

Stability of Doublons

Presented to the S. Daniel Abrahams Honors Program
in Partial Fulfillment of the
Requirements for Completion of the Program

Stern College for Women
Yeshiva University
May 22, 2020

Miriam Baitner

Mentor: Professor Lea F. Santos, Physics

Abstract

In this thesis, I discuss my research of the behavior and stability of doublons. I describe the dynamics of a one-dimensional closed chain of spins $\frac{1}{2}$. I show that by analyzing the eigenstates and eigenvalues of the Hamiltonian that describes the system, I can predict its dynamics. In the presence of strong interactions between the particles in the chain, particles can bind in pairs of excitations forming what is known as doublons. These doublons are very stable and they move together as a single particle, but contrary to it, doublons move slowly.

Doublons were observed experimentally by many different physicists with cold atoms. In those experiments, because of strong on-site interactions between atoms, they would see sites that were doubly occupied, which is how the term “doublon” was coined. These doublons could move to other sites, but they always moved together as a bounded pair. They were never found to be split up with one in each site, they always moved together. In my thesis, the doublons are equivalent to bounded pairs of neighboring excitations in a chain instead of pairs of atoms.

I. Quantum Mechanics

The mystery behind quantum mechanics is one that has been studied for many years, each experiment leading to even bigger and more innovative discoveries. The discussion of quantum mechanics began way back in the 1800’s in the industrial revolution. While working on building more efficient engines, engineers and other workers noticed that when the engines became very hot, they would start radiating. Thermal radiation was then born, and it was discovered that electrons emit radiation when they start moving at higher frequencies, which means more oscillations. In order to better understand the properties of thermal and electromagnetic radiation, the universal ideal mathematical body called the

blackbody was created. The blackbody absorbs all thermal radiation sent to it and does not reflect radiation, it only emits, and it depends only on temperature. The blackbody spectrum cannot be understood based on classical arguments, and physicists Wilhelm Wien, Josef Stefan, and Ludwig Boltzmann came up with different equations and constants in order to explain the spectral distribution of blackbody radiation. While trying to create a formula for blackbody radiation, scientists Rayleigh and Jeans accidentally discovered the ultraviolet catastrophe. Using the classical equipartition law, $\bar{E} = kT$, they predicted that the blackbody radiation should never diverge, and frequency should increase with radiation. However, their experimental results showed that it diverges with high frequency. Max Planck solves this issue with equation $E = nh\nu$ (using his constant h) which proves that energy is quantized. This concept has become one of the most basic principles of quantum physics. While Planck proved energy quantization for blackbody, Einstein extended this idea through the photoelectric effect and said that energy is quantized into lumps, which brought about the idea that light is composed of particles called photons.

One scientist who analyzed the behavior of particles and photons was Louis de Broglie, who studied the wave-like properties of particles and discovered the wave-particle duality. He did multiple experiments with some resulting in electrons behaving like particles and others with results showing that electrons behave like waves. Each experiment only gave one result and in a given measurement, only one model applies as to whether the electron behaves like a particle or wave. When the entity being studied was detected by some interaction with matter, it acted like a particle and was localized. When it moved or propagated, it behaved like a wave and it showed interference and was not localized.

The role of Quantum Mechanics was to resolve the continuous confusion of how things really behave. However, nobody really fully understands Quantum Mechanics, and the bottom line is that electrons and other like particles behave in their own unique way, which turns out to be both like particles and like waves. Physicist Richard Feynman describes several theoretical experiments, which help to explain the behavior of electrons. [1]

A. The Bullet Experiment

There was a famous thought experiment conducted involving two holes in order to prove the wave-particle duality and the mysterious nature of electrons, which became the basis for the theory of Quantum Mechanics. In the first part of the experiment, scientists tried to describe the behavior of particles by comparing it to the behavior of bullets. In this theoretical experiment, there was a machine gun that shot bullets from a distance to a plate with two slits, and a detector that counted the bullets passing through. It was determined that the bullets detected arrived in “lumps”, meaning that bullets equal in size either arrived or didn’t arrive in the detector or box, they never arrived in pieces. Furthermore, the bullets were only able to go through one hole at a time, so if one hole was closed it would only go through the other one. As the distance “x” from the center is varied, the amount of bullets that arrive also vary. The probability of arrival, the average number of bullets that arrive in a given length of time, was also measured using the sum of P1 (the probability of bullets entering hole 1 if hole 2 is closed) and P2 (the probability of bullets entering hole 2 if hole 1 is closed). These results are plotted on a graph showing two peaks, for P1 and P2, as seen in Figure 1b. The graph of P12 is interpreted as being the sum of two curves, $P_{12}=P_1+P_2$, implying that there is no interference, which means that the probability of arrival from two holes being open is the same as what you would get when you add each hole separately.

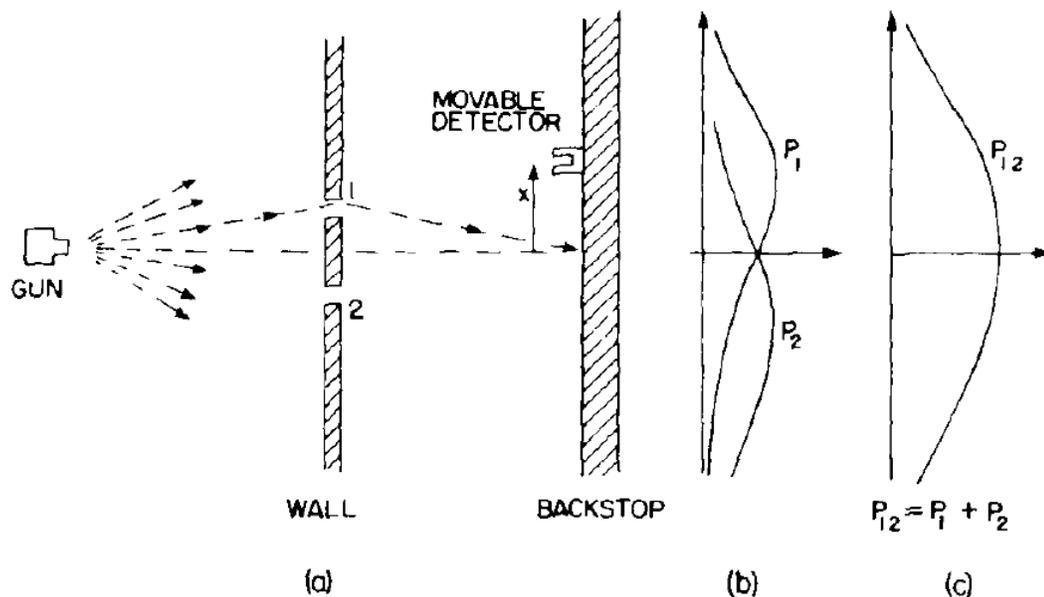


Figure 1: Experiment with bullets

B. The Wave Experiment

Then, there was a similar experiment done to determine the behavior of waves. Instead of bullets, there were waves released from a source to a wall with two holes and a detector behind the wall. This time however, instead of the detector measuring the amount of waves coming through, it measured the intensity of the waves coming through, which was the rate of energy generated by the waves at a certain point. It is important to note that the waves were able to come in any size and did not arrive in lumps like the bullets. The more ripples and motion in the wave, the higher the intensity would be. When one hole was closed, the result was similar to that of the bullet experiment and there was a simple peak at a point where the wave was most intense. The intensity of the waves is denoted as I_1 (when hole 2 is closed) and I_2 (when hole 1 is closed). However, when both holes were open, the result was not as a simple unified peak like that of the previous experiment. There is interference between the two waves when both holes are open and I_{12} (the intensity when both holes are

