Quantum Interference as the Cause of Stability of Doublons

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I. Abstract

Quantum mechanics describes the behavior of microscopic objects, as opposed to classical physics, which describes macroscopic systems. Since in our daily lives we deal with macroscopic objects, many of the phenomena described by quantum physics are sometimes counterintuitive. One such phenomenon is described in a recently published paper [1]. The experimentalists found that repulsively bound particles, also known as doublons, would remain together for long periods of time. As opposed to our general expectation that only attractive forces can bind objects together, the particles were able to remain united despite these repulsive forces.

I have studied a one dimensional quantum system with on-site repulsive interaction containing multiple sites and two particles. In my research, I compared two scenarios: one where both particles occupy the same site, and are thus subject to repulsive interaction, and one where the two particles occupy separate sites. I have investigated how the particles behave as a result of their interaction. In particular, I wanted to understand the conditions under which bound pairs would remain together and the conditions under which they would break apart. The long lifetime of the bound pairs is a result of the energy difference between these states and the states where each particle is on a singly occupied lattice site. I also introduced defects into the system to counterbalance energy differences between the two possibilities and to see if these different states would finally couple. My goal was to study how the interplay between the defects and interactions affects the behavior of the system and whether or not the bound pairs would split. Even when it was energetically favorable, I saw that the defect site does not always cause the bound pairs to split. I claim that this may be a result of destructive quantum interference.

My work was theoretical and heavily based on numerical studies. Under some conditions, analytical solutions are possible. I have shown analytical results for the simplest scenario of a single particle in the absence of defects. I have compared the numeric and analytic computations and they produced the same results.

II. A Glimpse into Quantum Mechanics

For thousands of years mankind has strived to describe faithfully the elegant operation of the physical world. The laws of classical physics suited that purpose: they were clear and concise, generalized to create consistency and precise in their specifics. These rules were obeyed and never broken. At the end of the 19^{th} century and into the 20^{th} century, researchers were able to begin experimenting on the quantum level. New technology allowed the discovery, isolation, and manipulation of single particles. The results obtained from experimentation with these particles were not what was hypothesized but, instead, seemed to undermine the validity of the classical laws. Those laws, once thought absolute, were not inviolate, after all, it seemed. Thus, over the past century, a new order was sought – one that would explain the mysteries of quantum physics – and that order is known today by the name of quantum mechanics.

There are some intrinsic differences between the study of classical physics and quantum mechanics, and they are best understood through the explanation of some of the experiments that founded quantum mechanics. For the purpose of this thesis, I will only need to discuss the "double-slit" experiment (as it is called), and this will be sufficient to explain

the foundational topics critical to understanding the methods and results of my numerical studies.

The "double-slit" experiment (Fig.1) was, at first, a gedanken (thought) experiment of Richard Feynman to evidence the wave-particle duality of quantum particles.

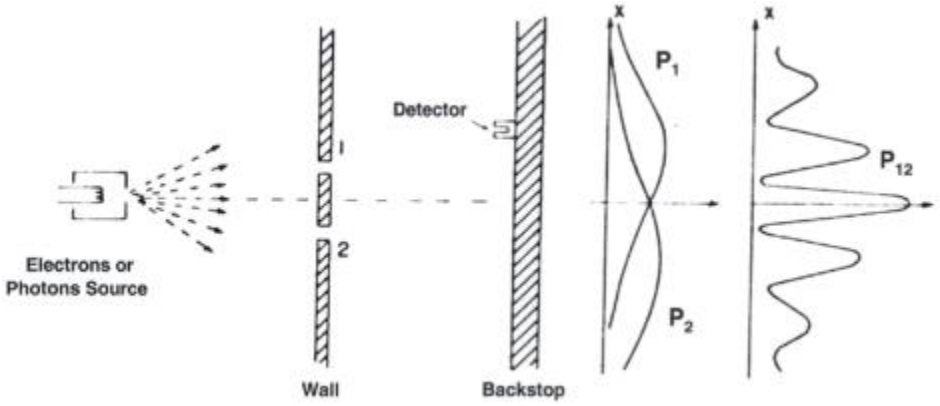

Figure 1: A light source emits electrons or photons toward a wall with two openings. A detector on the backstop counts the number of particles to hit it. P_1 and P_2 are the probability functions for each of the openings when they are opened individually and P_{12} is the probability function when both are opened at the same time.

