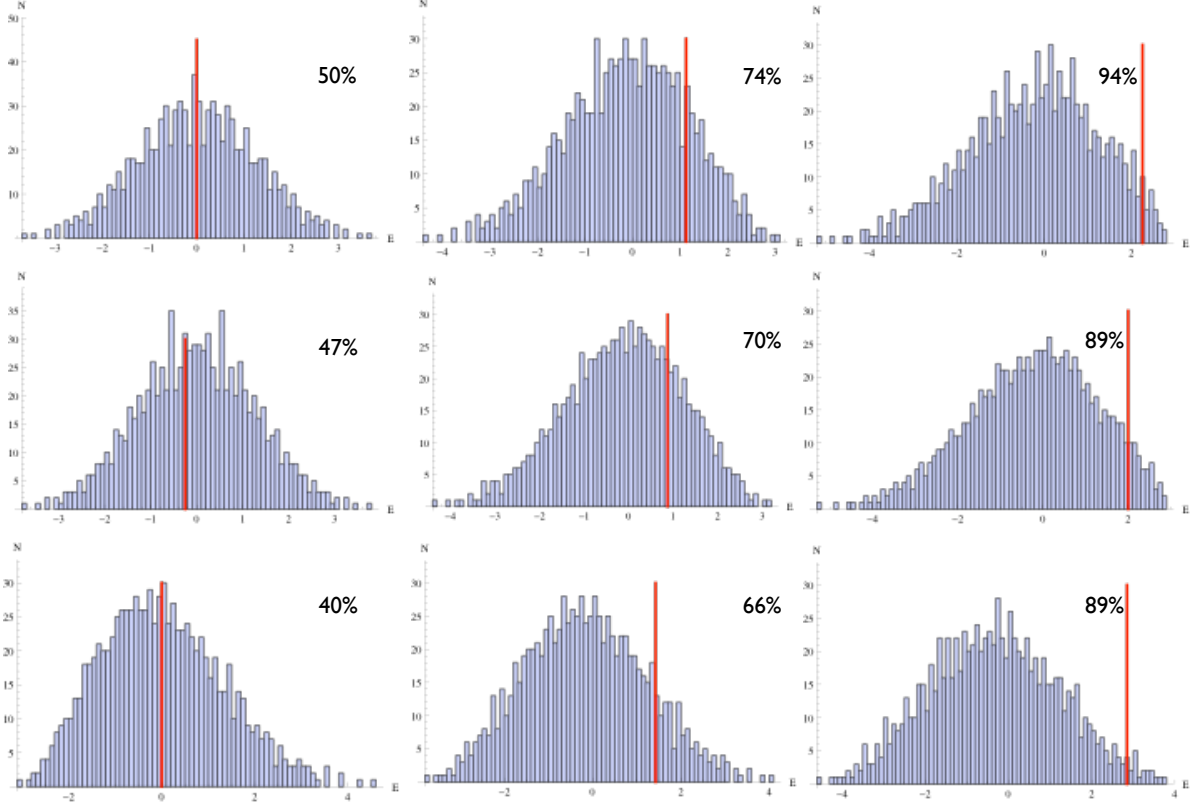
Fig 12. Plots denoting energy of initial state as compared to all eigenvalues of the system. Top row: clean integrable system. Middle row: impurity. Bottom row: NNN coupling. Left column: $\Delta=0$. Middle column: $\Delta=0.5$. Right column: $\Delta=1$

We studied the local magnetization of the system beginning with other initial states besides for the domain wall state to verify whether or not the strange behavior of the NNN system was related to the particular domain wall initial state. However, the strange phenomenon was again seen when the system had NNN coupling (figure not shown). Additionally, not only did the system with $\Delta=0.5$ decay more rapidly than the system with $\Delta=0$, but the system with $\Delta=1$ decayed most rapidly. This is even more surprising because at $\Delta=1$ the flip-flop term and the Ising interaction are equal in strength, while for the other two values of Δ the relative strength of the flip-flop term is greater, encouraging movement of the excitations. Despite these expectations, the local magnetization of the system with $\Delta=1$ decayed most rapidly.

Once we were unable to find an explanation for the anomalous behavior, the next step was to study different variations of the Hamiltonian. Originally, we were studying systems that had an Ising interaction and a flip-flop term for both the nearest neighbor interactions and the next nearest neighbor interactions, for a total of four terms. We looked at the effects of removing individual terms from this four-term Hamiltonian, such as removing only the NN Ising interaction, or only the NNN flip-flop term.