open) is not a sum of I_1 and I_2 , but rather forms a symmetrical curve with many peaks, as seen in Figure 2. When the two waves were released, they would reach a certain point at the same time and overlap, thus more ripples were formed resulting in a higher intensity at those points where they interacted. This interaction of the waves is known as interference. A peak of the I_{12} curve is referred to as the waves being “in phase”, where the amplitude and therefore intensity is very high, also known as constructive interference. On the other hand, destructive is when the curve of I_{12} is at a minimum, where the waves are “out of phase” and the intensity is very low. It was determined that the intensity is proportional to the square of the amplitude or height, which is why the graph of I_{12} looked so different than that of P_{12} .

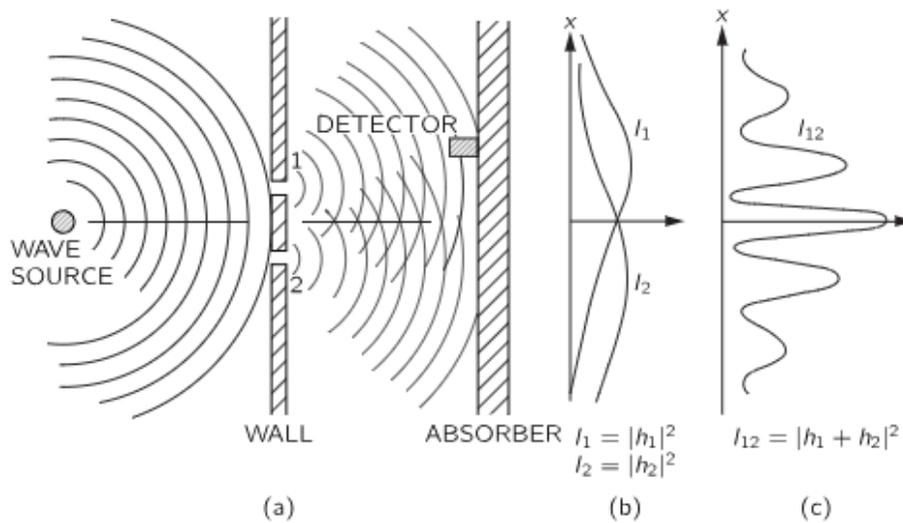


Figure 2: Experiment with waves

C. Experiment with Electrons

The final theoretical experiment was of the same nature as the first two, but with electrons. This time the source was an electron gun, which shot electrons to a wall with two holes in it, and a detector behind the wall. This detector is connected to a loudspeaker, so that every time an electron is detected a loud “click” is heard. The first thing the results showed is

that there are no “half-clicks”, every “click” is exactly the same. The clicks never changed size, or loudness, but the rate at which they were heard was able to change. If there were two detectors present, there would never be two clicks heard at the same time. Therefore, it was concluded that an electron will come in lumps because it has a definite size and it only arrives at one place at one time. When the probability of arrival was measured, which is the average rate of electrons coming in per hour, the result was the I12 graph as seen with the wave experiment, which indicates that there is some sort of interference. This seems to imply that the electron bullet could go through two holes at once, like the waves.

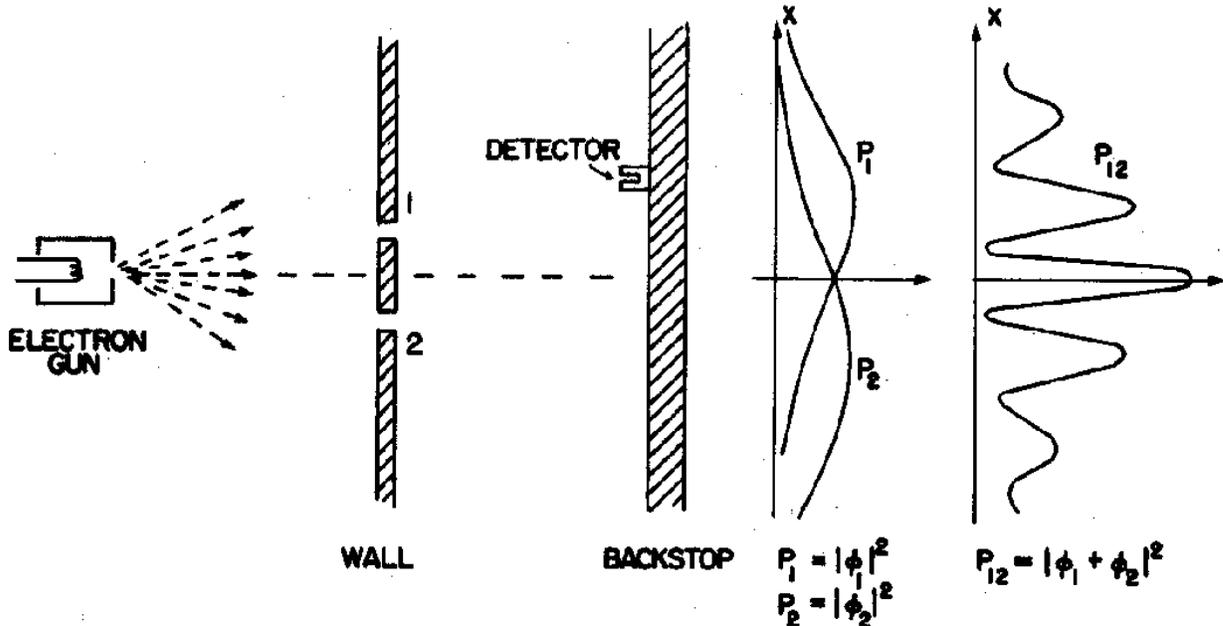


Figure 3: Experiment with electrons

The results of this experiment are confusing. It was determined first that electrons arrive in lumps like a particle but the probability of arrival of those lumps is determined like the intensity of waves. Is it possible that an electron can sometimes behave like a particle and other times like a wave?

In order to reduce the confusion, they investigated only Proposition A: that either the electron goes through hole 1 or hole 2. They added in a source of light so that every time an electron passed, a complete flash would be seen either behind hole 1 or hole 2 in addition to the “click” heard, but never behind both at one instant. The result here is surprising. With the light source on, the graph of probability of arrival becomes the P12 graph for the particles and it can be concluded that an electron behaves like a particle. But when the light source is turned off, the results show that the electron behaves like a wave!