When there is only one opening in the wall, the probabilistic function describing the particles hitting the detector is easy to understand: it has higher probability directly across from the slit and smaller probability as it moves to either side. The interesting part of this experiment comes when both slits are open at once. When this happens, there is an interference pattern, which is a shocking consequence of the wave nature of the particle. At detection we find the emitted particles at specific points, but their motion through the slits all the way to the screen is dictated by a wave. This experiment was later realized and served as another confirmation of the wave-particle duality of quantum particles.

III. Schrodinger's Equation and Time Evolution

In classical physics, the equations of motion along with specified initial conditions define the position and momentum of an object at any time, $x(t)$ and $p(t)$. In quantum mechanics, it is impossible to know at the same time the exact locations and momentum of the quantum particles. Both can only be known to a limited degree. This is known as the uncertainty principle.

The uncertainty principle is due to the fact that quantum mechanics is an intrinsically probabilistic theory: on the quantum level, only the *probability* that a particle is in a given range at a specific time can be known. The vehicle that relates this probability is the wave function, $\Psi(x,t)$, and it is obtained by solving Schrodinger's equation,

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

Similar to Newton's law, with initial conditions, $\Psi(x,t)$ is found for any time. The probability of finding the particle in a certain interval, $x + dx$, at time t is given by $|\Psi(x,t)|^2 dx$.

The narrower the wave function in x, the less uncertainty there is about the position. But a property of waves is that as the wave in x becomes narrower, the width of the wave number increases. Since momentum (p) is directly proportional to the wave number (k) [expressed mathematically, $p = \hbar k$, where ħ, the coefficient of proportionality, is Planck's constant], the more certain the position, the wider the range of possible values for the momentum. This produces the upper limit of certainty of position and momentum that can be attained for any particle at any time.

When a measurement is performed to try to find where the particle is at any given instant of time, the system collapses to one position and the wave properties are lost. If the same exact experiment is repeated several times, the particle may be found in different places every time the measurement is done. But when the system is undisturbed, the particle is in a superposition of different positions. It is not in only one state, but, rather, it is spread out among many states.

If the potential, V, in Schrodinger's equation (1) does not depend on time, the wave function can be separated into time-independent and position-independent components $\Psi(x,t) = \psi(x)f(t)$. The solution for the time-dependent part is simply: $f(t) = e^{-iEt/\hbar}$. The time-independent Schrodinger equation is

$$\mathrm{H}\,\psi(x) = E\,\psi(x) \tag{2}$$

H in the above equation is the Hamiltonian operator. The Hamiltonian is an essential tool in the study of Physics: it is associated with the energy and determines the dynamics of a system. From (1), the Hamiltonian operator corresponds to

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{3}$$

To solve (2) and find $\psi(x)$, the Hamiltonian must be known. Once the eigenstates, $\psi_n(x)$, and eigenvalues, E_n, are found, a more general solution for $\Psi(x,t)$ can be constructed

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar} \tag{4}$$

The coefficients c_n depend on the initial state of the system.

IV. Hamiltonian of our System and Analytics

We study the one-dimensional Bose-Hubbard model described by the following Hamiltonian

$$H = -J\sum_{i=1}^{L}\left(\hat{b}_i^{\dagger}\hat{b}_{i+1} + \hat{b}_{i+1}^{\dagger}\hat{b}_i\right) + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_i(\hat{n}_i - 1) + \sum_{i=1}^{L}\varepsilon_i\hat{n}_i \tag{5}$$

Only nearest neighbor couplings are considered $(i, i+1)$, ħ is set to 1, and periodic boundary conditions are assumed. That is, our system is in 'ring form' – for a system with L sites, the first site and the site L+1 are the same. $\hat{b}$ is the annihilation operator – it removes a particle from the site indicated by the index. $\hat{b}^{\dagger}$ is the creation operator – it adds a particle to the site indicated by the index; and $\hat{n}_i$, is the number operator – its operation is $\hat{b}_i^{\dagger}\hat{b}_i$. J represents the strength of the hopping term (the kinetic energy of the system), U represents the strength of the interaction (the potential energy), and ε_i is the energy of a particle on site i. When all ε_i are equal, the system is clean. A site i with ε_i different from the others corresponds to a defect or impurity.

