Dynamics of Quantum Systems with Interacting Particles

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1. Introduction

In this thesis, I study the static properties and dynamics of a quantum system of interacting particles. For this, I employ the laws of quantum mechanics, which differ from the laws of classical mechanics used to interpret the macroscopic world around us. Quantum mechanics is a branch of physics that describes how matter and light behave on a microscopic level. My focus is on a lattice system that has on each site a localized particle with spin ½. Spins are intrinsic properties of microscopic particles that tell us how they react to magnetic fields. The basic constituents of matter, such as electrons, protons, and neutrons, have spins ½, while atoms have higher values of spins. The interactions between the spins may lead to collective behaviors with macroscopic effects, such as ferromagnetism, where the spins line up parallel to each other, and antiferromagnetism, where neighboring spins point in opposite directions.

The model that I use to describe the spin-½ system is the Heisenberg model. This is one of the most important models of magnetism and has been investigated for decades [3]. Despite being a simplified theoretical model, it describes quantitatively well certain real materials found in nature or synthesized in a laboratory, such as magnetic compounds. It is also an important model in studies of quantum phase transition, the metal-insulator transition, and quantum computers.

The system that I study has all spins pointing down in the z-direction except for two that point up. This corresponds to the scenario where the lattice is subject to a strong magnetic field pointing down in z, which induces most spins to get aligned with it. I investigate how the properties of the system and its dynamics depend on the strength of the interaction between those two excitations. I assume that only neighboring spins are coupled. If the interaction is very strong, the eigenstates of the system are either superpositions of states with excitations on neighboring sites or superpositions of states where the excitations are separated. None of the eigenstates combine both kinds of states. This is reflected in the dynamics. If the system is prepared in an initial state where two up-spins are in neighboring sites, they move slowly together along the chain and never split up. Conversely, if in the initial state the two excitations are separated, throughout the evolution they avoid each other and never sit on neighboring sites. With my analysis, I therefore show that the dynamics of the system can be anticipated by studying its static properties.

2. What Distinguishes Quantum Mechanics from Classical Mechanics?

Quantum objects do not behave like the objects we are used to. Therefore, we cannot apply our experience or intuition to understand how they work. There are a few important elements that are unique to quantum physics.

- *Discreteness.* Firstly, the word "quantum" refers to the fact that in quantum physics everything is discrete, not continuous. For example, in a beam of light there are a discrete integer number of photons. Similarly an electron in an atom has certain discrete energy values.
- *Intrinsic probabilistic nature.* Second, quantum physics is based on probability. Physicists predict the probability of each possible outcome. This means that while physicists can predict the probability of finding a specific electron at point A and the probability of finding it at point B, they cannot say for certain where the electron will end up.

- *Uncertainty Relation.* Another characteristic of quantum physics is the uncertainty relation. The uncertainty relation means that we can precisely measure the position or momentum of a particle, but not both. The more precisely we measure the position, the less precise the momentum is, and vice versa. Since momentum is related to wavelength, this phenomenon can be illustrated with a wave on a string. In Figure 2.1 for example, you would be able to determine how long the wavelength is, but you cannot pinpoint precisely where the particle characterized by the wave is located. On the other hand if someone suddenly jerked the string to create a traveling pulse, as in Figure 2.2, it would be simple to determine precisely where the particle characterized by the wave is, but it would be difficult to assign it a wavelength. The inverse relationship between the uncertainty in position and the uncertainty in momentum can be seen from the following equation:

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \qquad (eqn\ 2.1)$$

where Δx is the standard deviation $\sqrt{<x^2> - <x>^2}$ or the uncertainty in position and Δp is the standard deviation , $\sqrt{<p^2> - <p>^2}$, in momentum. As Δx, decreases, Δp must increase to compensate, and vice versa.

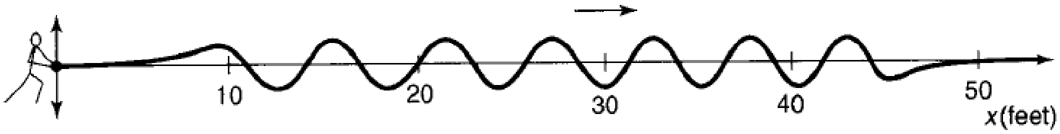


Figure 2.1: Well-defined Wavelength

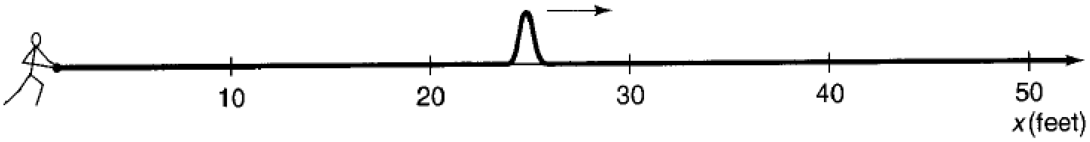


Figure 2.2: Well-defined Position

- *Wave-particle duality.* Lastly, from the study of the behavior of quantum particles, it was determined that they behave sometimes like waves and sometimes like particles. This wave-particle duality found for matter, is similar to the behavior of light. In fact, any quantum object presents this duality, including protons, atoms, and even molecules. An example of the latter is the carbon-60 molecule, the largest object so far to have demonstrated interference patterns typical of those occurring for waves [7].

To try to explain the wave-particle duality, we can imagine the following experiments. The first one is done with bullets. Bullets are shot from a gun toward a wall. The wall has two bullet-size holes in it, and behind the wall is a detector. Whenever a bullet is shot, either zero or one whole bullet arrives at the detector. We will describe this by saying that the bullets “arrive in lumps.” If hole 1 is closed, bullets can only enter through hole 2 and vice versa. The probability of a bullet arriving at the detector at different distances x from the center can be measured. Comparing the probabilities reveals that P_1 (the probability of a bullet passing through hole 1 when hole 2 is closed) and P_2 (the probability of a bullet passing through hole 2 when hole 1 is closed) add up to give P_{12} (the probability of a bullet passing through either hole 1 or hole 2, when both holes are open). This is illustrated in Figure 2.3. In addition to bullets arriving in lumps, we say that since $P_{12}=P_1+P_2$, there is no interference. The property of interference will be discussed more and explained later.

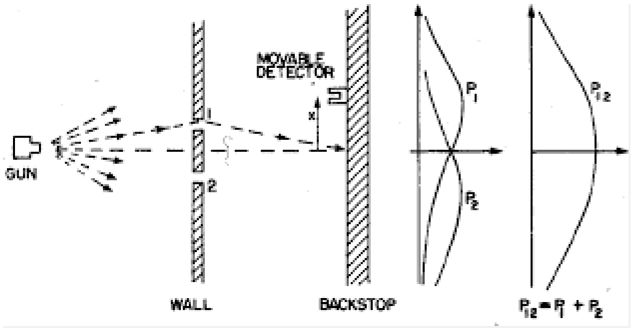


Figure 2.3: Bullet Experiment

A similar experiment can be done with water waves. A wave source with a motor makes circular waves. Again there is a wall with two holes and a detector behind the wall. The detector measures the intensity of the waves (the rate at which the energy is being carried to the detector). The first thing that is different from the bullets is that intensity can have any value and therefore cannot be described as arriving in lumps. Intensity depends on the motion at the wave source. If the wave source has more motion, the intensity at the detector is greater. The second difference is evident from looking at Figure 2.4. It is clear that I_{12} (the intensity when both holes are open) does not equal the sum of I_1 (intensity from hole 1 when hole 2 is closed) and I_2 (intensity from hole 2 when hole 1 is closed). Therefore, we describe the water waves (in I_1 and I_2) as having interference. There are two types of interference of the waves. Constructive interference occurs when the waves are “in phase”. In this case the peaks of the two waves add together to equal a large amplitude or intensity. When the waves are “out of phase,” the resulting intensity equals the difference of the two amplitudes. This is known as destructive interference.

