Stability of Doublons in One-Dimensional and Two-Dimensional Lattices with a Defect

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1. Introduction

As humans, we rely on our senses. Science teaches us to experiment through observation; through witnessing the world around us. How ironic is it then that the actual fundamental science is that which is not really discernable by eye; is that which is really counter-intuitive to any observations us humans could have. The science of quantum physics is the science of the universe in its most fundamental form. Its elegance, which is hidden in classical physics - in the bulky study of macroscopic objects - is revealed at last in the study of the microscopic building blocks of the universe, the tiny quantum particles.

This thesis explores the interaction of these particles in two quantum systems. It explores their energies and accessible states, and it explores the evolution of the systems through time. The systems in use are described by a one-dimensional (1D) model (a chain), and by a two-dimensional (2D) model (a plane). These models are employed in a variety of current studies of theoretical, experimental and technological interest, such as quantum computing, quantum cryptography, quantum sensors, spintronics, and the search for new phases of matter.

The quantum systems that we study have two particles, and because of the interaction between them, they may stick together and move together as a single heavier particle. These bound pairs, in which the particles occupy the same site, are often referred to as doublons, and they have been detected experimentally [1]. In the systems that we study here, the bounded excitations are in neighboring sites, but we will also refer to them as doublons, since the problem is analogous. In this thesis, I study how robust the doublons are - whether they survive the presence of impurities in the system and whether the geometry of the system, 1D or 2D, can make them more or less robust.

In order to begin the discussion of the research, some topics on Quantum theory and the needed mathematical tools from Linear Algebra must be reviewed.

2. What is Quantum Physics?

To get the discussion started, we are going to look at a few different experiments which clearly illustrate some key elements of quantum physics [2].

2.1 Double-slit experiment.

The first experiment is the classic double-slit experiment. In this thought experiment by Richard Feynman [3] (which was later realized in the lab [4]), a wall is set up with two slits a distance apart from each other. There is a detector on the backstop behind the wall which can detect particles. A source, which contains electrons is then beamed onto the wall.

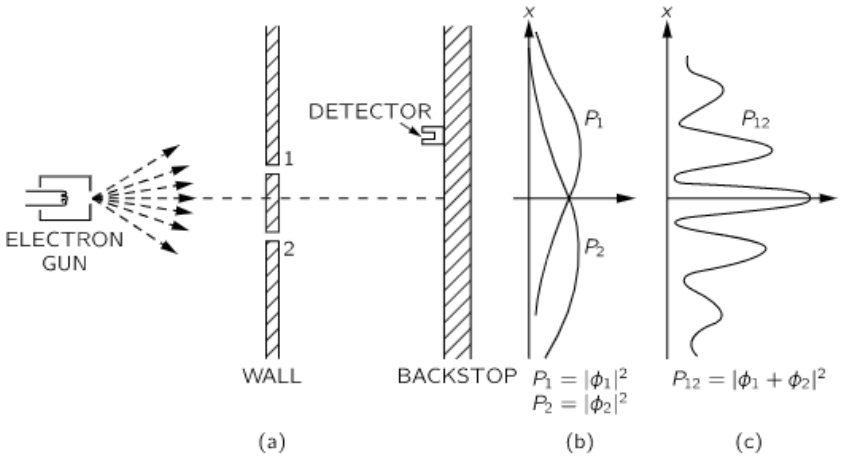


Figure 1: Schematic representation of the double-slit experiment proposed by Richard Feynman. (a) A wall with two thin slits, (b) probability of finding the electrons when only one slit is open: 2 distinct crests where the slits are, (c) the probability of the actual results when both slits are open, wave-like distribution.

When one of the slits is open and one of the slits is closed, the detection on the backstop is as would be expected if one were to shoot bullets at a wall through a little hole. The highest point of detection is that right behind the slit as in Fig.1 (b), where P_1 is for the probability of finding the particle that went through slit 1 and P_2 for the probability of finding the particle that went through slit 2, with smaller points of detection nearby and adjacent to that central spot. This illustrates the particle-like characteristic given to electrons. When both slits were open, however, something very unexpected would happen. In this scenario, instead of there being the two distributions overlapping into a new distribution peaked between the two, $P_{total} = P_1 + P_2$, there appeared to be an interference type of depiction on the backstop as shown in Fig.1 (c). Interference is wave language, not particle language. The interference pattern seen in Fig.1 (c) is typical of what we get when waves, such as water waves, go through the slits. And thus we must conclude that not only do electrons have particle-like characteristics, but they also have wave-like characteristics. This leads to the term "wave-particle duality" that is so much discussed in quantum physics. Furthermore, the wave-like nature of these electrons introduces an integral concept of quantum physics: Probability! Probability is a key concept in the Quantum ideas that will be discussed in this thesis. We do not know at the same time where an electron is and what its velocity is at any given moment, rather we know the probabilities of the different positions an electron may be in at a given moment in time. The sum of all these probabilities will equal 1, as the electron DOES of course exist indisputably.

The notion of probability when it comes to quantum particles such as electrons, raises the concept of superposition. We say loosely that an electron exists in different states at the same time, more formally, we say that a quantum object is in a superposition of various different states. It is only when we decide to find a precise location of the electron by doing a measurement that the

system collapses to a single state. The probability is then useful to say where we are likely to find the electron once we measure the system. If, however, the system remains un-collapsed, and the exact location of the electron unknown, Quantum theory states that the electron in fact exists in all of the possible forms for which we have probabilities.

2.2 Stern-Gerlach experiment.

A second experiment I would like to discuss is the Stern-Gerlach experiment. Essentially, this experiment proved that the electron has its own internal spin (its own intrinsic angular moment) and that the spin is quantized: that it has only two possible discrete values and not a continuum of values. The experiment is set up with a magnet apparatus. The electrons are beamed through a slit which then directs the electrons through a magnetic field and then onto a screen.

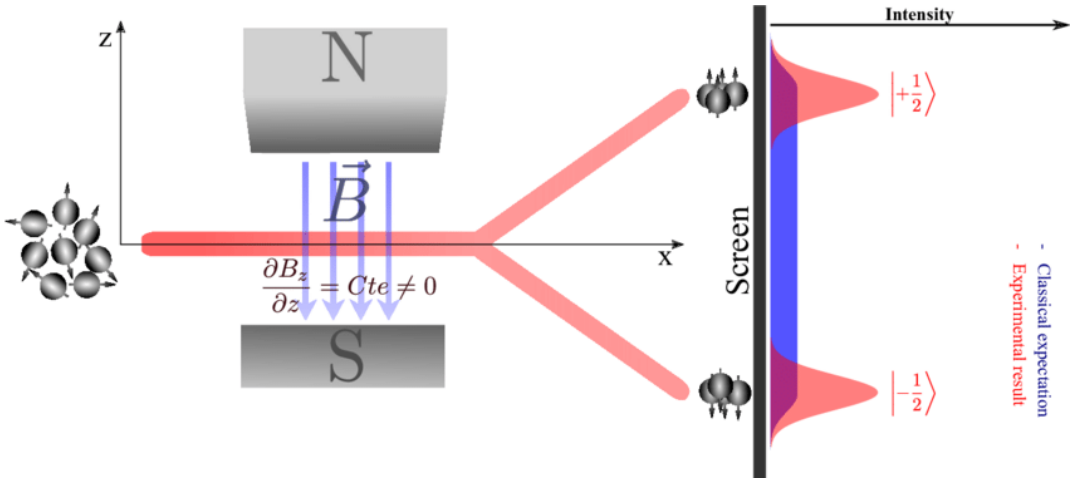


Figure 2: Sketch of Stern-Gerlach experiment: A beam of silver atoms is sent through an inhomogeneous magnetic field. The silver atoms come out of the magnetic field and hit a screen perpendicular to their initial path. On the right, the intensity distribution is observed on the screen; in blue is the classical expectation versus the quantum result in red. There are only two possible quantum results +1/2 or -1/2. The silver atom used in the experiment has a total of 47 electrons, 23 of one spin type, and 24 of the opposite. Because electrons of the same spin cancel each other out, the one unpaired electron in the atom will determine the spin of the silver atom.