When there is only one or two particles and $\varepsilon_i = 0$, the eigenvalues and eigenstates of this Hamiltonian can be found analytically. I will show this for the simple case of a single particle, where $(\hat{n}_i - 1) = 0$. For this case, the Hamiltonian reduces to

$$H = -J\sum_{i=1}^{L}\left(\hat{b}_i^{\dagger}\hat{b}_{i+1} + \hat{b}_{i+1}^{\dagger}\hat{b}_i\right) \tag{6}$$

Following the Bethe Ansatz [6], the time-independent wave function can be written as

$$\psi(x) = \sum_{x=1}^{L} a(x)\, \phi(x) \tag{7}$$

where $a(x)$ is the coefficient and $\phi(x)$ is the basis vector. Our basis corresponds to vectors that have one particle on one site. The expanded version of (7) is

$$\psi(x) = a(1)|100 \ldots 0> + a(2)|010 \ldots 0> + \cdots + a(L)|000 \ldots 1>$$

The time-independent Schrodinger equation (2) becomes

$$H \sum_{x=1}^{L} a(x)\, \phi(x) = \mathrm{E} \sum_{x=1}^{L} a(x)\, \phi(x) \tag{8}$$

Since there is only one particle in this example system, the reduced Hamiltonian (6) can be applied to each of our basis vectors and a simple expression is obtained:

$$H\, \emptyset(x) = -J(\emptyset(x-1) + \emptyset(x+1))$$

If this result is inserted into (8), it yields

$$-J \sum_{x=1}^{L} a(x)(\emptyset(x-1) + \emptyset(x+1)) = E \sum_{x=1}^{L} a(x)\, \phi(x)$$

Expanding this equation and gathering the matching basis vectors, $\emptyset(x)$, from both sides, this general equation is obtained:

$$E\, a(x) = -J\big(a(x-1) + a(x+1)\big) \tag{9}$$

In order to solve (9) for the coefficients of ψ(x) from (7), $a(x)$, the Bethe Ansatz trick is to use the boundary condition for the ring structure:

$$a(x) = a(x + L)$$

Next, a probable form for the solution to $a(x)$ can be guessed to be

$$a(x) = e^{ix\theta} \tag{10}$$

which, combined with the boundary condition, yields

$$e^{ix\theta} = e^{i(x+L)\theta} = e^{ix\theta}e^{iL\theta}$$

Therefore, $e^{iL\theta}$ must equal 1 which means that $L\theta = 2\pi$ n, resulting in

$$\theta = \frac{2\pi\, n}{L} \tag{11}$$

Inserting (10) into (9) yields

$$E\, e^{ix\theta} = -J(e^{ix\theta}e^{-i\theta} + e^{ix\theta}e^{i\theta})$$

$$E = -J(e^{-i\theta} + e^{i\theta})$$

$$E = -2\,J\cos\theta$$

Inserting (11) into the previous equation, leads to the equation for the eigenvalues:

$$E_n = -2\,J\cos\frac{2\pi\, n}{L}\text{, where } n = 0, \pm 1, \pm 2, \pm \ldots, +\frac{L}{2} \tag{12}$$

Combining (7), (10) and (11), the expression for the eigenvectors becomes

$$\psi_{\mathrm{n}}(x) = \sum_{x=1}^{L} e^{\frac{i2\pi xn}{L}} \phi(x) \tag{13}$$

The final step is to normalize each eigenvector with $\frac{1}{\sqrt{L}}$. This is because the sum of the probabilities for the basis vectors must equal to one.

For the case of a single particle, I obtained the eigenvalues and eigenvectors numerically and analytically. Analytically, for a chain with $L = 4$ sites and using (12), I found these values for the eigenvalues: two degenerate states with energy 0, one state with energy -2, and one with energy $+2$. Numerically, I found essentially the same values: $\{-2., 2., 2.3 \times 10^{-16}\ and\ 0\}$. The eigenvectors corresponding to eigenvalues 2 and -2 were exactly the same when found analytically using (13) and numerically. Since the others eigenvalues are degenerate the eigenvectors I obtained analytically were at first different than those obtained numerically. However, since any linear combination of degenerate eigenvectors is also an eigenstate of the system, I was able to match my analytical and numerical results.

The eigenvalues and eigenvectors can be found analytically for the case of two particles and even in the presence of an impurity, provided this impurity is very large [4]. In this thesis, however, I will study the case of two particles and an impurity numerically.