To investigate this disparity, it is considered that perhaps the light affects the behavior of the electron. As the light is turned down and the intensity is lowered, the size of the photons does not change at all, only the amount of photons being released is reduced.

Without being able to see which hole the electron is going through (i.e. without a light source), the result is the intensity graph found in the wave experiment, and with the ability to see which hole the electron is going through, the resulting graph is that of the bullets.

The conclusion of the experiment is then that it is impossible to predict ahead of time which hole the electron will go through without destroying the interference pattern. This conclusion is supported by Heisenberg’s uncertainty principle, which states that the location and momentum of a particle cannot be determined at the same time.

II. Probabilistic Nature of Quantum Particles

In classical mechanics, in order to determine the location of a particle at a given time, Newton’s second law $F=ma$ is applied. Quantum mechanics however functions based on probability because both the momentum and location are not able to be determined with infinite precision at the same time. Instead of looking for $x(t)$, we are trying to find the wave

function, $\Psi(x,t)$, of the particle. Just as in classical mechanics, $x(t)$ is found using Newton's second law, in quantum mechanics, the wave function is found using Schrödinger's equation:

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

Here, i is $\sqrt{-1}$ and \hbar is Planck's constant h divided by 2π :

$$\hbar = \frac{h}{2\pi} = 1.054573 \times 10^{-34} \text{ Js (eqn. 2).}$$

As we have already established, finding the position of a particle is based on probability. The probability that a particle will be found at a certain location x at a certain time t , also known as probability density, is used to describe the state of the particle:

$$|\Psi(x, t)|^2 dx \text{ (eqn 3).}$$

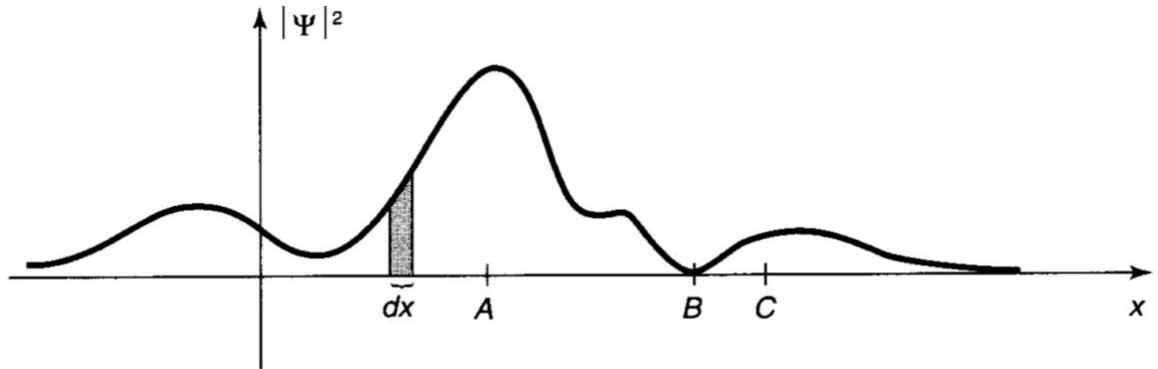


Figure 4: A wave function. There is a peak at point A and a minimum at B, showing that the particle is more likely to be found at point A than at point B. The shaded region dx shows the probability of finding the particle in that particular range.

The particle can be found anywhere along this wave function, but there is a much higher probability of the particle being found at point A than at point B. The wave function is simply providing all *possible* locations of the particle.

Though only the probability density is being measured, the particle still must be somewhere, which means that the wave function must be normalized:

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1 \text{ (eqn. 4).}$$

III. Stationary States

We have discovered the wave function and know that finding it will help us describe our system. Now we need to solve the Schrödinger equation to find $\Psi(x, t)$, and in order to do so we must use separation of variables so that lowercase ψ will be a function of x and f will be a function of t :

$$\Psi(x, t) = \psi(x)f(t).$$

Next, we separate the solutions and we get:

$$\frac{\partial \Psi}{\partial t} = \psi \frac{df}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} f$$

so when substituting these solutions back into the Schrödinger equation (eqn. 1), the equation then becomes:

$$i\hbar \psi \frac{df}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} f + V\psi f.$$

This equation can be further simplified by dividing everything by ψf :

$$i\hbar \frac{1}{f} \frac{df}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2 \psi}{dx^2} + V \text{ (eqn. 5).}$$

With this alteration of the Schrödinger equation, it is evident that the left side of the equation is solely a function of t and the right side is only a function of x , which can only be true if both sides are constant. So, we will call the right side, constant E and rewrite the equation:

$$i\hbar \frac{1}{f} \frac{df}{dt} = E,$$

which can also be written as,

$$\frac{df}{dt} = -\frac{iE}{\hbar} f \text{ (eqn. 6).}$$

We can also equate constant E to the right side of equation 5

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V = E,$$

and if you multiply everything by ψ , the result is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \text{ (eqn. 7).}$$

We have now transformed the original partial differential equations into two separate ordinary differential equations (Equations 6 and 7), which will help to more easily solve the Schrödinger equation. The first equation (Equation 6) can be solved easily by multiplying everything by dt and integrating, resulting in

$$f(t) = e^{-\frac{iEt}{\hbar}} \text{ (eqn. 8).}$$

The other equation is known as the time-independent Schrödinger equation, and in order to solve that, we need to find the potential V . To find the potential, we turn to classical mechanics, which tells us that the Hamiltonian is the observable which corresponds to the total energy of the system, kinetic plus potential:

$$H(x, p) = \frac{p^2}{2m} + V(x) \text{ (eqn. 9).}$$

To translate to quantum mechanics, we substitute p for $(\hbar/i)(\partial/\partial x)$ and we get

$$H = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x) \text{ (eqn. 10)}$$

which turns out to be exactly Equation 7, so we can equate the two and reduce the time-independent Schrödinger equation:

$$H\psi = E\psi \text{ (eqn. 11).}$$

The time-independent Schrödinger equation can now be solved using separation constant E which will yield the solutions needed to describe the system. One of the benefits of the separable solutions we found is that through linear combinations, an infinite number of solutions can be found ($\psi_1, \psi_2, \psi_3 \dots$) for each corresponding separation constant ($E_1, E_2, E_3 \dots$).

Additionally, we know through the separable solutions that the states we are describing from the time-independent Schrödinger equation are stationary states. Clearly, the wave function depends on t ,

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar} \text{ (eqn. 12)}$$

but the probability density does not because the time dependence cancels out

$$|\Psi(x, t)|^2 = \Psi^*\Psi = \psi^*e^{+iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2 \text{ (eqn. 13).}$$

Any non-stationary state that does change in time is considered to be dynamic. Now that we have learned about stationary states, we can discover more about the dynamics of non-stationary states.