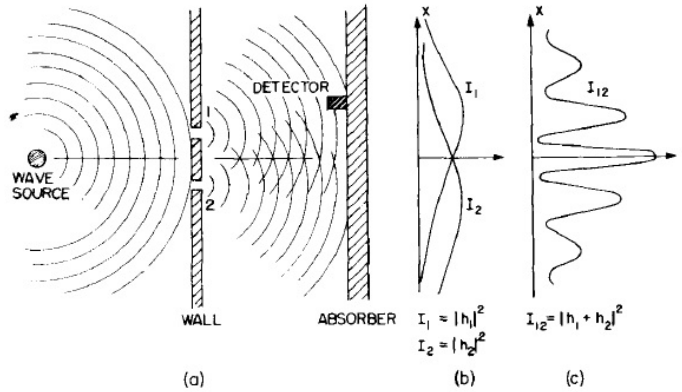


Figure 2.4: Water Wave Experiment

The last experiment is with electrons. An electron gun shoots electrons toward a wall with two holes, with a detector behind the wall. The detector is connected to a loudspeaker. Whenever an electron is detected, we hear a “click” from the loudspeaker. All the clicks are the same, with no half-clicks. If the detector moves, the rate of the clicks can get faster or slower, but the loudness of the clicks does not change. Also, if there were two detectors, one or the other would emit the “click,” but they would never both “click” at once. This shows that the electrons arrive in “lumps”. All lumps are the same size, they are whole, and arrive one at a time. In Figure 2.5 we can see the probability of a lump arriving at the backstop at different distances *x* from the center.

We can make a proposition based on the information we have so far. Since the electrons come in lumps, just like the bullets, the proposition is: Each electron either goes through hole 1 *or* it goes through hole 2. If this proposition was true, the probability of electrons passing through hole 1 (when hole 2 is closed) should add together with the probability of electrons passing through hole 2 (when hole 1 is closed) to equal the probability of electrons passing through either hole (when they are both open). But from

Figure 2.5, we see that since P_{12} does not equal P_1+P_2, it is more like the water wave experiment with interference. There are some points where more electrons pass through with one hole open than with both open. And there are some points where P_{12} is more than twice the value of P_1+P_2. It is very mysterious, and no explanation works. The only conclusion is that electrons arrive in lump-like particles, but they seem to move as waves. They show interference, which causes the probability of their arrival to be distributed like that of wave intensity. This is why we say that electrons behave sometimes like particles and sometimes like waves. We have also determined the proposition we made earlier to be false. It is not true that electrons either pass through hole 1 *or* pass through hole 2. Since they seem to propagate as waves, it is as if they had passed through both slits.

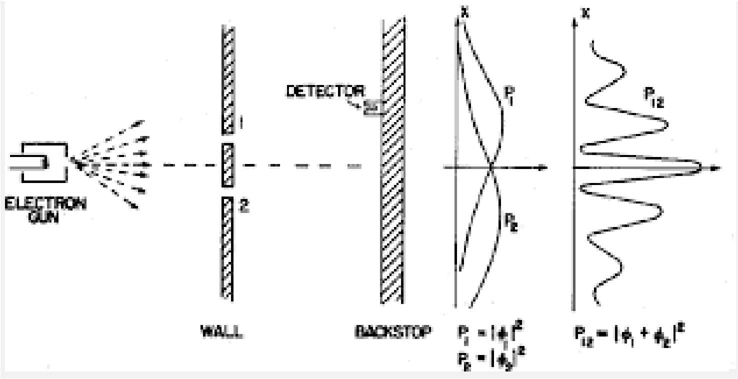


Figure 2.5: Electron Experiment

The experiment becomes even more remarkable if we try to detect which hole the electron actually passes through. When this is done, we get information about the electron’s position, but simultaneously lose the interference pattern! We say that by measuring the position, we “collapse the wave” [1].

3. Formalism of Quantum Mechanics

In classical mechanics the idea is to determine the position of a particle, $x(t)$, at a given time. With that information and Newton's second law, $F = ma$, we can find the particle's velocity, momentum, and kinetic energy. In quantum mechanics however, we cannot use classical properties. As we said above, we cannot know precisely position and momentum at the same time. Instead, to describe the system, we use the wave function, $\Psi(x, t)$. To find the wave function and to describe how it changes in time, we solve Schrödinger's equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \quad (eqn\ 3.1)$$

where i is the square root of -1 and ħ is Planck's constant (h) divided by 2π or:

$$\hbar = \frac{h}{2\pi} = 1.054573 \text{ x } 10^{-34}\text{J s} \quad (eqn\ 3.2)$$

All information about the system is contained in the wave function. As mentioned in Chapter 2, it is impossible to say for certain where a particle will be located, instead we use probabilities. The probability of finding the particle at point *x*, at time *t*, is the following:

$$|\Psi(x,t)|^2 dx \quad (eqn\ 3.3)$$

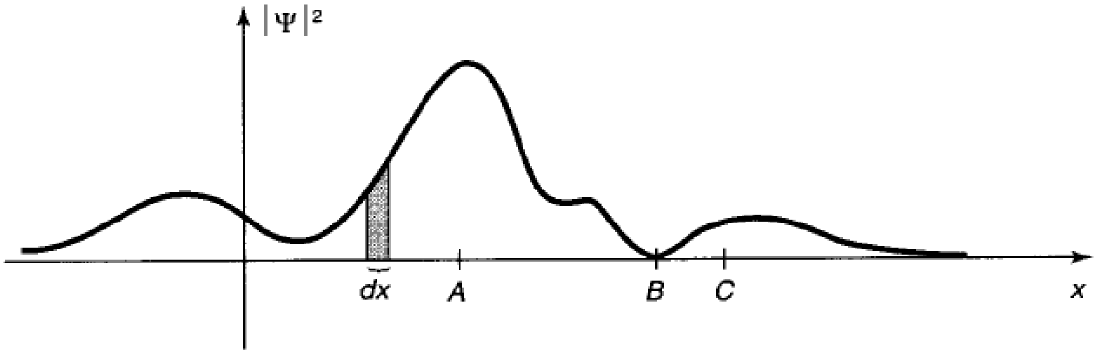


Figure 3.1: Wave Function

As seen in the graph in Figure 3.1, there is a high probability of the particle being found near point A and a very low probability of it being found near point B.

Since the wave has to be somewhere, the probabilities all add together to equal 100%. In this way, the wave function is normalized.

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1 \quad (eqn\ 3.4)$$

The position of the particle can be measured. If it is found to be at point C (see Figure 3.2), further measurements taken immediately after the first will cause the particle to be found again at C. The act of the first measurement causes the collapse of the wave function and the sharp peak at point C.

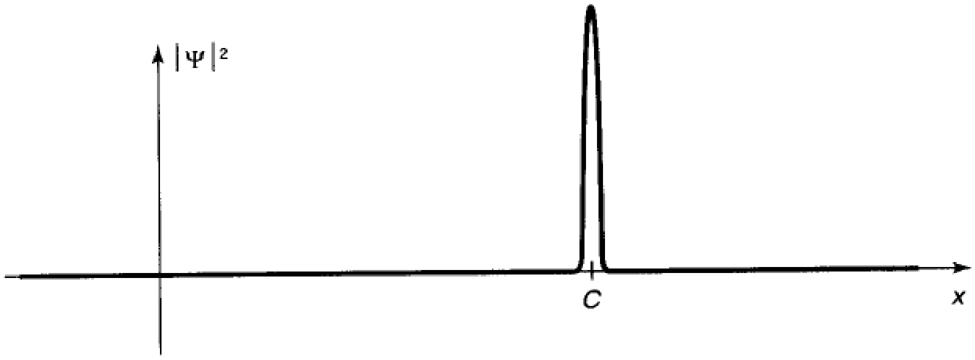


Figure 3.2 Collapse of the Wave Function

We will now discuss how to solve the Schrödinger equation to get the wave function. In Schrödinger's equation (equation. 3.1), the first term on the right side, $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$, is the kinetic energy and the second term, $V(x,t)\Psi$, is the potential energy. We start solving the equation through the separation of variables. Assuming *V(x)* has no dependence on time, we can guess that $\Psi(x,t) = \psi(x)f(t)$, it is the product of two functions, one dependent only on time and one dependent only on position. Then,

$$\frac{\partial \Psi}{\partial t} = \psi \frac{\partial f}{\partial t} \ (eqn\ 3.6)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial x^2} f \quad (eqn\ 3.7)$$

Thus,

$$i\hbar\psi \frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} f + V\psi f \quad (eqn\ 3.8)$$

After dividing through by ψf,

$$i\hbar \frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V \quad (eqn\ 3.9)$$

The left side is only a function of *t*, and the right side is only a function of *x*. This must mean that both sides are constant. Otherwise, if *t* changed, the value on the left side would change, and in order to keep the equality, the right side would need to change as well. But since the right side is not dependent on *t*, this cannot happen. Giving the name *E* to the value of this constant, we have

$$i\hbar \frac{1}{f}\frac{df}{dt} = E \quad (eqn\ 3.10)$$

and,

$$\frac{df}{dt} = -\frac{iE}{\hbar} f \quad (eqn\ 3.11)$$

The right side of equation 3.9 is equal to this constant as well,

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \quad (eqn\ 3.12)$$

And multiplying by ψ,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \quad (eqn\ 3.13)$$

We now have two ordinary differential equations (ODE), equations 3.11 and 3.13. The first can be simply solved as

$$f(t) = e^{-iEt/\hbar} \quad (eqn\ 3.14)$$

The second of the two is the time independent Schrödinger equation.