From classical physics, we would expect that the magnetic moment (spin) of the electron could take on a variety of different values – would be a continuous line on the back wall, as seen in blue on the right side of Fig.2. This is not what the result was in reality. In reality there were two distinct paths that the electron took, not a smudge of a variety of options, as seen in red on the right side of Fig.2. This indicates to us, that the electron must have its own internal spin, which is either attracted or repelled by a magnetic pole. It was concluded that the electron does indeed either have an up-spin (+1/2) or a down-spin (-1/2); the electron becomes parallel or anti-parallel to the magnetic field that it goes through.

To summarize, this Sec.2 introduced qualitatively some of the main concepts of quantum physics: the wave-particle duality, the existence of particles in a superposition of different states, the notion of the collapse to a single state after a measurement, the fact that quantum mechanics is an intrinsically probabilistic theory, and that quantization (of spin in the example above, but also of energy) is also present in the quantum world.

In the next sections, my descriptions will become more quantitative. I start by talking about probability and for that we need to introduce the notion of "wave function" and how to obtain it. As mentioned earlier, a key element of quantum physics, is the wave-particle duality that an electron (or another quantum particle) has. The "wave" aspect is at the core of the notion of probability.

3. Wave function and Schrödinger equation

In quantum mechanics, all information about the system and its dynamics is contained in the wave function. With the wave function we can compute the mean value of quantities, such as

position and momentum, and how they change in time. In order to derive the wave function of a particle and to explain its evolution throughout time, we must solve Schrödinger's equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \tag{1}$$

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

$$\hbar = \frac{h}{2\pi} = 1.054573 \times 10^{-34} \text{J s} \tag{2}$$

Psi (Ψ) is the wave function, m is the mass of the particle, and V is a potential. The wave function is an abstract mathematical tool, but its absolute square is physical. When written in terms of position, for example, as in the solution of Eq.(1), the absolute square of the wave function corresponds to the probability of finding the particle at position x and time t,

$$|\Psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } x \text{ and } (x+dx), \text{ at time } t. \end{array} \right\} \tag{3}$$

The integral of this probability over the entire space has to be 1, since the particles exists somewhere,

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

This process, of computing the integral of the square of the wave function over the whole space and forcing it to get a result of one, is called normalization. Schrodinger's equation ensures that no matter the change of the system throughout time, the normalization of the wave function still occurs.

To solve Schrödinger equation and obtain the wave function Ψ(x,t), we need to know the potential. In the case of a potential that is time independent, we can use the method of separation

of variables to solve the equation. The procedure goes as follows [2]. We write the wave function as a product of two functions, one dependent on position only and the other dependent on time only,

$$\Psi(x,t) = \psi(x)\, f(t), \tag{5}$$

This implies that the partial derivative on time becomes an ordinary derivative of f(t)

$$\frac{\partial \Psi}{\partial t} = \psi \frac{df}{dt} \tag{6}$$

and the partial derivative on position becomes an ordinary derivative of Ψ(x)

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2} f \tag{7}$$

Using Eq.(6) and Eq.(7) in Eq.(1) allows us to separate the time dependent Schrödinger into two parts, the equation for f(t)

$$\frac{df}{dt} = -\frac{iE}{\hbar} f, \tag{8}$$

and the equation for Ψ(x)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \tag{9}$$

In the two equations above, E is a constant, which actually represents the energy of the system. Equation (8) is easy to solve and gives us $f(t) = e^{-iEt/\hbar}$, while to solve Eq.(9) we need to know the potential.

Equation (9) can also be written in a more general form if we use the so-called Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{10}$$

which leads to

$$\hat{H}\psi = E\psi, \tag{11}$$

The Hamiltonian operator in quantum mechanics, just as the Hamiltonian in classical mechanics, gives us the energy of the system.

We use Eq.(9) for 1D systems where the particle can occupy any position in space. In lattice systems, however, the particle can only be in some fixed positions of space, known as sites. An illustration of a lattice is provided in the figure below, where each circle represents a particle. The particle can hop from one site to the other, but it cannot be between sites.

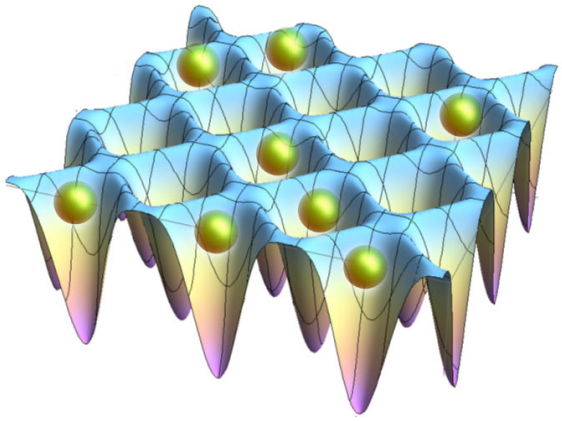


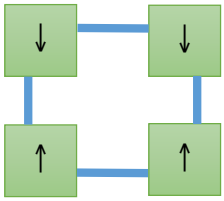
FIGURE 3: Sketch of a 2D quantum lattice, where the circles represent the particles. A particle can only be found on a site, not between sites.

Equation (11) is the time-independent Schrödinger equation in its most general form and it is therefore an appropriate equation to describe a lattice system, as the ones we study here. In this case, the Hamiltonian is a matrix and Ψ is a vector, as we show below.

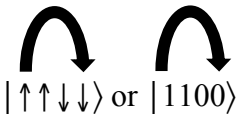
4. Spin-1/2 System

In our lattices, all sites are occupied with a fixed particle that has a spin $\frac{1}{2}$. There is a strong magnetic field pointing down in the z-direction and acting on the entire lattice, so that the spin of the particle either points up in the z-direction or down. We call the up-spin, which is anti-parallel to the magnetic field, an excitation and it can be denoted as $|\uparrow\rangle = |1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. A particle parallel to the magnetic field is in its ground state; it has less energy and is called a down-spin, denoted as $|\downarrow\rangle = |0\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.

Let me start by describing a lattice composed of only four sites, or in other words, four particles. The particles are on a chain with periodic boundary conditions, also called a "closed chain", that is, it is a ring, such that the "first" site also connects to the "last" site in our system. The figure below illustrates this 4-site lattice



We can represent the state of the lattice above as an array of up- and down-spins or, equivalently, an array of 0's and 1's as shown below, where the thick curved arrows remind us that the first and last sites are connected.



In the particular example above, there are 2 up-spins and 2 down-spins. As we will see, our system conserves the total number of up-spins and down-spins. In this scenario, our up-spins can be distributed throughout the four sites in a few different variations; namely a total of six variations:

{1, 1, 0, 0}, {1, 0, 1, 0}, {1, 0, 0, 1}, {0, 1, 1, 0}, {0, 1, 0, 1}, {0, 0, 1, 1}

We say for this that any eigenvector in our system will be composed of these six basis vectors. We symbolize the number of sites (or particles) in our system by denoting it with an "L". We calculate the dimension of the Hilbert space of our system, that is the number of basis vectors that exist in our system, by figuring out the number of permutations that we can configure with the number of up-spins.

L = number of sites (4 in our example)

up-spins = 2 (in our example)

down-spins = L – up-spins (4-2 = 2 in our example)

$$dim = \frac{L!}{up{-}spins!down{-}spins!} . \tag{12}$$

Notice that if there is a single up-spin in the system, the dimension of the Hilbert space equals the size of the chain, *dim=L*. However, as the ratio between up- and down- spins approaches 1, the dimension becomes significantly larger than L, especially when the chain is large. In our work, we only consider 2 up-spins, so that our Hilbert space grows quadratically on the size of the chain, *dim=L(L-1)/2*.