V. Remarkable Discovery of 'Doublons'

My numerical experiments are a motivated consequence of a recent discovery made by a group of scientists [1]. They found that although, typically, stable composite objects are

bound together with attractive forces, in their experiment, repulsive forces were able to accomplish the same thing. These repulsively bound atoms are called doublons. What is noticed in experimentation is that these pairs of particles stick together and remain with each other for long periods of time.

This experiment was performed on an optical lattice. Optical lattices are formed by criss-crossing laser beams to form standing waves. These waves localize the atom to confined regions of space, creating in this way an artificial crystal. A great advantage of this experiment is that the dissipation is almost null and therefore the particles can remain together for longer periods of time. They exhibit long lifetimes, about 700 ms, even when they collide. These repulsively bound pairs can be observed from their momentum distribution and spectroscopic measurements.

VI. My Numerical Analysis

I have done numerical studies on these doublons. Because my analysis is purely computational, it is, therefore, free of external forces and the pairs in my experiments last forever. Consequently, I am able to observe the way these pairs exist, move, and interact. Similar to the system used to detail the analytics, my experiments are done on a one-dimensional system in a ring form ($i = i + L$) with two particles. Because these systems are microscopic, the laws of quantum mechanics apply.

In order to obtain the Hamiltonian matrix for my one-dimensional system, a basis must be selected, where each vector corresponds to one possible configuration for the atoms

in the chain. The operations outlined in the Bose Hubbard model of the Hamiltonian are performed on each of the possible arrangements of our system.

The particles can either be in separate sites or in the same one. The equation

$$N = \frac{sites!}{particles!\,(sites - particles)!} + sites$$

is used in order to obtain the number of possible states of this system. For example, in the case of 4 sites and 2 particles, there are 10 possible arrangements for the particles. Each of these arrangements are written in the form, |1100>, |1010>,…|0002>. The collection of these arrangements (Fig.2) is called the basis.

Basis for L=4	
1	1 1 0 0
2	1 0 1 0
3	1 0 0 1
4	0 1 1 0
5	0 1 0 1
6	0 0 1 1
7	2 0 0 0
8	0 2 0 0
9	0 0 2 0
10	0 0 0 2

Figure 2: basis vectors of system with 4 sites and 2 particles

In order to obtain the Hamiltonian Matrix for this system, the Hamiltonian, (5), is applied to each of the elements of the basis. For the first sum, $-J\sum(\hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_{i+1}^\dagger \hat{b}_\iota)$, the basis vector couples to two different states for each element of the sum. When a particle is added to a site that has n elements, the expression is multiplied by $\sqrt{n+1}$; and when one particle is removed from a site that already has n particles, the expression is multiplied by

$\sqrt{n}$. The number operator $\hat{n}_i$ in the second sum in the Hamiltonian, $\frac{U}{2}\sum \hat{n}_i(\hat{n}_i - 1)$, will not change the basis; rather, it will only change the coefficient before the basis. If the annihilation operator is used on a site that doesn't have a particle, then the whole operation fails and that element produces nothing for the sum.

So, for example, if the Hamiltonian operator is applied to the first element of the basis vector, $|1100>$, the Hamiltonian operator would yield: $-J(\sqrt{2}\,|2000> + \sqrt{2}\,|0200> + |1010> + |0101>)$. The U component equals zero for this case and until later in the experiment the impurity, ε, will remain zero. An example in which the U component yields a result other than zero is when these operations are applied to the 7th element of the basis, $|2000>$: $-J(\sqrt{2}\,)|1100> \; -J(\sqrt{2}\,)|1001> + \frac{U}{2}(2)|2000>$. Performing these operations on each basis vector $|basis_j>$ gives $H|basis_j>$. When all these operations for each of the basis vectors are completed, the Hamiltonian matrix can be created. Using the basis as the rows and columns, a 10x10 matrix is produced. The values for the matrix elements are found by computing $<basis_i|H|basis_j>$ as i and j go from 1 to 10. The value of the matrix in the ith row and jth column is the coefficient of the basis vector in $H|basis_j>$ which is identical with the ith basis vector. For example, the element in the 7th row and 7th column would be $<2000|H|2000>$. It was computed above that $H|2000> = -\sqrt{2}\,J\,|1100> \; -J(\sqrt{2}\,)|1001> + U\,|2000>$, so applying $<2000|$ to this will destroy the J value because the elements of the basis $|1100>$ and $|1001>$ are orthogonal to $<2000|$. The value in the matrix will be U. Another example is the element in the 8th row and 7th column: $<0200|H|2000>$. Again, $H|2000> = -\sqrt{2}\,J\,|1100> \; -J(\sqrt{2}\,)|1001> + U\,|2000>$, and because $<0200|$ is orthogonal to all three basis vectors