IV. Spin- $\frac{1}{2}$ System

Many concepts in quantum mechanics stem from classical mechanics, and one of these concepts is what is known as the spin of a particle. Every object in classical mechanics has two types of momentum; orbital angular momentum and spin angular momentum, which seem very similar, but they have a key difference. Orbital momentum has to do with the motion of the center of mass, which can be seen in the earth's revolution around the sun. Spin on the other hand is the motion about the center of mass, which is related to the earth's rotation about its axis. In quantum mechanics, the concept is similar. There is both orbital momentum, which is associated with the electron orbiting around the nucleus, and also spin, which is different from the classical spin. The orbital and spin angular momentum of particles are otherwise known as extrinsic angular momentum and intrinsic angular momentum, respectively.

Every type of particle has a different fixed spin. For example, photons have a spin of 1 while electrons have a spin of $\frac{1}{2}$. The system that I am studying is a one-dimensional chain of spins $\frac{1}{2}$. In a system of spins $\frac{1}{2}$, there are only two basis vectors; spin up, indicated by vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and arrow $|\uparrow\rangle$, and spin down, indicated by vector $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and arrow $|\downarrow\rangle$. There are also spin operators, and in the case of spin $\frac{1}{2}$, they are known as the Pauli spin matrices:

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

As is evident here, the x and y matrices have off-diagonal elements, while the z matrix has diagonal elements. Each Pauli matrix has its own function and will be used in the Hamiltonian used to describe the spin $\frac{1}{2}$ system, which I will explain shortly.

In a chain with spins $\frac{1}{2}$, we assume that there is a strong magnetic field pointing down in the z direction, so the spins will either point up and be antiparallel to the field or be pointing down parallel to the field. Each up spin is therefore what we will refer to as an excitation. Interactions can occur between neighboring sites and as a result, the excitation can hop to the neighboring site on the right or the left.

The one-dimensional chain can be an open chain with open boundaries or a closed or periodic chain with closed boundaries, which has a ring structure (as seen in Figure 5).

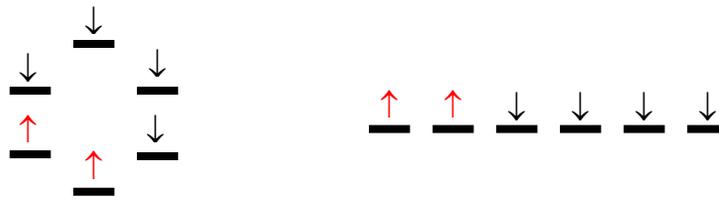


Figure 5: Left: Closed chain, Right: Open chain. Red arrows denote excitations.

We will be focusing only on a closed chain, which means that because of the ring structure, the first and last sites of the chain can also interact, and the excitation can move between those two sites if interaction occurs. Every chain has parameters and one parameter of the system is L , which represents the number of sites in the chain. In my case, I will have only two spins pointing up, so another parameter will be $L-2$, the number of spins pointing down. The excitations can occur at any two locations in the chain, but later on we will study the bound pairs, which are two excitations in neighboring sites in the chain.

The Hamiltonian of the system describes how the spins in the chain are coupled, and what role the Pauli matrices play in it:

$$H = \sum_{n=1}^L \frac{J}{4} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y] + \frac{J_z}{4} [\sigma_n^z \sigma_{n+1}^z] \text{ (eqn. 14)}$$

The first term in the Hamiltonian is known as the flip-flop term. When it acts on a state where it has a spin pointing up in one site and a spin pointing down in a neighboring site, it flips both. For example, when σ^x acts on a spin pointing up, it flips the spin to be pointing down, and vice versa.

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

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

Similarly, when σ^y acts on a spin, it flips the orientation but with an additional coefficient of i .

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

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

To look at it in terms of the Hamiltonian, when the flip-flop terms acts on a state with one spin pointing up and the spin in the neighboring site pointing down, it flips both terms and the state which was up down becomes down up. This is why it is called flip-flop, because it flips the terms. When the first term of the Hamiltonian,

$$\frac{J}{4} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y] |\uparrow\downarrow\rangle = \frac{J}{4} |\downarrow\uparrow\rangle$$

$$\frac{J}{4} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y] |\uparrow\downarrow\rangle = \frac{J}{4} |\downarrow\uparrow\rangle$$

acts on two spins in neighboring sites, the effect of the term is that it moves the excitation from one site to the neighboring site, from site n to site $n+1$. The flip-flop term is also equivalent to a term of kinetic energy.

The other term in my Hamiltonian is the term of interaction, known as the Ising interaction. This term tells us what the energy of each spin configuration is. When σ^z acts on a spin, it does not change the state like the flip-flop term, but it determines the energy. For example, when the σ^z sees a positive spin, it gives us positive energy and when σ^z sees a negative spin, it gives a negative energy but does not change the spin.

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

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

Therefore, when this term acts on parallel spins, it gives us this energy $+\frac{J_z}{4}$ and when it acts on a state with antiparallel spins, it gives us this energy $-\frac{J_z}{4}$.

$$\frac{J_z}{4} [\sigma_n^z \sigma_{n+1}^z] |\uparrow\uparrow\rangle = +\frac{J_z}{4} |\uparrow\uparrow\rangle$$

$$\frac{J_z}{4} [\sigma_n^z \sigma_{n+1}^z] |\uparrow\downarrow\rangle = -\frac{J_z}{4} |\uparrow\downarrow\rangle$$

A. Hamiltonian in Matrix Form

Now that we understand the different parts of the Hamiltonian, we will write it in matrix form. In order to write it in matrix form, I first have to choose a basis, which is the configuration of spins pointing up and down. The number of sites in the system is L and the number of up-spins is a fixed amount, which we will denote as n . As an example, I chose a system with 4 sites and 2 spins pointing up. The dimension, or permutations of the different basis vectors, can be found using the equation

$$\frac{L!}{n!(L-n)!} \text{ (eqn. 15).}$$

With $L=4$ and $n=2$, there are 6 different permutations or configurations:

$$|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle.$$

Each configuration can also be represented as a vector. For example, $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ represents the first

basis vector $|1100\rangle$, and $\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ represents the second basis vector $|1010\rangle$. In total for this

system, there Hamiltonian matrix will have a dimension of 6, with 6 rows and six columns.

In order to obtain each element of the matrix, we have two factors to include; the flip-flop term and the term of interaction. The diagonal elements of the matrix will be made up of

contributions coming from the Ising interaction, which is the energy of each of the spin configurations or basis vectors. The off-diagonal elements are the ones coming from the flip-flop term, which tell us which states are directly coupled.