The Hamiltonian of our system describes the interactions between the particles and is used to obtain the discrete energies of our isolated system. For each accessible energy, there is a corresponding eigenstate that describes the state of the system at that energy level.

5. A Brief Discussion of the Hamiltonian operator

The Hamiltonian that describes our systems includes three main elements: a defect, the J_z term, and the J_{xy} term [5].

$$H = \frac{1}{2}\epsilon_d \sigma_d^z + \frac{1}{2}\sum_{j=1}^{L} h\sigma_j^z + \frac{1}{4}\sum_{j=1}^{L}\left[J_z \sigma_j^z \sigma_{j+1}^z + J_{xy}(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y)\right] \quad (13)$$

where σ^z and σ^x, σ^y are the Pauli matrices,

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

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

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

d is the site where there is a defect, ε_d is the defect excess energy, h is the amplitude of the external magnetic field pointing down in the z-direction, J_z is the strength of the Ising interaction, and J_{xy} is the amplitude of the hopping term. We will now explain these terms.

5.1 First two terms

Let us explain the effect of ($\varepsilon\ \sigma^z + h\ \sigma^z$) first on one up-spin and one down-spin, then let us see the effect of ($\varepsilon\ \sigma^z + h\ \sigma^z$) on different spin configurations. This term means that we have an external magnetic field acting on all the sites that are providing energy, splitting h between the down-spin with energy $-\frac{h}{2}$ and the up-spin with energy $+\frac{h}{2}$. In addition to this field, there is an

additional small magnetic field that acts only on site d, which is the defect (or impurity) site, where a down-spin has energy $-\frac{h}{2}-\frac{\varepsilon}{2}$ and an up-spin has energy $+\frac{h}{2}+\frac{\varepsilon}{2}$.

Let's see an example with six sites and two excitations:

$\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow$ (down, down, up, up, down, down)

Since the energy from the homogeneous magnetic field for all spin configurations is just the constant -(L-4)h/2, we set it to zero, so that the only part that remains from this part of the Hamiltonian is the value $+\varepsilon_d/2$ or $-\varepsilon_d/2$, depending on the orientation of the spin on the defect site.

5.2 Ising interaction

In order to understand a little about the interactions between the particles, we must understand the role of the J_z term and the J_{xy} term. We note that according to Eq.(13), the couplings in our system exist only between neighboring sites, site *j* and site *j+1*.

This subsection is dedicated to the J_z term, which is known as the Ising interaction. Due to this term, spin configurations (basis vectors) with neighboring particles that have parallel spins have a different energy than configuration states with neighboring particles that have anti-parallel spins, as shown in the equations below

$$\frac{J_z}{4}\sigma_n^z\sigma_{n+1}^z\left|\uparrow_n\uparrow_{n+1}\right\rangle = +\frac{J_z}{4}\left|\uparrow_n\uparrow_{n+1}\right\rangle$$

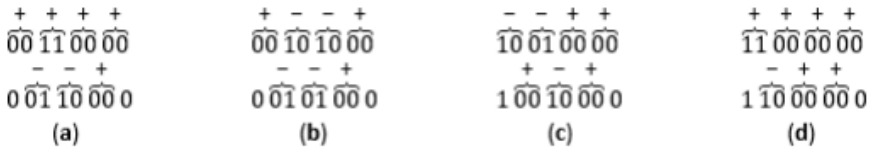
$$\frac{J_z}{4}\sigma_n^z\sigma_{n+1}^z\left|\downarrow_n\downarrow_{n+1}\right\rangle = +\frac{J_z}{4}\left|\downarrow_n\downarrow_{n+1}\right\rangle$$

$$\frac{J_z}{4}\sigma_n^z\sigma_{n+1}^z\left|\uparrow_n\downarrow_{n+1}\right\rangle = -\frac{J_z}{4}\left|\uparrow_n\downarrow_{n+1}\right\rangle$$

$$\frac{J_z}{4}\sigma_n^z\sigma_{n+1}^z\left|\downarrow_n\uparrow_{n+1}\right\rangle = -\frac{J_z}{4}\left|\downarrow_n\uparrow_{n+1}\right\rangle$$

Two neighboring parallel spins have energy $+J_z/4$, while anti-parallel spins have energy $-J_z/4$. If J_z is positive, the lowest energy is achieved with anti-parallel spins. In practice, to determine the energy of the basis vectors due to the Ising interaction, we count the number of parallel and

anti-parallel pairs. As shown below, for an up-spin that neighbors a downspin, a value of $-J_z/4$ is added to the Hamiltonian and for an up-spin neighboring an up-spin or a down-spin neighboring a down-spin, a value of $+J_z/4$ is added to the Hamiltonian



For the state (a) above, the energy due to the Ising interaction is $+J_z$, since there are 6 neighboring pairs of parallel spins (including the pair between the first and last site, due to the ring shape of our chain) and 2 neighboring pairs of anti-parallel spins, so $+6\frac{Jz}{4} - 2\frac{Jz}{4} = +J_z$. This is also the case of state (d), while states (b) and (c) have energy 0.

5.3 Flip-flop term

The J_{xy} term couples different basis vectors, specifically it connects basis vectors that are identical except for two neighboring sites, as shown in the equations below

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

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

The J_{xy} term is also termed "the flip flop term" because it reverses the spins of the basis if there are two opposite spins neighboring each other.

If, however, the neighboring sites have spins that are in the same direction, then the J_{xy} term does not contribute at all

$$\frac{J_{xy}}{4}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y)\,|\uparrow_n\uparrow_{n+1}\rangle = 0$$

$$\frac{J_{xy}}{4}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y)\,|\downarrow_n\downarrow_{n+1}\rangle = 0$$

It preserves the number of up-spins and down-spins found within a system.

As we will see later, when the initial state of the system is one of the basis vectors, the J_{xy} term is what contributes to its dynamics.

5.4 Hamiltonian in a matrix form

Now that I explained the different terms of the Hamiltonian, we can put it in a matrix form. For that we need to choose a basis. The basis that we use, as already mentioned, corresponds to states where on each site the spin either points up or down in the z-direction. Let us consider the case where L=4 and we have 2 up-spins.

To construct the Hamiltonian matrix, we identify each configuration state with an actual vector. For example, the state 1100, which can be written in the "ket" notation as $|1100\rangle$, is represented by the column vector

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

the state |1010> is represented by the column vector

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

and so on. We can also write these states in the "bra" notation $\langle 1100|$, which is represented by the row vector (100000). These vectors are orthonormal, that is, they are normalized,

$\langle 1100 \mid 1100 \rangle =$

$$(100000).\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} = 1$$

(14)

and orthogonal to each other.