obtained, the element in the Hamiltonian will be 0. This is done for every element of the basis. Fig.3 is the Hamiltonian obtained for the system with 2 particles and 4 sites:

$$\begin{bmatrix} 0 & -J & 0 & 0 & -J & 0 & -\sqrt{2}J & -\sqrt{2}J & 0 & 0 \\ -J & 0 & -J & -J & 0 & -J & 0 & 0 & 0 & 0 \\ 0 & -J & 0 & 0 & -J & 0 & -\sqrt{2}J & 0 & 0 & -\sqrt{2}J \\ 0 & -J & 0 & 0 & -J & 0 & 0 & -\sqrt{2}J & -\sqrt{2}J & 0 \\ -J & 0 & -J & -J & 0 & -J & 0 & 0 & 0 & 0 \\ 0 & -J & 0 & 0 & -J & 0 & 0 & 0 & -\sqrt{2}J & -\sqrt{2}J \\ -\sqrt{2}J & 0 & -\sqrt{2}J & 0 & 0 & 0 & U & 0 & 0 & 0 \\ -\sqrt{2}J & 0 & 0 & -\sqrt{2}J & 0 & 0 & 0 & U & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{2}J & 0 & -\sqrt{2}J & 0 & 0 & U & 0 \\ 0 & 0 & -\sqrt{2}J & 0 & 0 & -\sqrt{2}J & 0 & 0 & 0 & U \end{bmatrix}$$

Figure 3: Hamiltonian for system L=4, 2 particles

What is noticed when studying this Hamiltonian is that the diagonal elements [those elements that for $\langle basis_i|H|basis_j\rangle$, i=j] equal zero for the states when the two particles occupy separate positions (when the basis contains zeros and ones) and equal U for the paired states (when the basis contains zeros and two). For the off-diagonal sites, if the two elements of the basis are the same but differ by 1 in two neighboring sites, then: if neither basis has a 2, the Hamiltonian equals –J; if one basis has a 2, it equals $-\sqrt{2}J$. All other elements equal zero. The Hamiltonian is symmetric.

This Hamiltonian gives the energy of the system. The values U (potential energy), and J (kinetic energy), need to be defined. Once these have been defined, the eigenvalues, which represent the possible energies of the system, and the eigenvectors, which detail the probability that the system is in each of the ten possible states at the corresponding eigenvalues, can be computed.

Eigenvalues and eigenvectors can be computed by hand only for very small matrices or specific cases. In general, computers are needed. There are several ways to solve for the eigenvalues by hand. Here I will present two of them: if the Hamiltonian is already diagonal then the values on the diagonal are the eigenvalues. Alternatively, the eigenvalues can be solved for by subtracting Iλ from the Hamiltonian matrix, finding the determinant and equating this polynomial to zero, and then solving for the values of λ which are the eigenvalues. Once the eigenvalues have been obtained, the eigenvectors can be determined using the equation

$$H\psi_{\mathrm{i}} = E_i\psi_{\mathrm{i}}.$$

The number of eigenvalues corresponds to the dimension of the system and each eigenvalue represents a possible energy of the system. For each eigenvalue there is a corresponding eigenvector. The eigenvector is a vector where each element corresponds to the probability amplitude of a basis vector. When measured, though, the system collapses to one state with the probability given by the eigenvectors. The values of the eigenvectors should be normalized.

With these eigenvectors and eigenvalues, (4) can be used to obtain the wave function, $\Psi(\mathrm{t})$. The probability amplitude for each basis vector can be graphed to show their participation in time. These graphs will change for different initial configurations of the system such as changes in the value of U and different initial states. J = 1 sets the energy scale.

High potential energy systems. I began with a system of 4 sites and 2 particles. The particles were initially separated in the configuration, |1 0 0 1>, with one particle on the first

site and one particle on the fourth site and the middle two sites empty. The potential energy of the system, U, was set to 200 which is a much higher value than the hopping strength J (set to 1). For each possible basis vector (i.e. configuration) of the system, I graphed the probability in time that the system would move into that configuration from the initial configuration. Those probabilities each appear in Fig.4.