The total energy, kinetic and potential is represented by the Hamiltonian.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V = Hamiltonian \quad (eqn\ 3.15)$$

So equation 3.13 can be written as,

$$H\psi = E\psi \quad (eqn\ 3.16)$$

which is known as time-independent Schrödinger equation.

When we solve $H\psi = E\psi$, we find E, the eigenvalues which correspond to the energies of the system, and ψ, the eigenvectors or eigenstates, which correspond to the states of the system. The set of eigenvalues constitute the spectrum of the system.

Combining the solutions of the time-independent Schrödinger equation with equation 3.14, gives us the solutions for the time-dependent Schrödinger equation. They are stationary states. The wave function,

$$\Psi(x,t) = \psi e^{-iEt/\hbar} \quad (eqn\ 3.17)$$

depends on t, but the probability density does not,

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\, \psi e^{-iEt/\hbar} = |\psi(x)|^2 \quad (eqn\ 3.18)$$

because it does not depend on time. $|e^{-iEt/\hbar}|^2 = 1$ because $(e^{iEt/\hbar})(e^{-iEt/\hbar}) = 1$.

Other states are said to be dynamic rather than stationary because they change in time. In the next chapters we will be studying the dynamics of such non-stationary states.

4. Spin-1/2 Systems Described by the Heisenberg Hamiltonian Model

Until now we have been talking about continuous x, but the system we will be studying is a one-dimensional lattice with discrete sites. The lattice can either have open boundary conditions, in which case it is called an open chain, or it has closed (periodic) boundaries as in a ring. In the first case, a particle that reaches the edge of the chain hits an infinite wall and bounces back, while in the second case, it can move from the last site to the first site and vice-versa.

In classical mechanics, a charged, spinning object has magnetic properties. Elementary particles that move through a magnetic field are deflected in a way that suggests that they have similar magnetic properties. These subatomic particles are described as having a “spin” because to scientists it first seemed helpful to think about them as if they were rotating, just like in the planetary system, where the planets rotate around an axis. However, point-like particles are not really spinning, but the term “spin” remains. It refers to the total angular momentum of the particle. Protons, neutrons and electrons are particles with spin ½. There are only two values for the spin along a certain chosen direction, such as z: spin-up,

+½, and spin-down, -½. A single spin is therefore a two-level system. The Heisenberg model describes the interaction between particles of spin ½. Each site in the lattice holds one particle of spin ½.

The two states of the spins can be written in a few different ways. A spin-up in the z-direction can be represented with an arrow $|\uparrow\rangle$, $|1\rangle$ or a vector $\binom{1}{0}$. A spin-down can be written in a few ways as well, such as $|\downarrow\rangle$, $|0\rangle$ or $\binom{0}{1}$. There are three spin operators $S^{x,y,z} = \sigma^{x,y,z}/2$ where

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

are Pauli matrices. For a spin in the z-direction, if it is pointing up, σ^z gives a positive value:

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

If the spin is down, σ^z gives a negative value:

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

In contrast, σ^x and σ^y flip the direction of the spin. For example,

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

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

The Hamiltonian of a system with L spins described by the Heisenberg model is given by

$$H = \sum_{n=1}^{L-1} \frac{J_z}{4} \sigma_n^z \sigma_{n+1}^z + \frac{J}{4} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) \quad (eqn. 4.1)$$

This model is referred to as the XXZ model because the X and the Y term both have the same weight, while the Z term has a different weight. The Z term is in competition with the XY term.

To find E, the energies of the system, or the eigenvalues, and ψ, the eigenstates, we have to write the Hamiltonian in matrix form and then diagonalize it. In a 2x2 or 3x3 matrix we can do the diagonalization analytically. But with a larger matrix like the 6x6 we have below, we use the computer to diagonalize it numerically. To do the diagonalization, we need to define a basis. The basis is equivalent to the frame of reference that we choose when writing ordinary vectors, such as those for velocity or force. There are infinitely many options. For example, given a vector for velocity, we can choose a reference frame where the x-axis is aligned with the vector, or instead the y-axis, or the z, or none of them. To write the matrix for equation 4.1, we chose the basis composed of states where each spin either points up or down in the z-direction. We could, of course, have selected any other basis, but this turns out to be a very convenient one, as we explain below.

In our chain there are L sites, and because the Hamiltonian conserves the total spin in the z direction, there are a fixed number of spin-ups. If L = 4 sites and n_{up} = 2, there are 6 permutations: 1100, 1010, 1001, 0110, 0101, and 0011. Since for most values of L it would take too long to list all the basis vectors before counting them, the dimension, or the number of permutations of these basis vectors, can be written as a binomial, $\binom{L}{\mathrm{nup}}$, or calculated with the following equation:

$$\binom{L}{\text{nup}} = \frac{L!}{\text{nup}!(\text{L}-\text{nup})!} \quad (eqn\ 4.2).$$

Each basis vector can be represented in two ways. If we take the first basis vector as an example, it can be written in the more physical form $|1100\rangle$, where each number represents the state of each one of the four sites in the chain, or in the more abstract mathematical form, $\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix}$, where each element in the vector represents a state of the whole chain. Each basis vector multiplied by itself is 1, $\langle 1100|1100\rangle = 1$ and they are orthogonal, $\langle 1100|1010\rangle = 0$. This basis is therefore orthonormal.

To build the Hamiltonian matrix, we first analyze the effect of each term from equation 4.1 on the basis vectors. We note that the operator $\sigma_n^{x,y,z}$ acts on site *n* and $\sigma_{n+1}^{x,y,z}$ on site *n+1*. Thus, there are only couplings between neighboring sites. The first term in equation 4.1 is the Ising interaction. Since σ^z does not flip the state of the spin, this term is the diagonal part of the Hamiltonian matrix written in the z-basis. As shown in the equations below, a pair of adjacent parallel spins has higher energy than a pair of adjacent antiparallel spins.

$$(J_z/4)\sigma_n^z\sigma_{n+1}^z|\uparrow_n\uparrow_{n+1}\rangle = +(J_z/4)|\uparrow_n\uparrow_{n+1}\rangle \quad (eqn\ 4.9)$$

$$(J_z/4)\sigma_n^z\sigma_{n+1}^z|\uparrow_n\downarrow_{n+1}\rangle = -(J_z/4)|\uparrow_n\downarrow_{n+1}\rangle \quad (eqn\ 4.10)$$

To calculate the diagonal elements of the Hamiltonian we check whether each spin in the basis vector is parallel or antiparallel to the spin that follows it. If they are parallel, we add $+(J_z/4)$, if they are antiparallel $-(J_z/4)$. For example, the element $H_{11} = \langle 1100|\mathrm{H}|1100\rangle$ is calculated as

$$H_{11} = \langle 1100|\mathrm{H}|1100\rangle = +(J_z/4) - (J_z/4) + (J_z/4) = +(J_z/4)$$

The second term in equation 4.1 gives the off diagonal elements of the matrix. It is called the flip-flop term because it moves the excitations through the chain by flipping spins in two adjacent sites that have opposite spin direction, that is, spins that are antiparallel.

$$\frac{J}{4}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y)\,|\uparrow_n\downarrow_{n+1}\rangle = \frac{J}{2}|\downarrow_n\uparrow_{n+1}\rangle \quad (eqn\ 4.11)$$

$$\frac{J}{4}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y)\,|\downarrow_n\uparrow_{n+1}\rangle = \frac{J}{2}|\uparrow_n\downarrow_{n+1}\rangle \quad (eqn\ 4.12)$$

Contrary to the diagonal elements, whose values depend on the size of the chain and on the number of spins pointing up, the off-diagonal elements are all equal to J/2 if the two corresponding basis vectors are coupled, or zero otherwise. As an example for the first case, consider the states $|1100\rangle$ and $|1010\rangle$. The second and third spins are coupled via $\frac{J}{4}(\sigma_2^x\sigma_3^x + \sigma_3^y\sigma_3^y)$, so

$$H_{12} = \langle 1100|\mathrm{H}|1010\rangle = \frac{J}{2} = H_{21}.$$

As an example for the second case, consider the states $|1100\rangle$ and $|1001\rangle$. There are no terms in the Hamiltonian to couple them, so

$$H_{13} = \langle 1100|\mathrm{H}|1001\rangle = 0 = H_{31}.$$

5. Static Properties of the Heisenberg Model

5.1 Eigenvalues

The eigenvalues and eigenvectors depend on the parameters. Most importantly they depend on the competition between the two terms of the Hamiltonian. This competition is determined by the strengths of the flip-flop term, J_{xy}, and Ising interaction, J_z. The energies also depend on the system size, L, and the number of up-spins or excitations versus the number of down-spins, and on boundary conditions. In order to explain this, I will begin by focusing on a system of L = 6 sites with $n_{up} = 2$ and show some examples and figures.