$\langle 1100 \mid 1010 \rangle =$

$$(100000).\begin{pmatrix}0\\1\\0\\0\\0\\0\end{pmatrix} = 0$$

(15)

The entries of the matrix are obtained by "sandwiching" the Hamiltonian operator between one basis vector to the left in a row form ("bra") and one basis vector to the right in a column form ("ket"). For example, let us look at the "sandwich" between the basis vector 1100 with itself, which gives us the element H_{11} of the Hamiltonian matrix. We write it as

$$H_{11} = \langle 1100 \mid H \mid 1100 \rangle$$

From the description of the terms of the Hamiltonian, and assuming that the defect site is the first site, *d=1*, we have that

$H \left| 1100 \right\rangle = (+\varepsilon/2 + 0\ J_z) \left| 1100 \right\rangle + (\frac{J_{xy}}{2}) \left| 1010 \right\rangle =$

$$= +\varepsilon/2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \frac{J_{xy}}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

so,

$$H_{11} = \langle 1100 \left| H \right| 1100 \rangle = (10000).\ [+\varepsilon/2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \frac{J_{xy}}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}] = \varepsilon/2$$

as shown in the Hamiltonian matrix below,

	1,1,0,0	**1,0,1,0**	**1,0,0,1**	**0,1,1,0**	**0,1,0,1**	**0,0,1,1**
1,1,0,0	$H_{11} = \varepsilon/2$	$H_{12} = \frac{J_{xy}}{2}$	$H_{13} = 0$	$H_{14} = 0$	$H_{15} = \frac{J_{xy}}{2}$	$H_{16} = 0$
1,0,1,0	$H_{21} = \frac{J_{xy}}{2}$	$H_{22} = -J_z + \varepsilon/2$	$H_{23} = \frac{J_{xy}}{2}$	$H_{24} = \frac{J_{xy}}{2}$	$H_{25} = 0$	$H_{26} = \frac{J_{xy}}{2}$
1,0,0,1	$H_{31} = 0$	$H_{32} = \frac{J_{xy}}{2}$	$H_{33} = \varepsilon/2$	$H_{34} = 0$	$H_{35} = \frac{J_{xy}}{2}$	$H_{36} = 0$
0,1,1,0	$H_{41} = 0$	$H_{42} = \frac{J_{xy}}{2}$	$H_{43} = 0$	$H_{44} = -\varepsilon/2$	$H_{45} = \frac{J_{xy}}{2}$	$H_{46} = 0$
0,1,0,1	$H_{51} = \frac{J_{xy}}{2}$	$H_{52} = 0$	$H_{53} = \frac{J_{xy}}{2}$	$H_{54} = \frac{J_{xy}}{2}$	$H_{55} = -J_z - \varepsilon/2$	$H_{56} = \frac{J_{xy}}{2}$
0,0,1,1	$H_{61} = 0$	$H_{62} = \frac{J_{xy}}{2}$	$H_{63} = 0$	$H_{64} = 0$	$H_{56} = \frac{J_{xy}}{2}$	$H_{66} = -\varepsilon/2$

For the element H_{21}, we have

$$\langle 1010 \,|\, H \,|\, 1100 \rangle = (01000).\ [+\varepsilon/2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \frac{Jxy}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}] = \frac{Jxy}{2} \ .$$

And for $H_{31} = \langle 1001 \,|\, H \,|\, 1100 \rangle = 0$. In this way, we fill out the whole Hamiltonian matrix above. We see that the matrix is real and symmetric.

The diagonal elements in the matrix take on the values of the J_z elements and of the defect amplitude, while the off-diagonal elements need only take into consideration the J_{xy} effects. If we choose $\varepsilon=0$, $J_z = 1$, and $J_{xy} = 1$, we get the matrix

$$\begin{pmatrix} 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0.5 & -1. & 0.5 & 0.5 & 0. & 0.5 \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0.5 & 0. & 0.5 & 0.5 & -1. & 0.5 \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \end{pmatrix}$$

Figure 12: Hamiltonian matrix when $\varepsilon = 0$, $J_z = 1.0$ and $J_{xy} = 1.0$, and there are L=4 sites and 2 up-spins.

6. Diagonalization

By diagonalizing the Hamiltonian matrix, we obtain the energies accessible to the system (the eigenvalues) and the corresponding eigenstates.

6.1 $J_z < J_{xy}$

Looking back on the Hamiltonian matrix in figure 12, the J_z value is small: 1.0., it is of the order of J_{xy}=1. In this case, one sees that the energies of the basis vectors (the diagonal entries 0

and -1) get spread after diagonalization from -2.0 to 1.0. The eigenvalues that arise from this matrix are -2.0, -1.0, 1.0, 0.0, 0.0, 0.0 (rounded to one decimal place), as shown in the histogram below

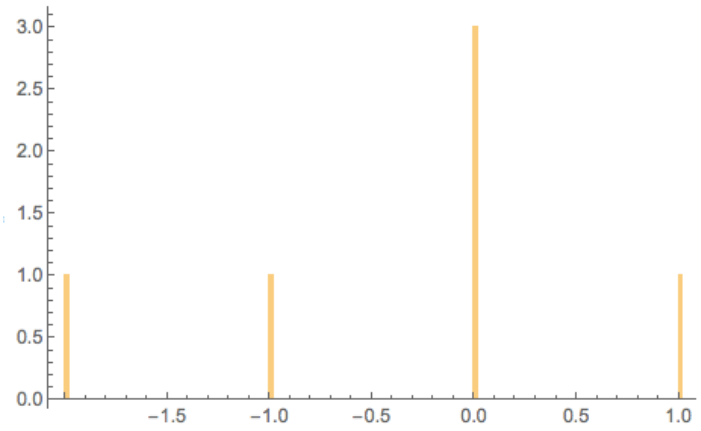


Figure 14: A Histogram of the eigenvalues when $J_{xy} = 1.0$ and $J_z = 1.0$.

The matrix with the eigenvectors of these eigenvalues as columns is

$$\begin{pmatrix} -0.29 & -0.41 & 0. & -0.29 & -0.79 & -0.21 \\ 0.58 & -0.41 & -0.71 & 0. & 0. & 0. \\ -0.29 & -0.41 & 0. & -0.29 & 0.21 & 0.79 \\ -0.29 & -0.41 & 0. & -0.29 & 0.58 & -0.58 \\ 0.58 & -0.41 & 0.71 & 0. & 0. & 0. \\ -0.29 & -0.41 & 0. & 0.87 & 0. & 0. \end{pmatrix}$$

(rounded to the nearest second decimal place). Recall that the basis vectors are

$$\{1, 1, 0, 0\}, \{1, 0, 1, 0\}, \{1, 0, 0, 1\}, \{0, 1, 1, 0\}, \{0, 1, 0, 1\}, \{0, 0, 1, 1\}$$

Take, for example, the first eigenstate. It has probability 0.29^2 to be found in the basis vector |1100>, probability 0.58^2 to be in the basis vector |1010>, etc.

The eigenvectors reflect the spreading in energy; in each eigenvector, we see contributions from all basis vectors, from basis vectors where the up-spins are neighbors and from basis vectors where they are not neighbors.

We refer to a pair of neighboring up-spins as a bound pair or as a doublon. The reason for it will become clear when we discuss the dynamics of the system.

6.2 $J_z >> J_{xy}$

When the $J_z = 10$, or just a higher value much larger than J_{xy}, the following Hamiltonian matrix appears,

$$\begin{pmatrix} 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0.5 & -10. & 0.5 & 0.5 & 0. & 0.5 \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \\ 0.5 & 0. & 0.5 & 0.5 & -10. & 0.5 \\ 0. & 0.5 & 0. & 0. & 0.5 & 0. \end{pmatrix}$$

with the eigenvalues of -10.2, -10.0, 0.2, 0.0, 0.0, 0.0 and the eigenvectors set up by columns in the following matrix,

$$\begin{pmatrix} 0.07 & 0. & -0.50 & -0.29 & -0.21 & -0.79 \\ -0.70 & -0.71 & -0.10 & 0. & 0. & 0. \\ 0.07 & 0. & -0.50 & -0.29 & 0.79 & 0.21 \\ 0.07 & 0. & -0.50 & -0.29 & -0.58 & 0.58 \\ -0.70 & 0.71 & -0.10 & 0. & 0. & 0. \\ 0.07 & 0. & -0.50 & 0.87 & 0. & 0. \end{pmatrix}$$

(rounded to the nearest second decimal place). We can observe from this set-up of our system, that the eigenvalues are very close to the diagonal terms, as shown in the histogram below.