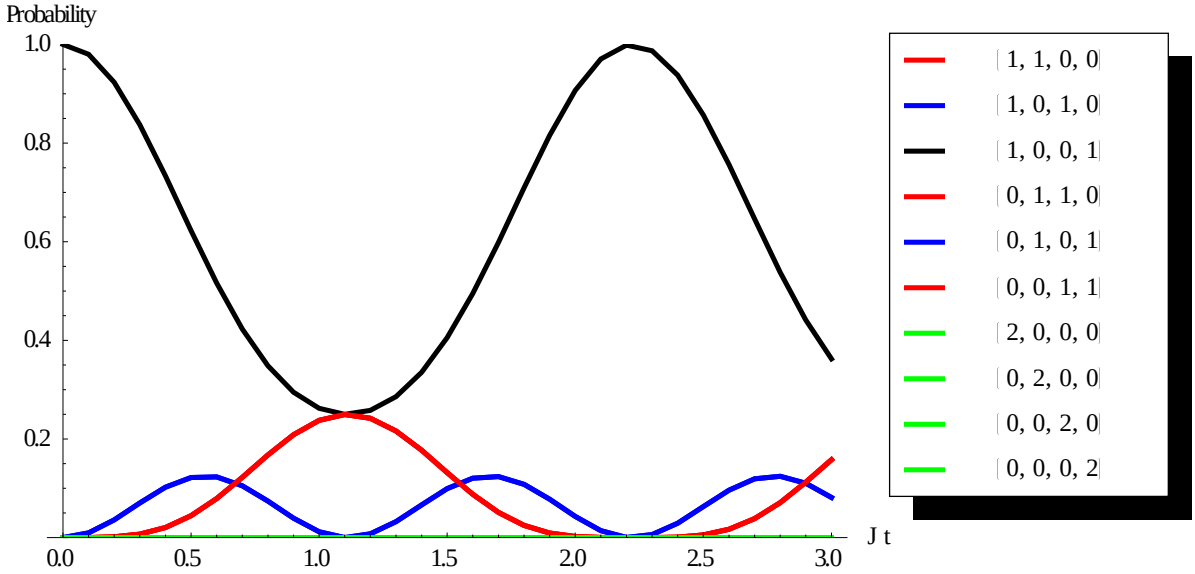

Figure 4: Probability of each basis vector in time. L=4, 2 particles, U = 200, Initial state: $\Psi(0) = |1\ 0\ 0\ 1\rangle$

If the system begins in a certain state or configuration and, upon running the experiment, another state has a probability other then zero of occuring, then the two states are said to couple with each other. This experiment ran for $t=3J^{-1}$ and within that time the initial state was able to couple with other states. One observation I made was that states one through six, the states where the particles are separated from each other, just like the initial state, couple with each other but the last four states, the states where the two particles occupy the

same site (also called paired states), did not couple at all. This means that there is practically zero probability under the specified conditions for the paired states to occur.

I repeated this exact experiment with the initial state set to each of the states where the particles are separated, states one through six, and each time I got the same result: the unpaired states couple with each other but did not couple with the paired states.

Another observation I made about this graph is that some of the states couple with the initial state, in exactly the same manner. For example, the probability plot for states 1, |1100>, 4, |0110>, and 6, |0011>, are all exactly the same which means they couple with state |1001>, in the same way. States 2, |1010>, and 5, |0101>, also have identical probabilities but lower than that for states 1, 4, and 6.

A possible explanation for this is the structure of the states. I noticed that the states that interacted similarly have similar structures. States 1, 4, and 6 are the states where the two particles are in sites that are directly next to each other. States 2 and 5 are the two states where the two particles are separated by one site on each side. Because the system is a ring, state 3 (initial state) is also in a configuration where the two particles are next to each other. The graph indicates that states 1, 4 and 6 (the red line) interact more with state 3 (black line) than do states 2 and 5 (blue line). And this makes perfect sense in terms of structure. State 3 has the same structure as states 1, 4, and 6.