We start by just focusing on the diagonal elements of the Hamiltonian, which are the J_z energies. For an open system of L = 6 sites, the state $|001100\rangle$ has an energy of $+ J_z/4$ because there are 3 adjacent pairs with parallel spin, $(3*(+ J_z/4))$, and 2 adjacent pairs with antiparallel spins, $(2*(- J_z/4))$.

Whether the chain is open or closed can change the value of its energy. Consider the state $|101000\rangle$. If the chain is closed, it will have the same energy as the state $|010100\rangle$, because in both cases we count four pairs of antiparallel spins on neighboring sites, including the pair on sites 1 and 6, and two pairs of parallel spins. But in an open chain, the two states will have different energies. Because $|101000\rangle$ has three pairs with adjacent antiparallel spins and only two pairs with adjacent parallel spins, it will have an energy of $-J_z/4$, while $|010100\rangle$ has an energy of $-3J_z/4$ because it has four pairs with adjacent antiparallel spins and only one pair with adjacent parallel spins. This difference in energy between a state that has an up-spin, or excitation, on the border of an open chain, such as $|101000\rangle$, and a state that does not, such as $|010100\rangle$, is called the border effect.

Now let us focus on a system of L = 8 with $n_{up} = 2$. Using equation 4.2, the dimension is $\frac{8!}{2!6!}$ or 28. We can demonstrate the border effect by the creating histograms of the eigenvalues. If we fix $J_{xy} = 1$ and set $J_z = 10$, we get the following histograms. For the closed chain:

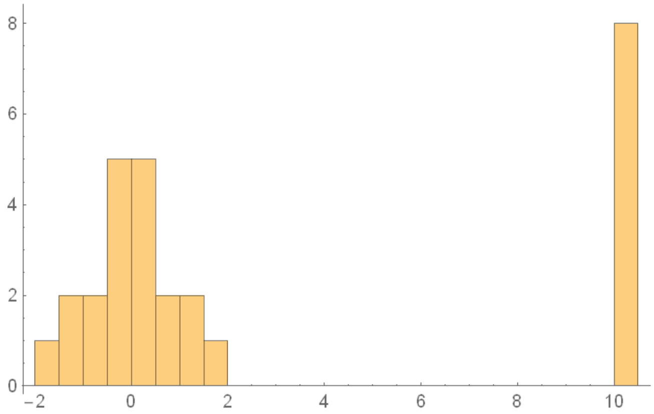


Figure 5.1: Histogram of the Energies of Heisenberg Model Closed Chain with $J_{xy} = 1$, $J_z = 10$, L = 8, and $n_{up} = 2$ (Arbitrary Units)

For the open chain:

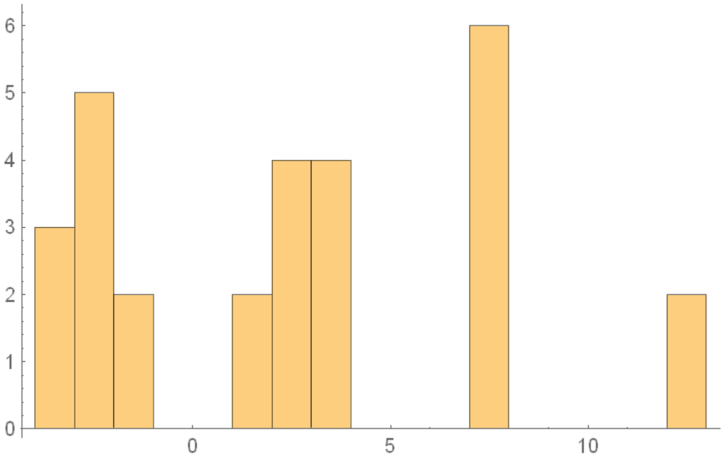


Figure 5.2: Histogram of the Energies of Heisenberg Model Open Chain with $J_{xy} = 1$, $J_z = 10$, L = 8, and $n_{up} = 2$ (Arbitrary Units)

Consistent with our discussion, the histogram of the closed chain has only two bands of energy, while for the open chain there are four bands because some states which have different energies in the open chain, for example $|10100000\rangle$ and $|01010000\rangle$, have the same energy when in a closed chain. In Figure 5.2, the four distinct bands of energy represent the four categories of energies that can result in the system we are studying. The first has an energy of $-J_z/4$. This is the energy of the state $|00100100\rangle$ or states similar to that with the up-spins not adjacent and neither one on the border. The next energy is $+J_z/4$. This results when the up-spins are not adjacent to each other and one of them is on the border. For example the state $|10010000\rangle$. When the 2 up-spins are adjacent to each other but not on the border, $|00110000\rangle$ for example, the energy that results is $+3J_z/4$. A special case where the up-spins are not adjacent to each other but still have this energy is the state $|10000001\rangle$, where the up-spins are on either end. This is due to the border effect. The last band of energy is $+5J_z/4$. This corresponds to the two states where the up-spins are adjacent and on the ends, either $|11000000\rangle$ or $|00000011\rangle$. Consistent with this discussion are equations 4.11 and 4.12. A pair of adjacent parallel spins has a higher energy than a pair of adjacent antiparallel spins. The two states that have an energy of $+5J_z/4$ are the states with the most adjacent pairs of parallel spins.

We now compare the histogram in Figure 5.2, where the value of J_z is large with respect to J_{xy}, with that of an open chain where the value of J_z is small, at 0.5. We get the following histogram for the eigenvalues:

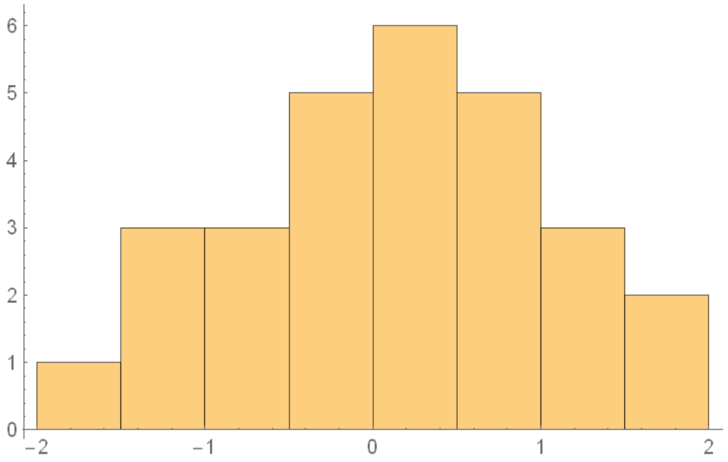


Figure 5.3: Histogram of the Energies of Heisenberg Model Open Chain with J_{xy} = 1, J_z = 0.5, L = 8, and n_{up} = 2 (Arbitrary Units)

From these figures, it is clear that when J_z is small there are no distinct energy bands, but when J_z is large, as in Figure 5.2, the histogram for the eigenvectors shows the different bands of energies. When J_z = 10, the energy difference between two of the bands is much greater than $J_{xy}/2$ and there is no overlap, causing the bands of energy to persist. When J_z = 0.5, the energy difference between the bands is small. It is clear on the histogram that the energy values are close to each other, and that is why no energy bands form.