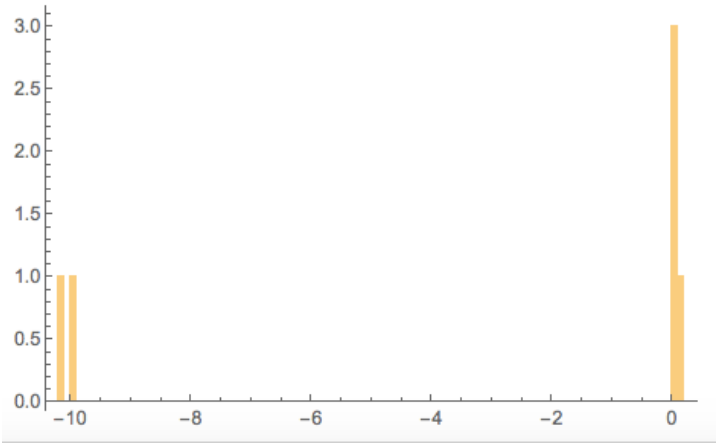


Figure 15: A Histogram of the eigenvalues when $J_{xy} = 1.0$ and $J_z = 10.0$.

Additionally, the eigenvector will only have a high probability of having a state with a pair of parallel up-spins if its eigenvalue is one which is similar in value to a diagonal term obtained with basis vectors that contain a pair of parallel up-spins. For example, the first eigenvector (first column above) has eigenvalue -10.2. This value is very close to a diagonal term obtained with basis vectors that do not contain a pair of parallel up-spins (do not contain a doublon). Indeed, this first eigenvector has probability 0.7^2 to be found in the basis vector |1010>, probability 0.7^2 to be in the basis vector |0101>, but almost no probability to be found in states with bound pairs, such as |1100>. Conversely, the fourth eigenstate, which has eigenvalue 0, is a superposition with high contributions only from basis vectors with a doublon.

6.3 Delocalization vs Localization

We can conclude from this, that the higher the J_z value, the more defined the eigenvalues become, and the closer they are to the values of the diagonal terms of the Hamiltonian matrix. Consequently, the eigenvectors become more localized as well and will consist of specific configurations.

We can measure/quantify the level of delocalization of the eigenstates with the Participation Ratio, which is given by,

$$PR = \frac{1}{\sum |C_k|^4} \tag{16}$$

Where C_k is each coefficient of a given eigenstate. A large value of the PR means that the eigenstate is very much delocalized (spread out in the basis vectors), since we have many small C_k's, that is, we have the participation of several different basis vectors. If the eigenstate is localized, then the PR is small. The extreme case of localization is when the eigenstate is not a superposition, but equals a single basis vector, in which case PR=1.

The graph below plots the average of the participation ratio over all eigenstates as a function of the J_z value for a chain with L=6 sites and 2 up-spins.

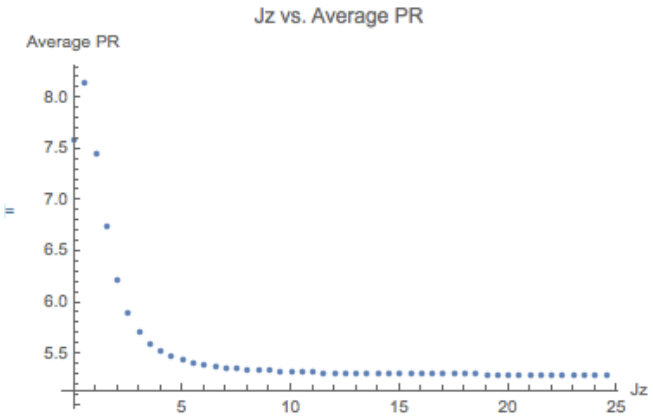


Figure 16: The Participation Ratio averaged over all eigenstates written in the site-basis vectors as a function of the J_z values.

L = 6, up-spins = 2 and down-spins = 4. J_z values range from 0 to 25 in units of J_{xy}=1.

The Participation Ratio stabilizes as the J_z value increases (Fig. 16).

7. Dynamics of a System

When we talk about dynamics, we are talking about the evolution of a system. In order for a system to evolve, it must include: an initial state that it will evolve from (this initial state must not be an eigenstate of the system), and it must include time. Our system changes as a function of time. The special feature in quantum physics, that all possible states and energies are occurring at the same time, is not how our system starts out. Our system begins with one specific spin configuration, and no probability of being in another spin configuration; the probability of being in a specific spin configuration at time zero is one.

As time evolves, our system does not remain in the initial state, rather it acquires the probability of being in other basis vectors as well, but this is not random, rather it is dependent on a number of factors.

7.1 Equation for Evolution

Our initial state is Ψ_0 and our evolved state is given by

$$|\Psi(t)> = e^{-iHt}|\Psi_0>$$

(17)

By utilizing the Taylor Expansion, we get,

$$e^{-iHt}|\Psi_0> = \left[1 - iHt - \frac{(Ht)^2}{2!} + \frac{(iHt)^3}{3!} + \frac{(Ht)^4}{4!} \ldots\right] * |\Psi_0>$$

(18)

At time t=0, $|\Psi(t=0)> = |\Psi_0>$. As time passes, the first states to appear are those directly connected with the initial state. For example, if $|\Psi_0> = |1100>$, the first states that will contribute to $|\Psi(t)>$ are |1010> and |0101>. As more time passes, due to the flip-flop J_{xy} term in the Hamiltonian and the contribution from the higher order terms in the Taylor Expansion, the probability for the initial state further decreases and other states appear as well.

The exact evolution is done as follows: after diagonalizing the Hamiltonian, we have all eigenvalues E_k and eigenstates $|\psi_k>$, with them, Eq.(17) gives us the evolved state as

$$|\Psi(t)> = \sum_{k=1}^{D} c_k\, e^{-iE_k t}|\psi_k>$$

where D is the dimension of the Hilbert space (dimension of the Hamiltonian matrix). The evolved state above can be written in terms of the basis vectors.

For example, in the case of L=4 and 2 up-spins, we have

$$|\Psi(\mathrm{t})> = \begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \\ c_4(t) \\ c_5(t) \\ c_6(t) \end{pmatrix}$$

In the equation above $|c_1(t)|^2$ is the probability of finding the evolved state at time *t* in the basis vector |1100>, and $|c_2(t)|^2$ is the probability of finding the evolved state in the basis vector |1010>, etc.

7.2 Factors affecting the Dynamics

The evolution of the system can almost be predicted once a few key elements are known:

- The set up of our initial state; where the up-spins are placed and whether they are placed next to each other.
- The value of the J_z term which affects the strength of the interactions between the particles.
- The strength and placement of the defect in our system.

For example, if we start with two up-spins in sites that are neighboring each other, a doublon, there is a higher amount of energy in that state than in another basis state in which there is no doublon, due to the fact that the up-spins interact with each other. As stated earlier, the strength of the interaction of the bounded pairs is dependent on the value of the J_z. If the J_z has a large value, then the bounded pairs are heavily bounded to each other, and will stick together as the system evolves. If the J_z has a small value, then it is possible for the bounded pairs to separate in the course of the evolution. The strength of the interaction affects the evolution of the system, because the system will only evolve in a way that will maintain that same amount of energy as the initial state.

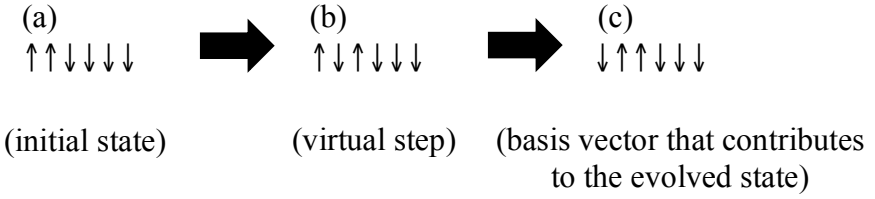
The J_z, however, is not the only thing that determines the energy of the initial state; the defect determines the energy of the system as well. While a system with an initial state of a bounded pair might maintain its energy by only spreading into other basis vectors with other

doublons, it could in principle also maintain its energy by splitting and placing an up-spin on the site of the defect, if the defect excess energy is exactly equal to J_z. This is a scenario that we will also explore in our analysis of the dynamics.