The four combinations we studied included:

1) No NN Ising interaction:

$$H = \sum_{n=1}^{L-1} J\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) + \alpha\left[\sum_{n=1}^{L-2} J\left[\left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y\right) + \Delta S_n^z S_{n+2}^z\right]\right.$$

2) No NNN Ising interaction :

$$H = \sum_{n=1}^{L-1} J\left[\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) + \Delta S_n^z S_{n+1}^z\right] + \alpha\left[\sum_{n=1}^{L-2} J\left[\left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y\right)\right]\right]$$

3) No NN flip-flop term:

$$H = \sum_{n=1}^{L-1} J\Delta S_n^z S_{n+1}^z + \alpha\left[\sum_{n=1}^{L-2} J\left[\left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y\right) + \Delta S_n^z S_{n+2}^z\right]\right.$$

4) No NNN flip-flop term:

$$H = \sum_{n=1}^{L-1} J\left[\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) + \Delta S_n^z S_{n+1}^z\right] + \alpha\left[\sum_{n=1}^{L-2} J\Delta S_n^z S_{n+2}^z\right]$$

From the four combinations considered, the only one that exhibited this strange behavior was the case in which NNN Ising was removed (case 2). The only difference between this case and the clean integrable system in which there was no anomalous behavior is an additional NNN flip-flop coupling. Though we can still not conclude exactly what causes this anomalous behavior, we can narrow down the options and suggest that this phenomenon stems from the interplay between the NNN flip-flop and the NN Ising terms.

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6. Heat Transfer

After the detailed analysis of static and dynamic properties of integrable and chaotic spin-1/2 systems, we were ready to couple the system to baths and study heat transfer. In order to do so we use a model to describe the effects of the interaction with the baths. We attach baths of different temperatures to each end of the chain [9]. In this case, the total magnetization is no longer conserved, because the baths can add or remove excitations from the chain. The cold bath takes energy from the system and can therefore take an up-spin and turn it into a down-spin, while the hot bath adds energy to the system and can make a down-spin into an up-spin.

For such non-isolated systems, the dimension of the Hamiltonian to be diagonalized increases significantly because it now includes the whole Hilbert space. The dimension of this matrix is 2^L. We consider a generic initial state which in this case is a random superposition of all 2^L basis vectors. In order to create a random initial state, we created a random Hermitian matrix. This random matrix had to be symmetric, so in order to ensure that this was so, we used the sum of a matrix with random elements from a Gaussian distribution and the transpose of that same random matrix. The resulting matrix was then diagonalized and an eigenvector of this matrix was used as the initial state. The system is evolved according to Schrödinger's equation. We do this by continuously applying the propagator $U(t) = \exp(-iHt)$ to the initial state so that the system evolves for a long time until it reaches an equilibrium.

The state evolves freely during equal successive intervals of time. In between two such intervals, the edge spins of the system are reset to model the effects of heat baths. The method used to determine whether or not the hot/cold baths change the orientation of an edge

spin is through generation of random numbers. The cold bath (on the left of the system) and the hot bath (on the right side of the system) each have a chemical potential μ associated with it. For the cold bath, μ_L is set to 0.35, and for the hot bath, μ_R is set to 0.75.

Randomly generated numbers ξ_L and ξ_R are compared with their respective chemical potential. If $\xi_L < \mu_L$, which is less likely, the edge spin will be oriented up. In the case which is more likely, that $\xi_L > \mu_L$, the cold bath causes the edge spin to be a down-spin. Similarly, majority of the time the hot bath will cause the edge spin to be an up-spin, but sometimes, when $\xi_R > \mu_R$, the edge spin will be a down-spin. This process continues as the system evolves until an equilibrium is reached.

Once a steady equilibrium is reached, the magnetization of each site can be measured. Based on these measurements we can determine whether or not the system follows the Fourier Law. If the system is chaotic, we expect that the magnetizations will be a gradient, where the magnetization steadily increases as we move from the site closest to the cold bath to the site closest to the hot bath. This situation follows the Fourier Law. For an integrable system we expect there to be no gradient. We expect that along the chain the magnetization would be approximately zero and this system does not follow the Fourier Law.

At this point we have written the code that models the chain attached to the cold bath on one end and the hot bath on the other end. According to the process described above, the system evolves and is appropriately adjusted due to the baths. However, further work must be done to have this process continue until the system reaches an equilibrium state. Once that is completed, we can produce results in an effort to confirm the expectations of seeing a gradient in the magnetization for chaotic systems and no gradient for integrable systems.

7. Conclusions

In this work we studied the static and dynamic properties of both integrable and chaotic spin-1/2 systems described by the Heisenberg model. Using the observables magnetization and probability to study the evolution of the integrable system, we saw several factors that can limit the evolution of the system, including the magnitude of the anisotropy parameter as well as symmetries of the initial state. While studying chaotic systems we studied the anomalous behavior detected when a system had next nearest neighbor coupling. An exact cause for this behavior was not determined, but we were able to narrow down the possible causes, concluding that it is related to the interplay between the NNN flip-flop and the NN Ising terms. Finally, we modeled a chain attached to a cold bath on one end and a hot bath on the other, and we are in the process of using this model to study heat transfer in integrable and chaotic systems.

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