5.2 Eigenstates

Now let us have a closer look at the eigenstates associated with the two scenarios of Figure 5.2 and Figure 5.3. The eigenstates or eigenvectors are denoted by $|\psi\rangle$. They are superpositions of the basis vectors, which are represented by $|basis_k\rangle$ where k goes from 1 to dim (dim being the dimension of the Hamiltonian matrix),

$$|\psi\rangle = \sum_{k=1}^{dim} C_k |basis_k\rangle. \quad (eqn\ 5.1)$$

A superposition indicates that more than one state, or basis vector, is available for the system at the same time. Before making a measurement, it is as if the system was simultaneously in all basis vectors. However, once a measurement is performed, the wave function collapses (as discussed in Sec.2) and the outcome is a single basis vector. The probability to get each basis vector is given by $|C_k|^2$. When L = 6 and n_{up} = 2, and thus dim = 15, the eigenstates are vectors with 15 numbers. Each number gives the probability of one basis vector, as shown in the list below.

$\vert C_1\vert^2$	$\vert 110000\rangle$		$\vert C_6\vert^2$	$\vert 011000\rangle$		$\vert C_{11}\vert^2$	$\vert 001010\rangle$
$\vert C_2\vert^2$	$\vert 101000\rangle$		$\vert C_7\vert^2$	$\vert 010100\rangle$		$\vert C_{12}\vert^2$	$\vert 001001\rangle$
$\vert C_3\vert^2$	$\vert 100100\rangle$		$\vert C_8\vert^2$	$\vert 010010\rangle$		$\vert C_{13}\vert^2$	$\vert 000110\rangle$
$\vert C_4\vert^2$	$\vert 100010\rangle$		$\vert C_9\vert^2$	$\vert 010001\rangle$		$\vert C_{14}\vert^2$	$\vert 000101\rangle$
$\vert C_5\vert^2$	$\vert 100001\rangle$		$\vert C_{10}\vert^2$	$\vert 001100\rangle$		$\vert C_{15}\vert^2$	$\vert 000011\rangle$

When two parallel spins-up are adjacent to each other, the pair is called a doublon. In the case of Figure 5.2, where $J_z > J_{xy}$ and the energy bands are formed, we see that the eigenstates are either superpositions of basis vectors that have a doublon or instead, superpositions where none of the basis vectors have a doublon. By that we mean the components $|C_k|^2$of the eigenstate in the first case are extremely small for any basis vector that does not have a doublon, while for the second case they are approximately zero for the basis vectors with a doublon. Examples of each of these two eigenstates are shown below for L = 6 and n_{up} = 2.

First, we show an eigenstate with corresponding eigenvalue 2.52481, which is very close to $+J_z/4$ when $J_z = 10$ and $J_{xy} = 1$. The energy $+J_z/4$ is that of the basis vectors with a doublon away from the borders, such as $|011000\rangle$. We see that only basis vectors $|011000\rangle$, $|001100\rangle$, and $|000110\rangle$ contribute to the eigenstate.

1.6542×10^{-5}	$\|110000\rangle$		0.1671	$\|011000\rangle$		4.0742×10^{-4}	$\|001010\rangle$
0.001638	$\|101000\rangle$		4.0742×10^{-4}	$\|010100\rangle$		4.0743×10^{-6}	$\|001001\rangle$
4.0743×10^{-6}	$\|100100\rangle$		4.0541×10^{-6}	$\|010010\rangle$		0.1671	$\|000110\rangle$
2.7458×10^{-14}	$\|100010\rangle$		2.7458×10^{-14}	$\|010001\rangle$		0.001638	$\|000101\rangle$
4.4596×10^{-11}	$\|100001\rangle$		0.6617	$\|001100\rangle$		1.6542×10^{-5}	$\|000011\rangle$

The second studied eigenstate has a corresponding eigenvalue -6.91082 which is close to $-3J_z/4$, when Jz = 10 and Jxy = 1. The energy $-3J_z/4$ is that of a basis vector without a doublon and without an up-spin on any edge, such as $|010100\rangle$. We see that only basis vectors $|010100\rangle, |010010\rangle, and\ |001010\rangle$ contribute to the eigenstate.

8.6790×10^{-8}	$\|110000\rangle$		7.0425×10^{-4}	$\|011000\rangle$		0.241074	$\|001010\rangle$
7.2095×10^{-5}	$\|101000\rangle$		0.2411	$\|010100\rangle$		0.002311	$\|001001\rangle$
0.002311	$\|100100\rangle$		0.4975	$\|010010\rangle$		7.0425×10^{-4}	$\|000110\rangle$
0.005688	$\|100010\rangle$		0.005688	$\|010001\rangle$		7.2095×10^{-5}	$\|000101\rangle$
6.4220×10^{-5}	$\|100001\rangle$		0.002722	$\|001100\rangle$		8.6790×10^{-8}	$\|000011\rangle$

These two distinct kinds of eigenstates are a consequence of the energy difference between basis vectors with or without a doublon, as discussed in Sec.5.1. If $J_z > J_{xy}$, the flip-flop term is not strong enough to couple basis vectors that have different energies. In contrast, when $J_z < J_{xy}$ as in Figure 5.3, all basis vectors can mix and we get eigenstates such as the one below.

Now we consider $J_z = 0.5$ and $J_{xy} = 1$. We select an eigenstate with corresponding eigenvalue 1.35198. Now we see equivalent contributions to the eigenstate from almost all basis vectors, the ones that have a doublon as well as the ones without.

0.01071	$\vert 110000\rangle$		0.04597	$\vert 011000\rangle$		0.1049	$\vert 001010\rangle$
0.04090	$\vert 101000\rangle$		0.1049	$\vert 010100\rangle$		0.07810	$\vert 001001\rangle$
0.07810	$\vert 100100\rangle$		0.1303	$\vert 010010\rangle$		0.04597	$\vert 000110\rangle$
0.08964	$\vert 100010\rangle$		0.08964	$\vert 010001\rangle$		0.04090	$\vert 000101\rangle$
0.05954	$\vert 100001\rangle$		0.06969	$\vert 001100\rangle$		0.01071	$\vert 000011\rangle$

6. Dynamics

Now that we know the eigenvalues and eigenvectors we can use this information to predict the dynamics. We start with one of the basis vectors as the initial state. Over time, the state will evolve, because it is not an eigenstate of the Hamiltonian, so it is not a stationary state. To describe the evolution, we first project our initial state $|\Psi(0)\rangle = |basis_k\rangle$ into the eigenstates $|\psi_\alpha\rangle$ of the total Hamiltonian, so that

$$|\Psi(0)\rangle = \sum c_\alpha \, |\psi_\alpha\rangle \, ,$$

where $c_\alpha = \langle \psi_\alpha | \Psi(0) \rangle$ We can have the evolution of the initial state by adding to each term above the phase $e^{-iE_\alpha t}$.

$$|\Psi(t)\rangle = \sum c_\alpha \, e^{-iE_\alpha t} |\psi_\alpha\rangle \quad (eqn\ 6.3)$$

The orientations of the spins in the different sites in the system will change, causing a different state than the original one to be present. The dynamics are strongly dependent on the ratio between J_z and J_{xy} and again we identify two different cases, when $J_z > J_{xy}$ and when $J_z < J_{xy}$.

6.1 Case where $J_z > J_{xy}$

When J_z is larger than J_{xy}, states with a doublon have significantly larger energy than states without a doublon. Therefore if there is a doublon in the initial state, the doublon will hop to different sites without separating. If the initial state is basis 14, $|00110000\rangle$, over time it can have a significant probability for being in state $|01100000\rangle$, but the probability of it becoming $|01010000\rangle$ is very low.

Using the Mathematica program we can calculate the probabilities of the different states over time and graph them. Such graphs are shown in Figures 6.1-6.3. The probabilities of the three states shown in Figure 6.1 are high. This is because the initial state, $|00110000\rangle$, has a doublon and so do the other two. In Figure 6.2 however, we start with the same initial state, but the other two states do not have a doublon, instead the two up-spins are not adjacent. The probability of either of those states is very low and therefore is not visible on the graph in Figure 6.2. In Figure 6.3, we zoom in on Figure 6.2 and see just how small the probability for each of those states is, the highest either one reaches is 0.003.