Finding the diagonal elements is relatively simple. First, for each term we look at the number of pairs parallel and antiparallel spins there are. For each pair of parallel spins, you will add $\frac{J_z}{4}$, and for each pair of antiparallel spins you will subtract $\frac{J_z}{4}$. Let us use the first configuration as an example, $|1100\rangle$. The spins in the first and second sites are parallel, so $\frac{J_z}{4}$ is added. Sites 2 and 3 have anti-parallel spins, so $\frac{J_z}{4}$ is subtracted. Sites 3 and 4 have parallel spins $\frac{J_z}{4}$ is added again. We also look at sites 4 and 1 because as I mentioned early, the spins are on a closed chain, which means that the first and last sites also interact. The spins on sites 4 and 1 are antiparallel, so $\frac{J_z}{4}$ is subtracted. We total these results to find the first diagonal element in the matrix, H_{11} . We find that $\frac{J_z}{4} - \frac{J_z}{4} + \frac{J_z}{4} - \frac{J_z}{4} = 0$, so the H_{11} element is 0. This process is done for all the diagonal elements in the matrix.

Next, we have to find the off-diagonal elements, which is a little more difficult to calculate. Each element in the matrix is the result of two vectors acting on each other, and the result will tell us whether the two states are coupled. For example, the element H_{12} (the element in row 1 and column 2) is the result of the vectors $|1100\rangle$ and $|1010\rangle$ acting on each other, which can also be written as: $\langle 1100|H|1010\rangle$. In order to see if the states can be coupled, the spins of both sites are compared. If only two neighboring sites differ, then there is a coupling matrix element. In other words, if the two states can be made equal by moving an excitation by only one site, then the states can be coupled. Using the example of element

H_{12} , if the excitation in site 2 from $|1100\rangle$ was moved over one site, it would become $|1010\rangle$. These states only differ by two neighboring sites, site 2 and site 3. So, the states can be directly coupled, and the result is $\frac{J_{xy}}{2}$. Additionally, this means that the opposite element H_{21} of row 1 and column 2 will also be coupled. Therefore, $H_{12} = \langle 1100|H|1010\rangle = \frac{J_{xy}}{2} = H_{21}$. This same process can be done for all the remaining elements in the matrix, and the remaining elements in the Hamiltonian matrix can now be filled. It is evident when looking at the matrix which states are directly coupled and which are not, because if the resulting element is non-zero, then the states can be directly coupled.

This is the Hamiltonian matrix for the system with 4 sites and 2 excitations which we have been studying until now:

$$H = \begin{matrix} & \begin{matrix} 1100 & 1010 & 1001 & 0110 & 0101 & 0011 \end{matrix} \\ \begin{matrix} 1100 \\ 1010 \\ 1001 \\ 0110 \\ 0101 \\ 0011 \end{matrix} & \begin{pmatrix} 0 & \frac{J_{xy}}{2} & 0 & 0 & \frac{J_{xy}}{2} & 0 \\ \frac{J_{xy}}{2} & -J_z & \frac{J_{xy}}{2} & \frac{J_{xy}}{2} & 0 & \frac{J_{xy}}{2} \\ 0 & \frac{J_{xy}}{2} & 0 & 0 & \frac{J_{xy}}{2} & 0 \\ 0 & \frac{J_{xy}}{2} & 0 & 0 & \frac{J_{xy}}{2} & 0 \\ \frac{J_{xy}}{2} & 0 & \frac{J_{xy}}{2} & \frac{J_{xy}}{2} & -J_z & \frac{J_{xy}}{2} \\ 0 & \frac{J_{xy}}{2} & 0 & 0 & \frac{J_{xy}}{2} & 0 \end{pmatrix} \end{matrix}$$

It is important to note that we can never create or annihilate excitations. If you have two spins pointing up, you will forever have two spins pointing up. This conservation of excitations implies that there is a symmetry in the system and the sum of total magnetization in the z direction is conserved.

B. Eigenvalues and Eigenvectors

Once I have the Hamiltonian matrix, I will diagonalize it in order to get the eigenvalues and eigenvectors. I will also choose values for the parameters of the Hamiltonian, meaning the interaction strength J_z , and the coupling strength J_{xy} . I will do so for a closed chain with $L=6$ sites and $n=2$ excitations, which will be the parameters of the chain I am working with from now on. To find the dimension of the chain, we will use Equation 15, $\frac{6!}{2!(6-2)!} = 15$. The Hamiltonian matrix will therefore be 15×15 , and there will be 15 basis vectors. The eigenvalues of the Hamiltonian represent the energy of each basis vector, so there will be 15 different eigenvalues and each eigenvalue will have 15 different corresponding eigenvectors or eigenstates. For each eigenvector, each element gives the probability amplitude for a particular basis vector, or spin configuration. For instance, eigenvalue E_1 is associated with eigenvector Ψ_1 . The probability amplitude to find eigenstate Ψ_1 in the basis is C_1 , which is a complex number. If we perform a measurement on a system in state Ψ_1 , at energy E_1 , we have $|C_1|^2$, which is the probability of finding it in the first state $|1100\rangle$. The sum of all the probabilities should equal 1,

$$\sum_{n=1}^{dim} |C_n|^2 = 1 \text{ (eqn. 16)}$$

because there must be a probability of finding something. Before making any calculations, using the Mathematica software I checked and verified that indeed each eigenstate is normalized.

V. Case Studies

We will now choose values for the coupling strength and the interaction strength in order to find the eigenvalues and eigenvectors. We want to find out if there is participation in the system of configurations with bound pairs and how the interaction strength will affect the participation. We will study two cases, one in which J_z is much larger than J_{xy} and the other in which they are of the same order. After doing so, we will see the effects of both through the probability amplitudes and dynamics for each case.

A. Case 1: $J_z \gg J_{xy}$

For the first example, I will choose the J_{xy} term, the flip-flop term, to be 1 in any arbitrary unit of energy, and I chose the J_z interaction strength to be much larger than the strength of the flip-flop term. In this case it will be 100 times larger. This is the resulting histogram of the energies with the chosen parameters:

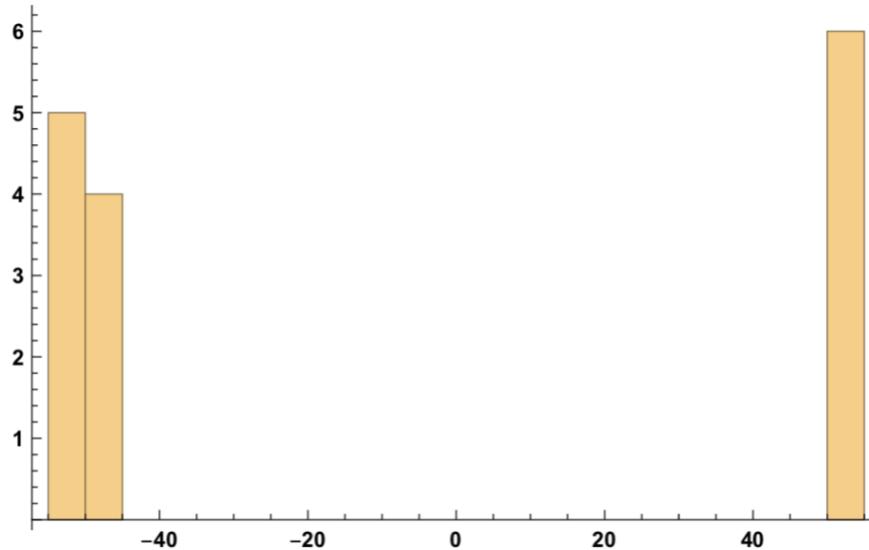


Figure 6: Histogram for the case where $J_z = 100$, showing well separated bands of energy

These are the eigenvalues I get with the chosen parameters: $\{-51.4192, -50.7083, -50.7083, 50.01, 50.0075, 50.0075, -50.0075, -50.0075, 50.0025, 50.0025, 50., -50., -49.2942, -49.2942, -48.5908\}$. As an example, I will choose eigenvalue -50.0075 and show the probability amplitudes of the corresponding eigenvector for each of the basis vectors.