7.3 Movement of Doublon

When J_z is large and we have an initial state that has a doublon, the system will only evolve to include states that also have a doublon, consequently, states with the same energy as the initial state [6-8].

A doublon moves in two steps: one virtual step separating the doublon and one other step moving the up-spin back next to the other up-spin.



If (a) is the initial state, the virtual step will be (b), where the two up-spins separate, and the second step will be (c), where the two up-spins join together again to become a doublon.

We now have the necessary tools to quantitatively investigate the dynamics.

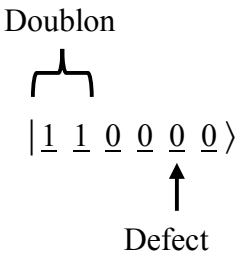
8. Evolution of 1D System

The system we will examine first is a 1D system. In this system we will look at a chain of six sites with two up-spins and four down-spins. The evolution of our system is dependent on the many factors discussed earlier in this thesis and we will look specifically at the influence of the defect, or interaction with the defect site, on the system and the effect that the presence of doublons has on the system.

8.1 Energy of an Initial State

Our system will evolve in such a way that will preserve the energy of the initial state of the system. Let's examine the energy of a few initial states in our 1D system with six sites and the following parameters: J_{xy}=1, J_z = 10, ε = 10. We place our defect on the site d=5.

Case (a): The initial state is a doublon on sites 1 and 2:



Using the Hamiltonian described above, we can determine that the energy of this system is $\frac{Jz}{2}$ (due to the doublon) - $\frac{\varepsilon}{2}$ (due to the down-spin on the site of the defect).

$$\frac{Jz}{2} - \frac{\varepsilon}{2} = 5 - 5 = 0$$

Only states with energy zero can participate in the evolution of this initial state. This includes, for example, the state |011000> and it excludes the state |101000>.

Case (b): The excitations of the initial state are separated and one of them is on the defect site

$$-\frac{Jz}{2} + \frac{\varepsilon}{2} = -5 + 5 = 0$$

Only states with energy zero can participate in the evolution of this initial state. This includes, for example, the state |100010> and it excludes the state |101000>. One of the main questions we plan to address here is whether a state such as state (a) could also evolve into state (b) and vice

versa. We could expect this to happen by energy conservation, however, as we will show, this case is forbidden!

Case (c): The initial state is a doublon, where one of the excitations is on the defect site

Doublon

$|\underline{0}\ \underline{0}\ \underline{0}\ \underline{1}\ \underline{1}\ \underline{0}\rangle$: $+\frac{Jz}{2} + \frac{\varepsilon}{2} = 5 + 5 = 10$

Defect

The only other state with the same energy as this initial state is |000011>

Case (d): The excitations of the initial state are separated and none of them is on the defect site

$|\underline{1}\ \underline{0}\ \underline{0}\ \underline{1}\ \underline{0}\ \underline{0}\rangle$: $-\frac{Jz}{2} - \frac{\varepsilon}{2} = -5 - 5 = -10$

Defect

If we take this scenario (d), we can conclude that any configuration that includes, up-spins that are not neighboring each other, as well as a down-spin on the site of the defect, will all have the same energy of -10. As such, we can expect to find such configurations in the evolution of our system with an initial state like the one in (d). This includes, for example, the states |101000>, |010100>, etc.

8.2 Quantum Interference

If we examine the scenarios above carefully, we notice that there are two different configurations, case (a) and case (b) that result in the same energy of the system. This was illustrated above, with both cases having an energy of 0. We have specifically chosen the defect value and the J_z value so that this might occur and we might observe what happens.

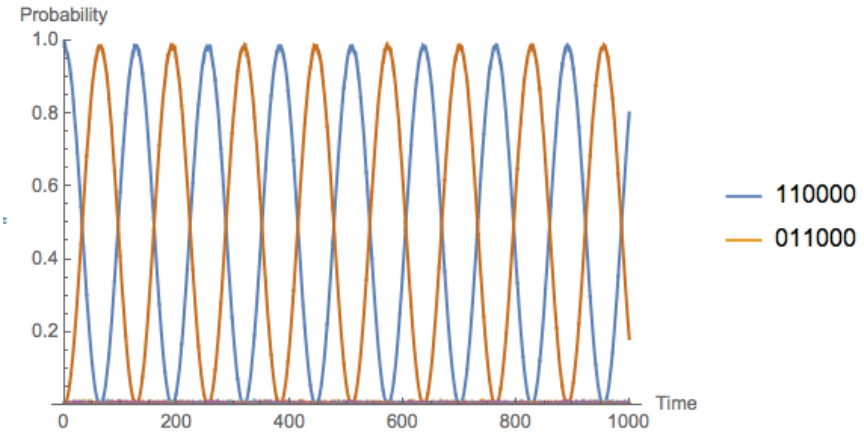


Figure 17: The dynamics of a system with an initial state of 110000 where $\varepsilon = J_z$

As observed in Fig. 17, the only states that occur in this system are states where there is a bounded pair more than one site away from the site of the defect. Though the energy would be the same if we had a split pair with one up-spin on the site of the defect, this does not happen in the evolution of the system. The reason this does not happen, is due to the fact that there is quantum interference.

If we examine the state $|011000\rangle$ that *does* appear in the dynamics in Fig. 17, keeping with the rules of dynamics that we stated above, that a bounded pair moves in a two-step process, there are two configurations that can theoretically occur by conservation of energy as the two excitations move to the right:

Initial state	Step 1	Step 2	
↓↑↑↓↓↓	↓↑↓↑↓↓	↓↓↑↑↓↓	(A)
	↓↑↓↑↓↓	↓↑↓↓↑↓↓	(B)

On the line (A) above, we recovered a doublon after two steps and on the line (B), one of the excitations moved to the defect site. Both cases maintain the energy of the initial state. However, due to the fact that there are two possible ways for the configuration ↓↑↑↓↓↓ to evolve, the two

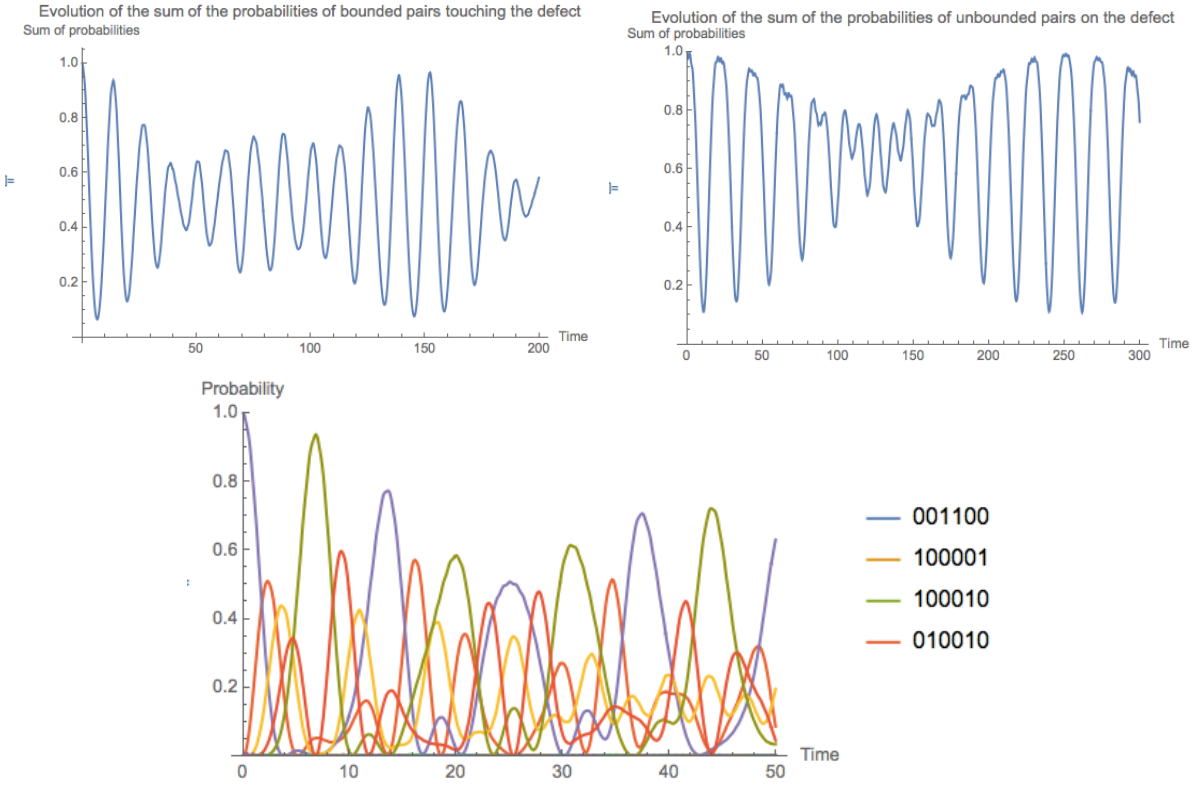
possible configurations interfere destructively with each other and neither occurs within the dynamics of the system.