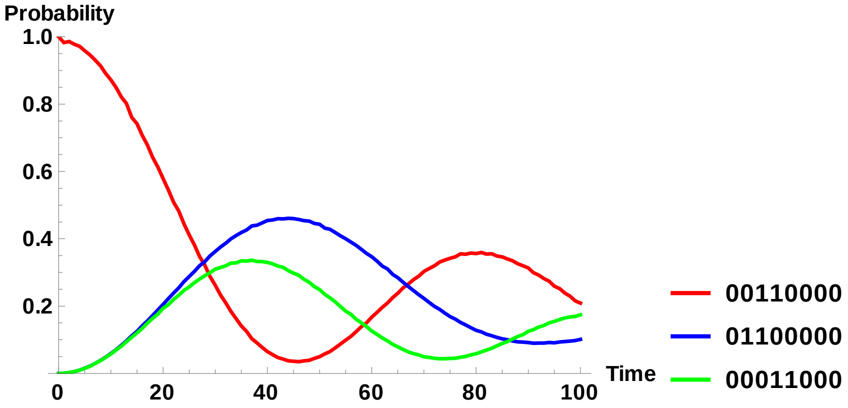


Figure 6.1: Probabilities of some basis vectors over time in an open chain with $J_{xy} = 1$, $J_z = 10$, $L = 8$, $n_{up} = 2$, and initial state $|00110000\rangle$ (Arbitrary Units)

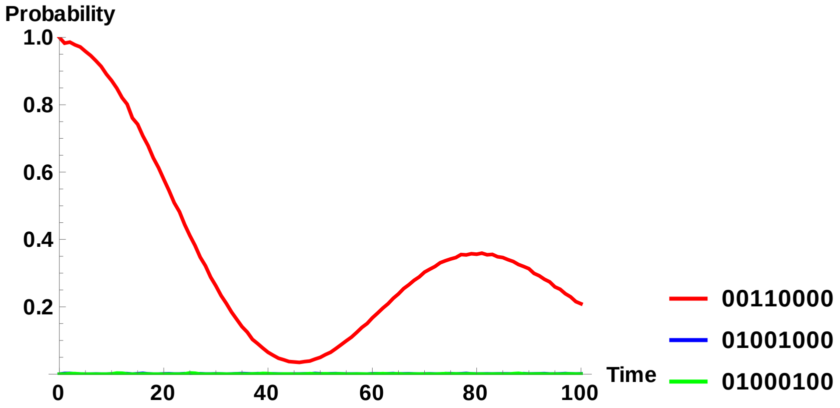


Figure 6.2: Probabilities of some basis vectors over time in an open chain with $J_{xy} = 1$, $J_z = 10$, $L = 8$, $n_{up} = 2$, and initial state $|00110000\rangle$ (Arbitrary Units)

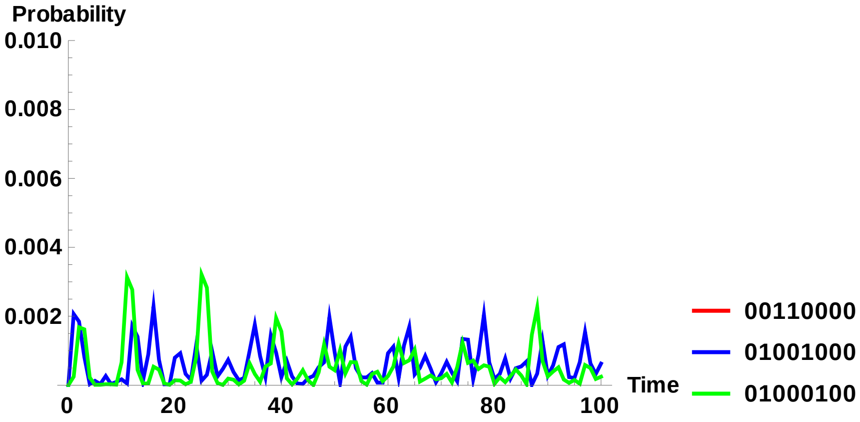


Figure 6.3: Probabilities of some basis vectors over time in an open chain with J_{xy} = 1, J_z = 10, L = 8, n_{up} = 2, and initial state $|00110000\rangle$ (Arbitrary Units)

As discussed in Sec 5.1, due to the border effect in an open chain, the state $|11000000\rangle$ has a greater energy than the state $|00110000\rangle$ and there is only one other state with that same energy, $|00000011\rangle$. This is demonstrated in Figure 6.4. When the initial state is $|11000000\rangle$, the graph of the probabilities of different states in time only has two visible curves, and no others.

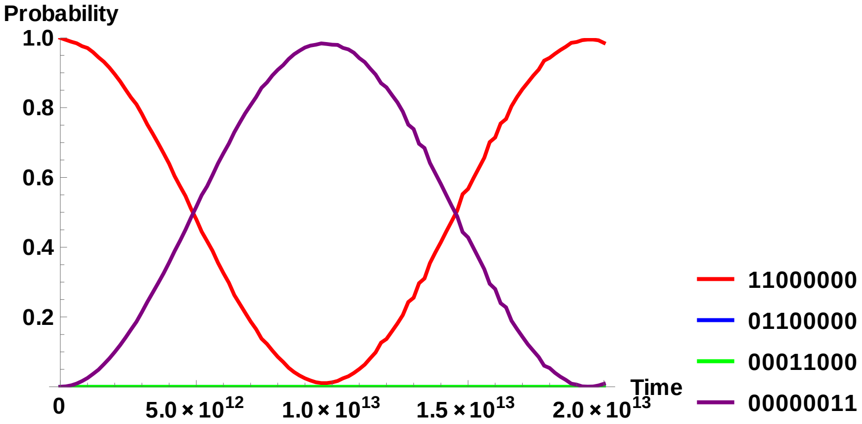


Figure 6.4: Probabilities of some basis vectors over time in an open chain with J_{xy} = 1, J_z = 0.5, L = 8, n_{up} = 2, and initial state $|11000000\rangle$ (Arbitrary Units)

On the other hand, Figure 6.5 shows that in a closed chain with the same initial state, every state with a doublon will participate and will have a significant probability.

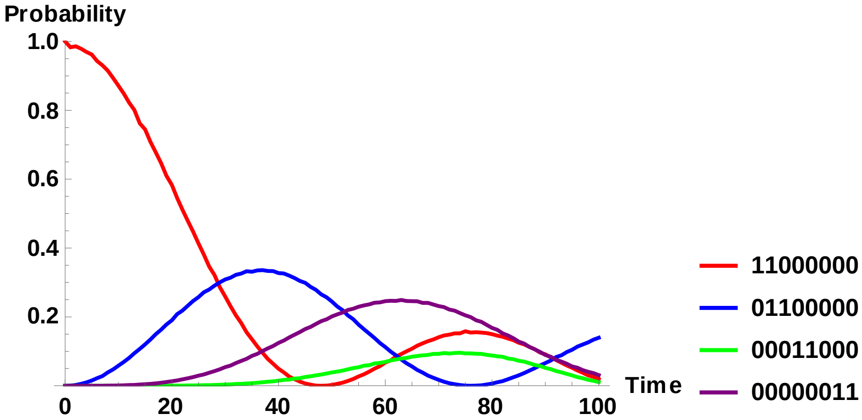


Figure 6.5: Probabilities of some basis vectors over time in a closed chain with $J_{xy} = 1$, $J_z = 10$, $L = 8$, $n_{up} = 2$, and initial state |11000000⟩ (Arbitrary Units)

6.2 Case where $J_z < J_{xy}$

When J_z is smaller than J_{xy}, the difference in energy between states with and without a doublon is small. If we begin with the same state as before, basis 14, |00110000⟩, we get a different result. Over time, many states will participate, not just the other states that have a doublon. As shown in Figure 6.6, the other states that have a doublon have smaller probabilities than they did in the open chain because there are other additional states that are participating, as seen in Figure 6.7.