0.493138	↑↑↓↓↓↓	-0.0134155	↓↑↑↓↓↓	-0.00499809	↓↓↑↑↓↓
0.00239843	↑↑↑↓↓↓	-0.00259965	↓↑↑↓↓↓	-3.13985×10^{-16}	↓↓↑↓↓↑
-1.11022×10^{-16}	↑↓↓↑↓↓	4.85723×10^{-16}	↓↓↓↑↑↓	-0.493138	↓↓↓↑↑↓
0.00259965	↑↓↓↑↑↓	0.00499809	↓↑↓↓↑↑	-0.00239843	↓↓↓↑↑↑
0.506554	↑↓↓↑↑↑	-0.506554	↓↓↑↑↓↓	0.0134155	↓↓↓↑↑↑

Table 1: Eigenvectors corresponding to eigenvalue -50.0075 when $J_z \gg J_{xy}$

You will immediately notice after examining the values that the probability amplitude for the states with bound pairs are very large. For example, the states $|110000\rangle$, $|100001\rangle$, and $|001100\rangle$ have probability amplitudes of approximately 0.49, 0.51, and -0.51 respectively. In contrast, if you look at states where the excitations are separated, the value is approximately 0, meaning there is almost no probability amplitude. For the chosen eigenvalue, only states with bound pairs contributed to the eigenstate.

Now we will look at eigenvalue -49.2942 and its corresponding eigenvectors.

0.000485865	↑↑↓↓↓↓	-0.00197118	↓↑↑↓↓↓	-0.391454	↓↓↑↑↓↓
0.294967	↑↑↑↓↓↓	0.0964871	↓↑↑↑↓↓	-0.136697	↓↓↑↑↑↑
0.554586	↑↓↑↑↓↓	-0.41789	↑↓↑↑↑↓	0.000485865	↓↓↓↑↑↓
0.0964871	↑↓↑↑↑↓	-0.391454	↓↑↓↑↑↑	0.294967	↓↓↓↑↑↑
0.00148532	↑↓↑↑↑↑	0.00148532	↓↓↑↑↓↓	-0.00197118	↓↓↓↑↑↑

Table 2: Eigenvectors corresponding to eigenvalue -49.2942 when $J_z \gg J_{xy}$

Here, we see that there are contributions only from states with *no* bound pairs, and the participation ratio for configurations with bound pairs is almost 0. Because of very strong interactions, either we will have states where there will only be contributions from configurations with bound pairs, or there will be eigenstates where there will only be contributions from configurations that do not have bound pairs. So, either there is an existence of a bound pair, or there is not.

In order to further explain why this is the case, I will go back to the Hamiltonian matrix with 4 sites and 2 excitations. It is clear that there is a direct coupling between the first state $|1100\rangle$ where there is a bound pair, and the second state $|1010\rangle$ where there is no bound pair, because there is a resulting element of $\frac{J_{xy}}{2}$. The energy of the state $|1100\rangle$ is 0 and the energy of the state $|1010\rangle$ is $-J_z$, which means that the energy difference, $0 - J_z = J_z$. In the case we just examined where J_z is very large, the energy difference here is very large as well, and as a result the coupling is ineffective. For any spin configurations, they will get coupled if they have the same energy, even if they are not directly coupled, because of high

order of perturbation theory. (The perturbation theory is a system created in order to correct any perturbations in a problem and find approximate solutions created from the unperturbed solutions.) So, there are some states that will be indirectly coupled, and other states that will be directly coupled, but the energy difference is so large that the coupling is ineffective.

B. Case 2: $J_z \sim J_{xy}$

Now, I will change the interaction strength to be the same order as the coupling strength and compare the results to what happens when the interaction strength is much larger than the coupling strength. We will set $J_z = 0.5$ and $J_{xy} = 1$ and this is the Histogram of energies:

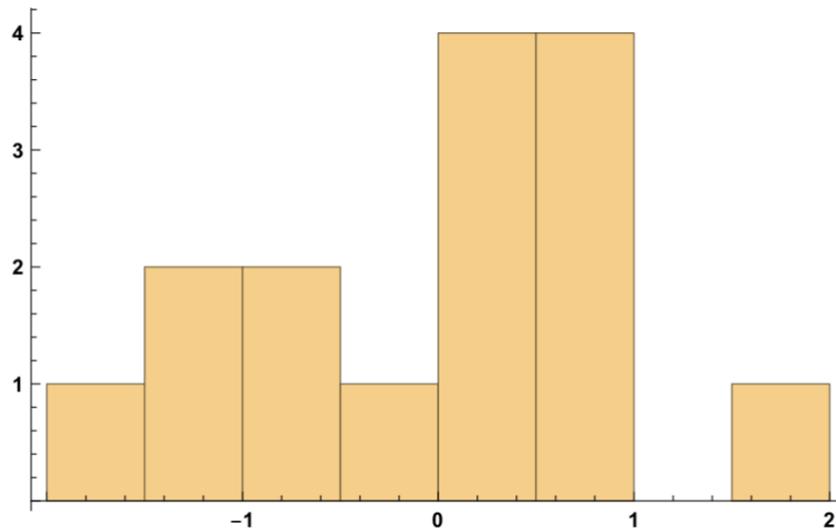


Figure 7: Histogram of energies for case of $J_z = 0.5$, where all eigenvalues are close in values.

These are the resulting eigenvectors to the chosen eigenvalue -1.05902 .