After examining this unique case, we can now move on to discussing the dynamics of the other initial states in our system.

8.3 Dynamics due to different Initial States

1. When our initial state is a bounded pair right next to the site of the defect (on site 5) $|001100\rangle$, these are our results

(a) (b)



(c)

Figure 19: These figures represent the dynamics that occur as a result of a doublon being adjacent to the site of the defect. (a) shows the sum of participation of the bounded pairs touching our defect, (b) shows the unbounded pair with one upspin on the defect, and (c) illustrates all the participating bases in the dynamics.

In this scenario the system evolves such that the only bases that appear in the system will be bases that maintain the same energy as the initial state.

$|001100\rangle$: $+\frac{Jz}{2} - \frac{\varepsilon}{2} = 5 - 5 = 0$

$|010010\rangle$: $-\frac{Jz}{2} + \frac{\varepsilon}{2} = -5 + 5 = 0$

As such, our system will evolve and have the probability of having states from either category: bounded pair not on the defect, but right *next* to it, and unbounded pair with one excitation on the defect. The bounded pair not on the defect will have to be next to the defect because we are keeping with the "one hop" idea. Starting with the state |001100>, with a single hop, the excitation falls on the defect site: |001010>. As such the up-spin next to the defect will move one site over and be on the defect, separating itself from the other up-spin. This case is different from the previous one in Sec.8.2, where the motion of the bound pair necessarily required two steps to find another state with its energy.

2. When our initial state is a bounded pair on the defect $|001100\rangle$, these are our results

(a) (b)

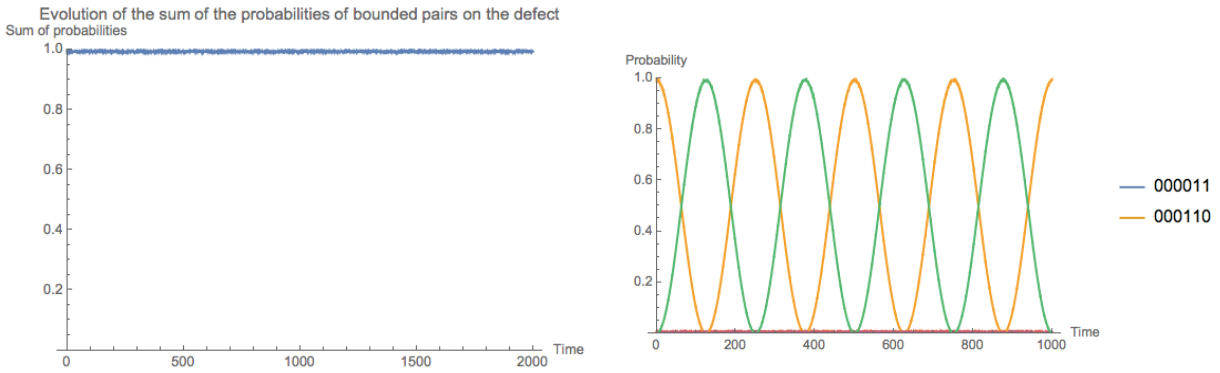


Figure 20: in (a) the only participating configurations in the dynamics are ones with a doublon that has one up-spin on the site of the defect (site 5). In (b) the participating configurations in this dynamics are clearly exposed.

This is the case (c) described in Sec.8.1. In this scenario, the only way for the system to maintain its energy is to evolve into other bounded pairs on the defect. An evolution to a state that includes an unbounded pair, would not have the same energy, and an evolution to a state not on the defect, would also not maintain the energy of our system.

3. When our initial is an unbounded pair on defect, these are our results

(a) (b)

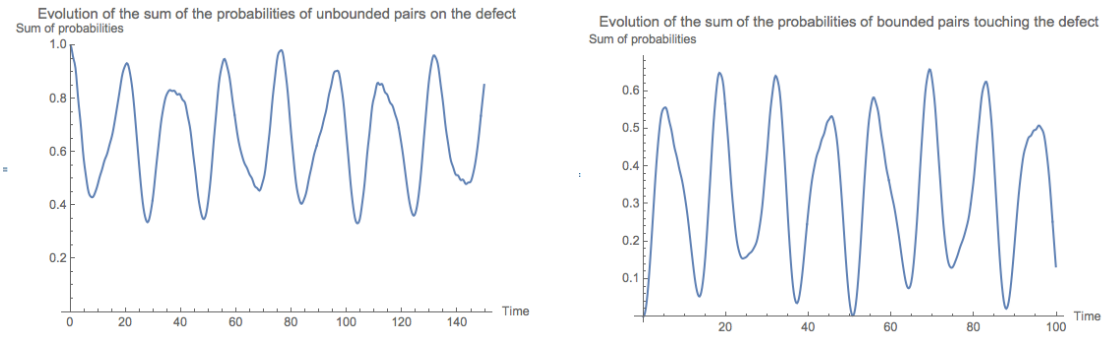


Figure 21: These figures represent the dynamics that occur as a result of the unbounded pair having one up-spin on the site of the defect. (a) shows the sum of participation of an unbounded pair with one up-spin on the defect, (b) shows the sum of participation of the bounded pairs touching our defect.

These graphs reflect the evolution of our system due to an initial state with an unbounded pair on defect. In this scenario the system evolves such that the only bases that appear in the system will be bases that maintain the same energy as the initial state. This results in the same scenario discussed earlier in the case (1) above where the initial state was the bounded pair adjacent to the defect.

4. When our initial state is an unbounded pair with neither up-spins on the defect, these are our results

(a) (b)

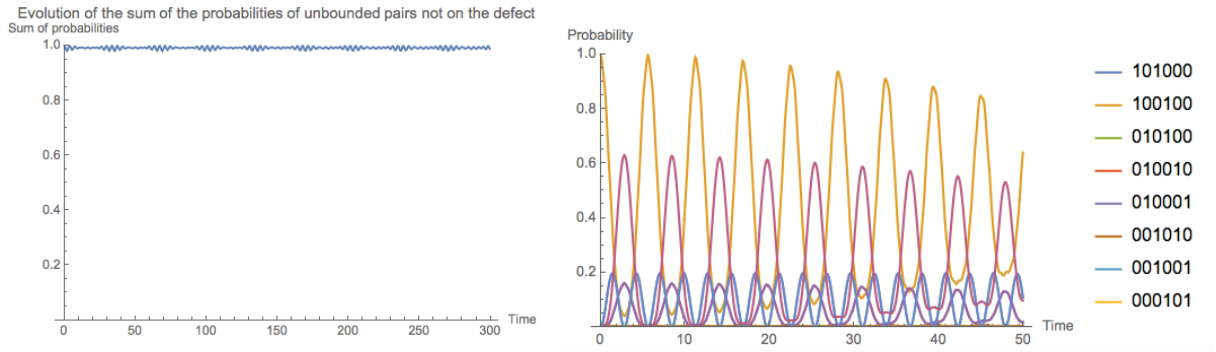


Figure 22: in (a) the only participating configurations in the dynamics are ones with an unbounded pair where neither up-spin is on the site of the defect (on site 5). In (b) the participating configurations in this dynamics are clearly exposed.