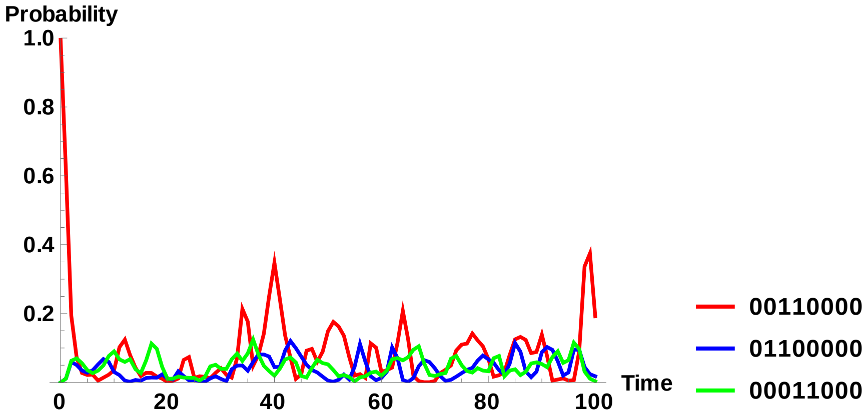


Figure 6.6: Probabilities of some basis vectors over time in an open chain with J_{xy} = 1, J_z = 0.5, L = 8, n_{up} = 2, and initial state |00110000⟩ (Arbitrary Units)

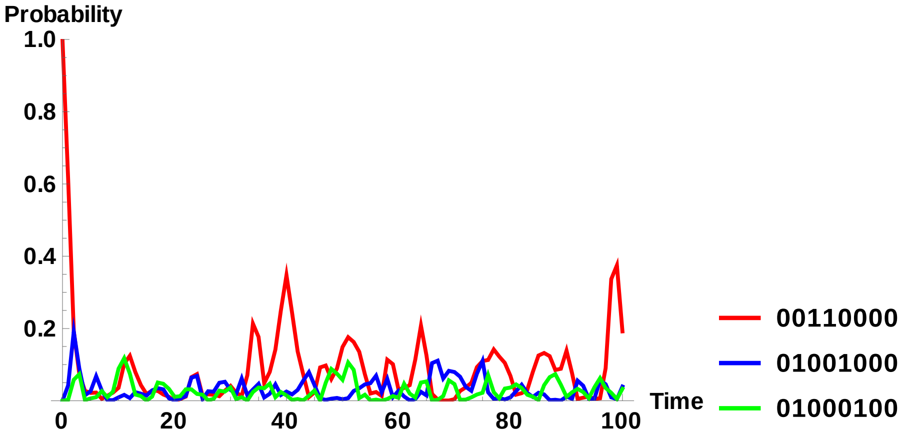
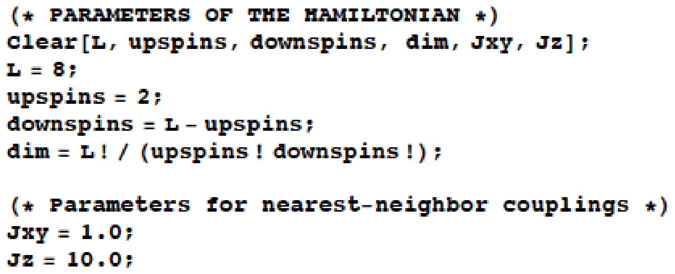


Figure 6.7: Probabilities of some basis vectors over time in an open chain with J_{xy} = 1, J_z = 0.5, L = 8, n_{up} = 2, and initial state |00110000⟩ (Arbitrary Units)

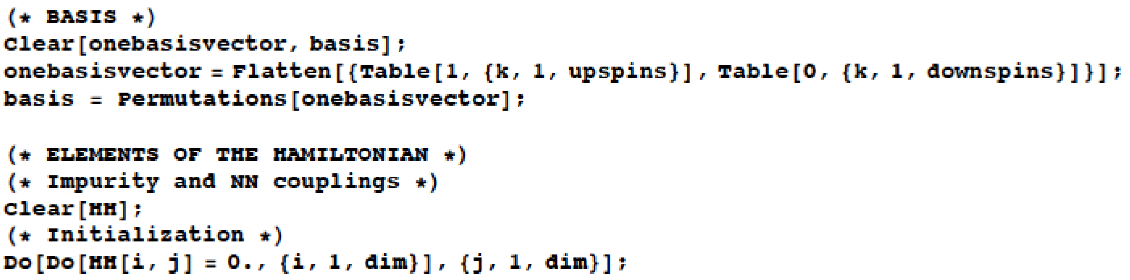
7. Instructions for Writing the Computer Codes

I show below pieces of the computer code used to obtain the results presented in this thesis.

- Definition of the parameters and basis, and initialization of the elements of the Hamiltonian matrix:

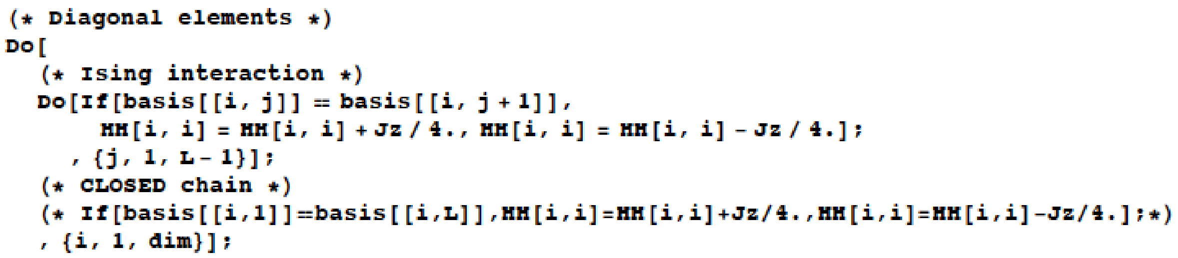


```
(* PARAMETERS OF THE HAMILTONIAN *)
Clear[L, upspins, downspins, dim, Jxy, Jz];
L = 8;
upspins = 2;
downspins = L - upspins;
dim = L! / (upspins! downspins!);

(* Parameters for nearest-neighbor couplings *)
Jxy = 1.0;
Jz = 10.0;
```



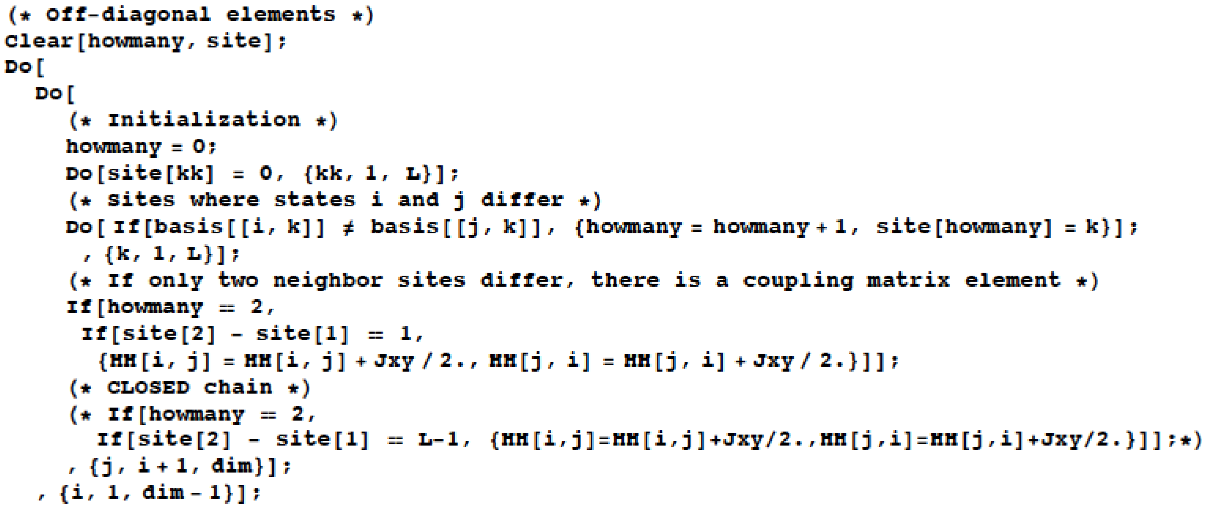
```
(* BASIS *)
Clear[onebasisvector, basis];
onebasisvector = Flatten[{Table[1, {k, 1, upspins}], Table[0, {k, 1, downspins}]}];
basis = Permutations[onebasisvector];

(* ELEMENTS OF THE HAMILTONIAN *)
(* Impurity and NN couplings *)
Clear[HH];
(* Initialization *)
Do[Do[HH[i, j] = 0., {i, 1, dim}], {j, 1, dim}];
```

- How to obtain the diagonal elements of the Hamiltonian matrix: As it is, the chain considered is open. If the reader would like to study a closed chain, he/she needs to remove the part that is commented out with “(*…*)”