0.070406	$\uparrow\uparrow\downarrow\downarrow\downarrow$	-0.159221	$\downarrow\uparrow\uparrow\downarrow\downarrow$	-0.416847	$\downarrow\downarrow\uparrow\downarrow\downarrow$
0.232522	$\uparrow\downarrow\uparrow\downarrow\downarrow$	0.184325	$\downarrow\uparrow\uparrow\downarrow\downarrow$	0.227839	$\downarrow\downarrow\uparrow\downarrow\uparrow$
-0.515251	$\uparrow\downarrow\uparrow\downarrow\downarrow$	0.287413	$\downarrow\uparrow\downarrow\uparrow\downarrow$	0.070406	$\downarrow\downarrow\uparrow\uparrow\downarrow$
0.184325	$\uparrow\downarrow\downarrow\uparrow\downarrow$	-0.416847	$\downarrow\uparrow\downarrow\downarrow\uparrow$	0.232522	$\downarrow\downarrow\uparrow\downarrow\uparrow$
0.0888154	$\uparrow\downarrow\downarrow\uparrow\downarrow$	0.0888154	$\downarrow\downarrow\uparrow\uparrow\downarrow$	-0.159221	$\downarrow\downarrow\uparrow\downarrow\uparrow$

Table 3: Eigenvectors corresponding to eigenvalue -1.05902 when $J_z \sim J_{xy}$

It is evident here that all spin configurations can participate. When the energy difference was very large, for each eigenvalue there were contributions either from spins with bound pairs or from spins without bound pairs. With an interaction strength of the same order as the flip-flop term, there is a probability amplitude for the first configuration with a bound pair, but a probability amplitude also exists for the second configuration when they are separated. The that all spin configurations can participate is because the interaction is weak and so the coupling is effective. Using this information, we will be able to anticipate the dynamics of the system.

C. Dynamics

Suppose I prepare my system in an initial state where I have a bound pair, for example this first configuration $|110000\rangle$. If there is a strong interaction, as with the case where $J_z = 100$, I would expect the bound pair to move as a pair and never split up. In the second example where the interaction is weak ($J_z = 0.5$), the bound pair should be able to split. Using Mathematica, I can calculate the probability amplitudes and graph them to anticipate the dynamics.

In the plot below, you can see that each curve in the plot gives you the probability to find the spin configurations in time. I set $J_z = 100$ and my initial state here is $|110000\rangle$ with the bound pair on sites 1 and 2. As time passes, I only see contributions from other bound pairs. Note that excitations on sites 1 and 6 on basis $|100001\rangle$ is also a bound pair, because it is a closed chain. On the graph, only the configurations with bound pairs can be seen, because there is no participation from the spin configurations with no bound pairs.

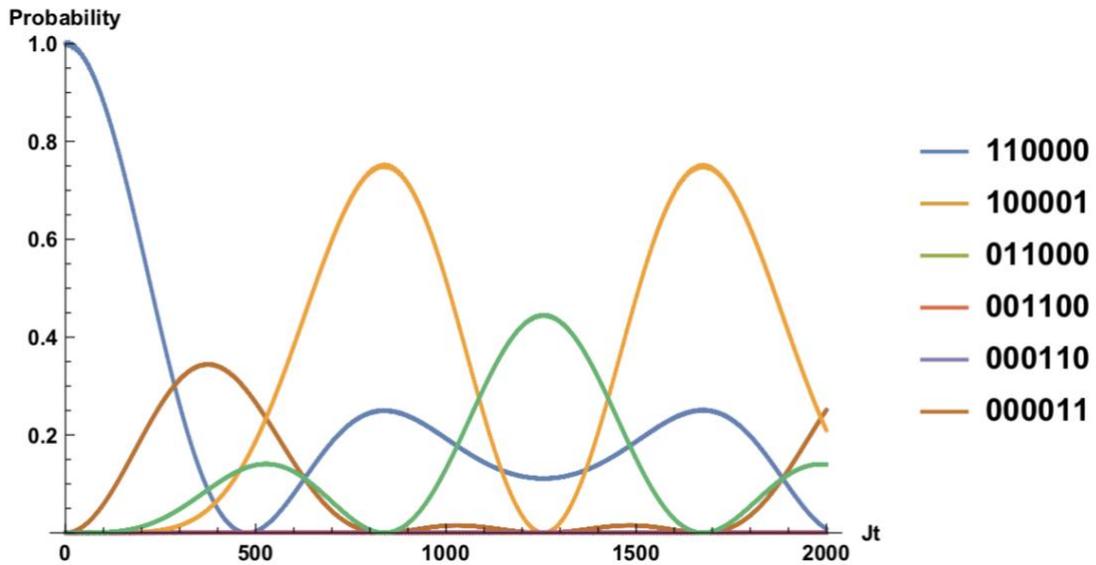


Figure 8: Probability to find spin configurations in time for $L=6$, $n=2$, $J_z=100$, $J_{xy}=1$, in a closed chain

Let us now compare this to the results when $J_z = 0.5$. As we saw earlier, when the interaction strength is weak and of the same order of the strength of the coupling term, there will be participation from many different spin configurations, not only ones with or without bound pairs. I will graph the system with $J_z = 0.5$, with the same initial state $|110000\rangle$.

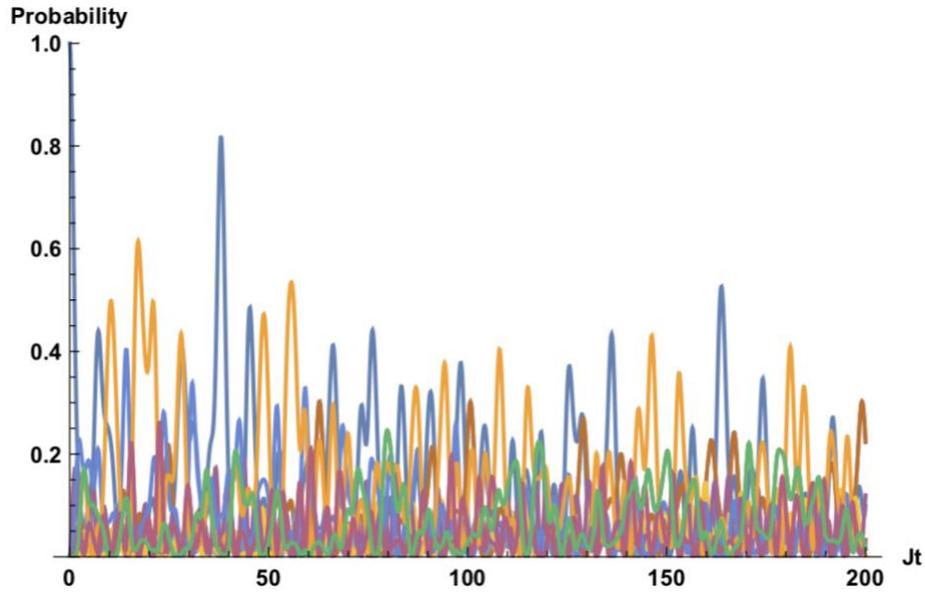


Figure 9: Probability to find spin configurations in time for $L=6$, $n=2$, $J_z=0.5$, $J_{xy}=1$, in a closed chain

It is evident that the dynamics here are much faster than the dynamics when I had a strong interaction. In Figure 3, there is a shorter time scale to better identify each curve. My initial state is the same, but as time goes on you see contributions both from states with and without bound pairs.