This is the case (d) discussed in Sec.8.1. In this scenario, the only way for the system to maintain its energy is to evolve into other unbounded pairs not on the defect. An evolution to a state that included a bounded pair, would not have the same energy, and an evolution to a state on the defect, would also not maintain the energy of our system.

Now that we have discussed the dynamics of our system in a 1D chain, let's discuss the two-dimensional (2D) plane.

9. Two-dimensional System

In this section, we will discuss the structure of a 2D system as well as the dynamics of such a system and how it compares to a 1D system.

9.1 Description of the System

The 2D system behaves similarly to the 1D system: the first and last site connect, forming a ring. With a 2D system, the first and last site of every column connect as well as the first and last site of every row. Ultimately, this forms a donut-like shape, as displayed in the image below on the right Fig.23(b). It's important to note in the donut diagram that the the inner circle does not correspond to a stronger interaction, despite the closer proximity between the sites.

(a) (b)

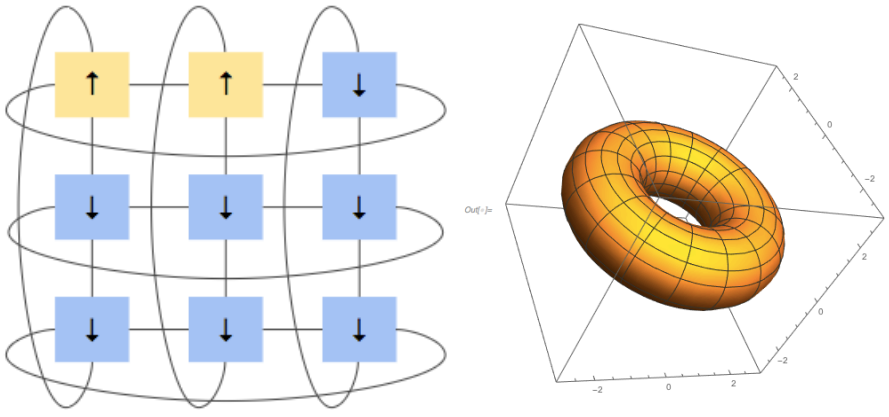


Figure 23: The structure of the 2D system is portrayed in (a) as the connection between the first and last sites in rows as well as columns. (b) presents a more visual representation, in the shape of a donut.

Much as we denoted the 1D system in a chain of 1's and 0's, with the 1's representing the up-spins and the 0's the down-spins, we can represent the 2D system in a matrix form with 1's and 0's as well.

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

The up-spins are free to move to their right, left, up, and down, with the full flexibility of the donut-like shape of the 2D system.

9.2 Evolution of the 2D System

The main question we need to examine, is whether or not the doublons are as robust in the 2D system as they are in the 1D system. In the 1D system, the doublons (away from the defect site by at least one site) do not break, rather the system evolves to maintain the structure of the two up-spins neighboring each other. Can the same thing be said for the 2D system where there are many more channels in which the up-spins can move?

By taking one example with one type of initial state, we can sufficiently explore this question and find the answer.

If our initial state is $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}$, with the site of the defect being the top left corner, then our configuration would be one of a bounded pair more than one site away from the site of the defect. If our doublon is indeed so robust, we would expect the system to evolve in such a way that we would only find configurations with a bounded pair more than one site away from the site of the defect.

(a) (b)

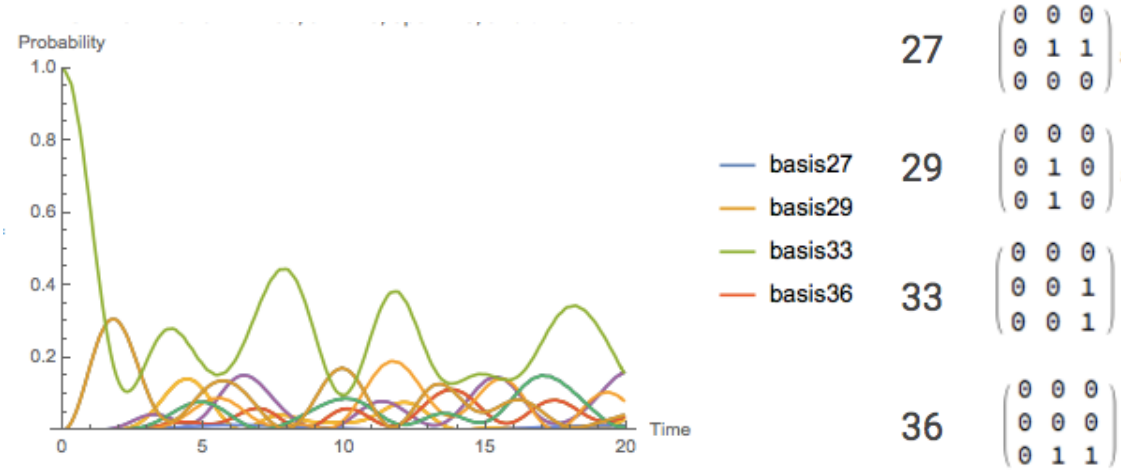


Figure 24: In (a) we observe the evolution of the system and the bases that clearly participate in its evolution. On the right, (b) shows the configurations of each of the participating bases.

As shown in Fig. 24, the bases that appear within the dynamics are the bases with a configuration of a doublon more than one site away from the site of the defect. From this we can conclude that the 2D system behaves much like the 1D system. The doublons in the 2D system are just as robust as the doublons in the 1D system, despite the extra channels for movement. Observing the graph carefully in Fig.24(a) will reveal that there appears to be some other configurations participating in the dynamics of the system as well. This is noise due to the fact that our system is of such a small size. The many channels in such small quarters, give rise to some noise. We tested larger systems with more sites, and in those systems the noise disappears entirely and the 2D system behaves just like the 1D system.

My analysis of the 2D system was extensive. We investigated several initial states, but the example above summarizes well our results.

10. Conclusions:

In this study we examined two different types of systems: a one-dimensional chain and a two-dimensional plane. We used the spin ½ model to represent the particles and sites in our system. We examined the influence of the J_z Ising interaction between neighboring sites, as well as the effect the defect site had on our system. After observing these factors in a static system, we then observed our 1D system as it evolved throughout time. We specifically looked at the configurations with two up-spins neighboring each other (doublons) to see if these doublons persist throughout the evolution of our system. We introduced the defect site in order to allow for other configurations without doublons to have the same energy as configurations with a doublon to study the robustness of the doublon: was the persistence of the doublon configuration due solely to energy conservation? Or did the doublon have a unique robustness that endured throughout evolution? We discovered that while energy conservation is, of course, required in order to evolve into other configurations with a doublon, it is not sufficient to break the doublon – the doublon is robust.

After concluding this about 1D systems, we set out to see if the same quality exists in 2D systems. We had our doubts: the 2D system has many more avenues in which the up-spins could move; we would expect that due to these extra channels the doublon would split. We were surprised to note that, in fact, the doublon behaved precisely as it did in the 1D system and thus we concluded – the doublon is robust in the 2D system as well.

While these experiments were done computationally, these results could be tested in a lab in experiments with cold atoms in optical lattices, such as those where the doublons were already studied.

11. Acknowledgements:

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