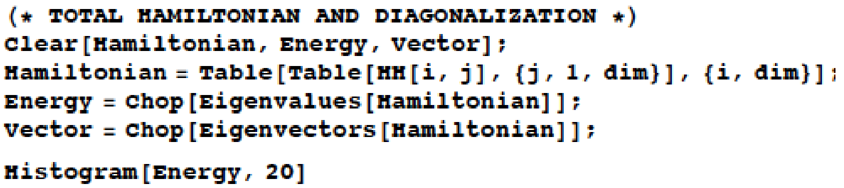
```
(* Diagonal elements *)
Do[
  (* Ising interaction *)
  Do[If[basis[[i, j]] == basis[[i, j + 1]],
       HH[i, i] = HH[i, i] + Jz / 4., HH[i, i] = HH[i, i] - Jz / 4.];
    , {j, 1, L - 1}];
  (* CLOSED chain *)
  (* If[basis[[i,1]]==basis[[i,L]],HH[i,i]=HH[i,i]+Jz/4.,HH[i,i]=HH[i,i]-Jz/4.];*)
  , {i, 1, dim}];
```

- How to obtain the off-diagonal elements of the Hamiltonian matrix: As it is, the chain considered is open. If the reader would like to study a closed chain, he/she needs to remove the part that is commented out with “(*…*)”



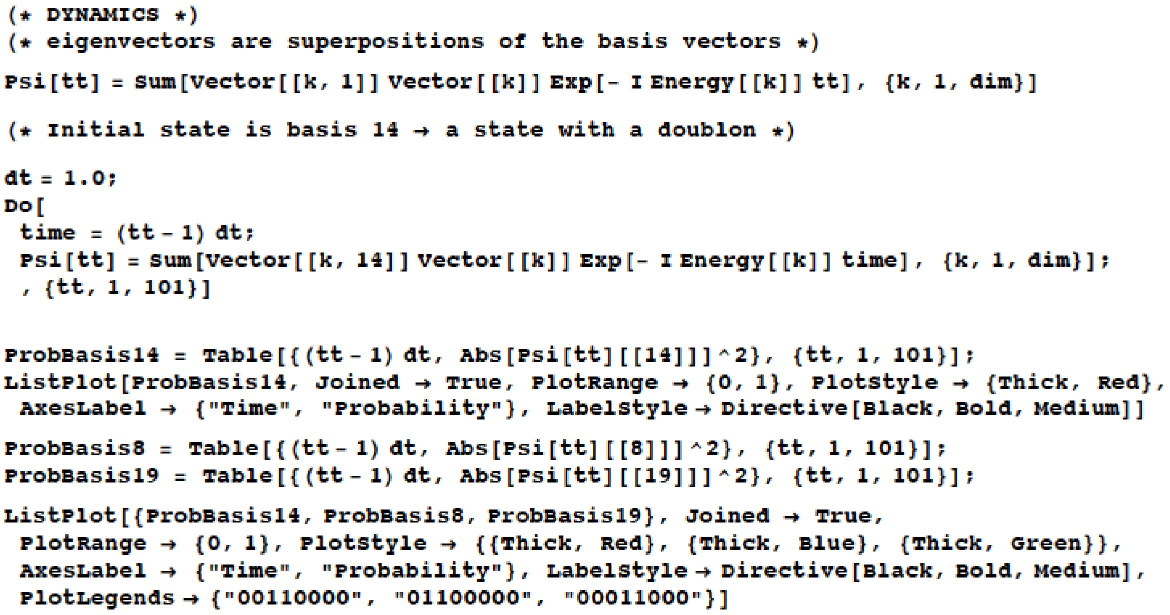
```
(* Off-diagonal elements *)
Clear[howmany, site];
Do[
  Do[
    (* Initialization *)
    howmany = 0;
    Do[site[kk] = 0, {kk, 1, L}];
    (* Sites where states i and j differ *)
    Do[ If[basis[[i, k]] ≠ basis[[j, k]], {howmany = howmany + 1, site[howmany] = k}];
     , {k, 1, L}];
    (* If only two neighbor sites differ, there is a coupling matrix element *)
    If[howmany == 2,
     If[site[2] - site[1] == 1,
      {HH[i, j] = HH[i, j] + Jxy / 2., HH[j, i] = HH[j, i] + Jxy / 2.}]];
    (* CLOSED chain *)
    (* If[howmany == 2,
      If[site[2] - site[1] == L-1, {HH[i,j]=HH[i,j]+Jxy/2.,HH[j,i]=HH[j,i]+Jxy/2.}]];*)
    , {j, i + 1, dim}];
  , {i, 1, dim - 1}];
```

- Diagonalization and histogram of the eigenvalues:



```
(* TOTAL HAMILTONIAN AND DIAGONALIZATION *)
Clear[Hamiltonian, Energy, Vector];
Hamiltonian = Table[Table[HH[i, j], {j, 1, dim}], {i, dim}];
Energy = Chop[Eigenvalues[Hamiltonian]];
Vector = Chop[Eigenvectors[Hamiltonian]];

Histogram[Energy, 20]
```

- Evolution of the initial state and how to make the plots for the probability in time of some of the basis vectors:



```
(* DYNAMICS *)
(* eigenvectors are superpositions of the basis vectors *)

Psi[tt] = Sum[Vector[[k, 1]] Vector[[k]] Exp[- I Energy[[k]] tt], {k, 1, dim}]

(* Initial state is basis 14 → a state with a doublon *)

dt = 1.0;
Do[
 time = (tt - 1) dt;
 Psi[tt] = Sum[Vector[[k, 14]] Vector[[k]] Exp[- I Energy[[k]] time], {k, 1, dim}];
 , {tt, 1, 101}]


ProbBasis14 = Table[{(tt - 1) dt, Abs[Psi[tt][[14]]]^2}, {tt, 1, 101}];
ListPlot[ProbBasis14, Joined → True, PlotRange → {0, 1}, PlotStyle → {Thick, Red},
 AxesLabel → {"Time", "Probability"}, LabelStyle → Directive[Black, Bold, Medium]]

ProbBasis8 = Table[{(tt - 1) dt, Abs[Psi[tt][[8]]]^2}, {tt, 1, 101}];
ProbBasis19 = Table[{(tt - 1) dt, Abs[Psi[tt][[19]]]^2}, {tt, 1, 101}];

ListPlot[{ProbBasis14, ProbBasis8, ProbBasis19}, Joined → True,
 PlotRange → {0, 1}, PlotStyle → {{Thick, Red}, {Thick, Blue}, {Thick, Green}},
 AxesLabel → {"Time", "Probability"}, LabelStyle → Directive[Black, Bold, Medium],
 PlotLegends → {"00110000", "01100000", "00011000"}]
```

8. Conclusions

This thesis has demonstrated some of the dynamics of interacting particles in a quantum system. We have seen that when the strength of the Ising interaction, Jz, is stronger than the strength of the flip-flop term, the states with a doublon have higher energies than states without a doublon. Therefore if the initial state has a doublon, over time only other states with a doublon will have significant probabilities. However, when the interaction is weak, the energy difference between basis vectors with and without a doublon is smaller and all states will participate on the evolution regardless whether or not they have a doublon.

In the case of strong Ising interaction, we have also observed differences between open and closed chains. In an open chain, a state with a doublon on the border has a higher energy than a state where the doublon is not on the border. This is called the border effect. As a result, if the initial state has a doublon on the border, the only other state that will participate in the dynamics is when the doublon is on the other border. If the initial state has a doublon that is not on the border, only the other states with a doublon not on the border will participate. In a closed chain on the other hand, there are only 2 different energy values. The states with a doublon have a higher energy than those without. Since all states with a doublon have the same energy regardless of its location, if the initial state has a doublon, all other states with a doublon will participate, whether or not it is located on the border.

All the results found for the dynamics were anticipated by first studying the static properties of the system. The dynamics of many-body quantum systems is currently a subject of intense investigation due to remarkable experimental developments that allow systems isolated from the environment, as the one treated here, to be tested in the lab.

Acknowledgements

I would like to thank Dr. Lea Ferreira dos Santos, Professor of Physics at Stern College for Women, for mentoring me through the process of writing this thesis. Over the last year and a half she has consistently guided me with patience and kindness. I am fortunate to have had the opportunity to work with such a knowledgeable and generous professor whom I regard as a role model. I would also like to thank the S. Daniel Abraham Honors program for providing me with the opportunity of writing this thesis and for allowing me to participate in this program.

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