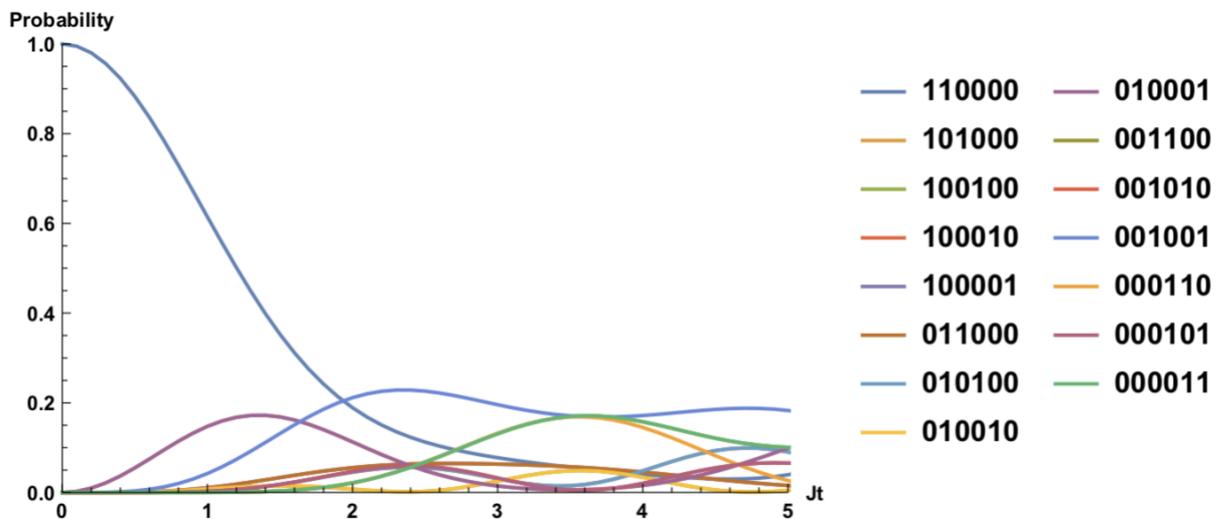


Figure 10: Probability to find spin configurations in time for $L=6$, $n=2$, $J_z=0.5$, $J_{xy}=1$, in a closed chain

VI. Mathematica Codes

Many of the results in my thesis were found using Mathematica codes, which are presented below.

- How to define the parameters Hamiltonian, find the basis vectors and initialize the Hamiltonian:

```
(* PARAMETERS OF THE HAMILTONIAN *)
Clear[L, upspins, downspins, dim, Jxy, Jz];

L = 6;
upspins = 2;
downspins = L - upspins;
dim = L! / (upspins! downspins!);

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

(* Parameters for nearest-neighbor couplings *)
Jxy = 1.0;
Jz = 100.;

(* ELEMENTS OF THE HAMILTONIAN *)

Clear[HH];
(* Initialization *)
Do[Do[HH[i, j] = 0., {i, 1, dim}], {j, 1, dim}];
```

- To find the diagonal elements of the Hamiltonian which are composed of the ising interaction terms and add the additional parameter of the closed chain:

```

(* 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 find the off-diagonal elements of the Hamiltonian matrix, which are composed of the coupling terms, including the additional parameter of the closed chain:

```

(* 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] = Jxy/2., HH[j, i] = Jxy/2.}]];

    (*closed chain*)
    If[howmany == 2,
      If[site[2] - site[1] == L - 1, {HH[i, j] = Jxy/2., HH[j, i] = Jxy/2.}]];

    , {j, i + 1, dim}];
  , {i, 1, dim - 1}];

```

- Compiling the completed Hamiltonian matrix and finding the eigenvalues and eigenvectors as well as the Histogram of the energies:

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

Histogram[Energy, 20]
```

- Finding and plotting the dynamics of the system:

```
(*** DYNAMICS ***)
(* time increment and total final time *)
dt = 0.1;
tfinal = 20001;

(* Initial state *)
chosenBasis = 1;
PSI0 =
  Flatten[{Table[0, {k, 1, chosenBasis - 1}], 1, Table[0, {k, chosenBasis + 1, dim}]}];

(* Basis Vectors *)
Do[
  basisPos = j;
  basisVec[j] =
    Flatten[{Table[0, {k, 1, basisPos - 1}], 1, Table[0, {k, basisPos + 1, dim}]}];
  , {j, 1, dim}];

Do[
  time = (k - 1) dt;
  PsiT = MatrixExp[- I Hamiltonian time].PSI0;
  Do[
    Prob[j, k] = Abs[basisVec[j].PsiT]^2;
    , {j, 1, dim}];
  , {k, 1, tfinal}];

Do[
  lisT[j] = Table[{(k - 1) dt, Prob[j, k]}, {k, 1, tfinal}];
  , {j, 1, dim}];
```

```
ListPlot[Table[list[j], {j, 1, 15}], Joined → True, PlotRange → {0, 1},  
AxesLabel → {Jt, Probability},  
PlotLegends → {"110000", "100001", "011000", "001100", "000110", "000011"}]
```

VII. Conclusions

In this thesis, we were successfully able to predict the dynamics of a quantum system and demonstrate the stability of doublons. In our case, however, instead of doubly occupied sites as in experiments with cold atoms, we investigated the lasting nature of a bound pair of neighboring excitations. We saw that we were able to create these bound pairs through interaction, when the interaction strength was much larger than the coupling strength. The stability of these bound pairs is caused by the energy difference between configurations where we have a bound pair and configurations where the two pairs are split up. We also saw that the dynamics were very slow in the case where the interaction strength was much larger than the coupling strength, compared to the case where they were of the same order.

This research can take many future directions. One of which can be to add an impurity or defect to the chain and see its effects. An additional study could be to analyze open chains as well, both with and without an impurity. Once one defect is added, we can include more than one defect, and consider coupling not just between direct neighbors, but second neighbors as well. An even more challenging direction may be to extend the studies to a 2-dimensional system. Many of these future directions are all extensions of my research that can be done experimentally with cold atoms in optical lattices.

VIII. Acknowledgements

I would like to thank Dr. Lea F. Santos, for teaching me, guiding me and spending hours on end helping me through this project and research, especially in this difficult pandemic. She was an amazing mentor throughout this whole process, and I am lucky to have been her

student. I would also like to thank the S. Daniel Abraham Honors program for giving me the privilege to conduct this research and to participate in all of the opportunities the Honors program had to offer.

IX. References

[1] Richard P. Feynman, Robert B. Leighton, Matthew Sands, *The Feynman Lectures on Physics, Vol. III* (Addison Wesley, 1971)

[2] David J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, New Jersey, 1995).

[3] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J.H. Denschlag, A. J. Daley, A. Kantian, H.P. Büchler, and P. Zoller, *Repulsively bound atom pairs in an optical lattice*, Nature **441** 853 (2004).

[4] L.F. Santos and M. Dykman, *Quantum interference-induced stability of repulsively bound pairs of excitations*, New J. Phys. **14** 095019 (2014).

[5] Kira Joel, Davida Kollmar, and Lea F. Santos, *An introduction to the spectrum, symmetries and dynamics of spin-1/2 Heisenberg chains*, Am. J. Phys. **81**, 450-457 (2013).