Again, I repeated this experiment but this time the initial state was one of the paired states:

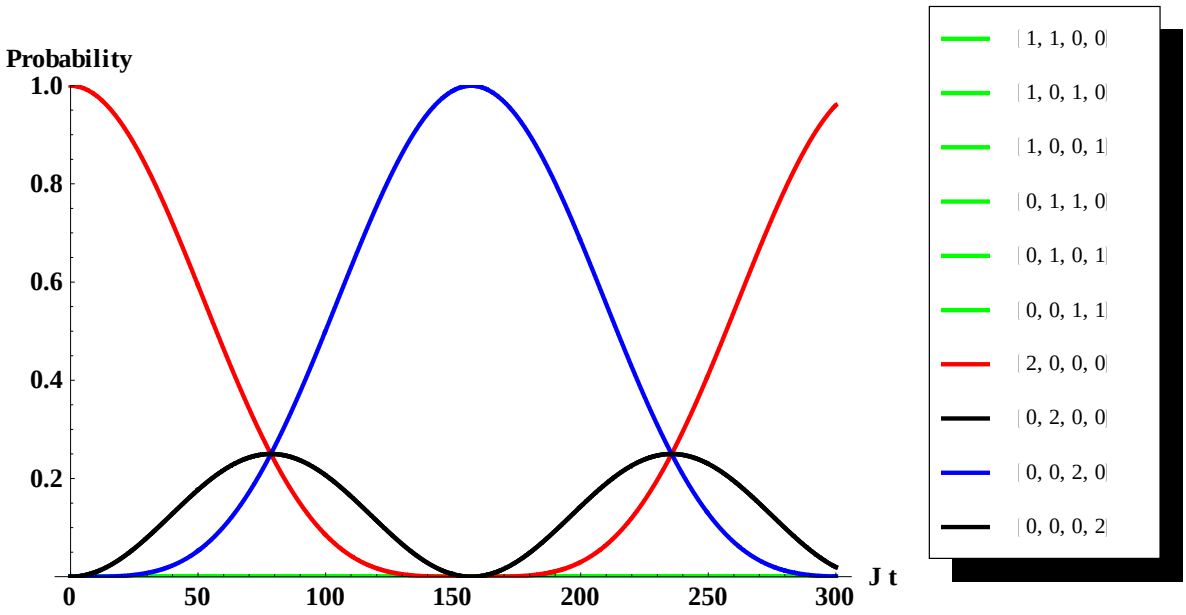

Figure 5: Probability of each basis vector in time. L=4, 2 particles, U = 200, Initial state: $\Psi(0) = |2\ 0\ 0\ 0\rangle$

Very noticeably, only the paired states appear in this graph. States one through six, the unpaired states, have zero probability of occuring. When the experiment was repeated, setting each of the paired states as the initial state, the same result was obtained – each time states one through six did not appear.

Another observation I made was that when starting with a paired state, it took the system a lot more time for the decay of the initial state and emergence of the others. This experiment ran for $t=300J^{-1}$ (as opposed to $t=3J^{-1}$ when starting with an unpaired system). Comparison of Fig.4 and Fig.5 will show that it takes a lot longer for the particles to move when they are in pairs than when they are moving separately.

The question of whether or not the paired and unpaired states communicate with each other is the same question as whether the bound pairs will remain together or will separate. Under these conditions, it is clear that the bound pairs will remain bound and will not separate.

Low potential energy systems. The above results were obtained for systems whose potential energy was very high. I then changed the potential energy of the system to $U = 0.5$, which is lower than the hopping strength, J. Besides for the change in potential energy, the two graphs that follow, Fig.6 and Fig.7, have the same initial conditions as Fig.4 and Fig.5, respectively. What we notice now, though, is that all the states appear in both graphs:

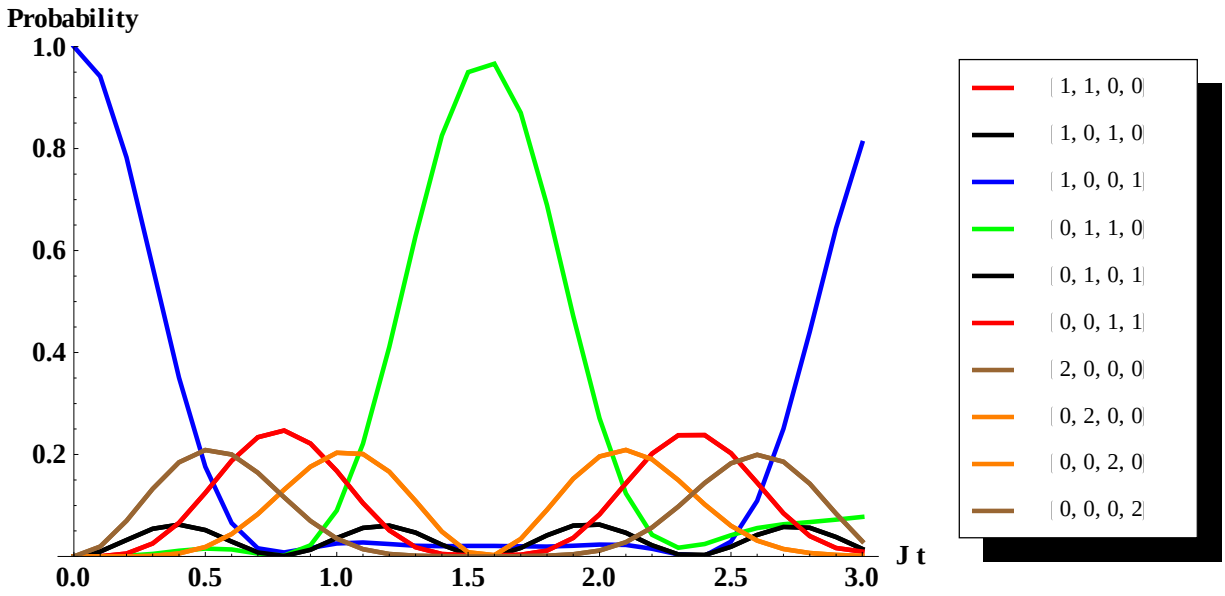

Figure 6: Probability of each basis vector in time. L=4, 2 particles, U = 0.5, Initial state: $\Psi(0) = |1\ 0\ 0\ 1\rangle$

The system in Fig.6 is initially in an unpaired state but, in this case, even the paired states couple with it. This is an interesting result and indicates that energy is the reason the states do interact sometimes and do not interact at other times.

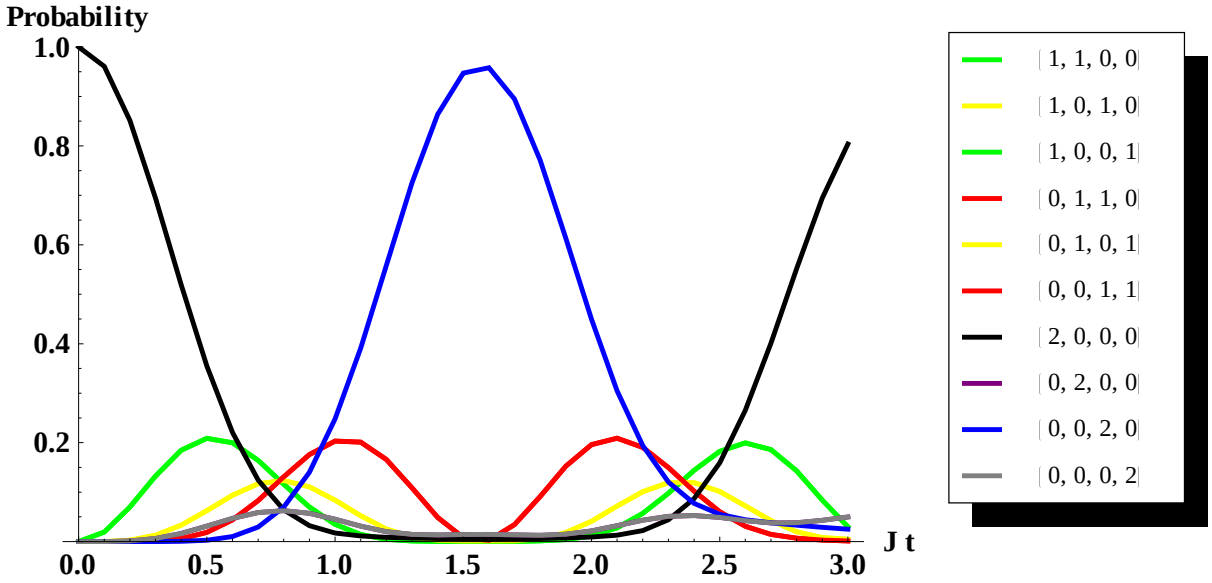

Figure 7: Probability of each basis vector in time. L=4, 2 particles, U = 0.5, Initial state: $\Psi(0) = |2\ 0\ 0\ 0\rangle$

Similarly, the graph in Fig.7 represents a system that begins in a paired state but communicates with all the possible states, even the unpaired ones.

I also noticed that this time the system did not need more time to interact with the other states. As opposed to before, when there was a delay in the experiment that began in a paired state, this experiment is very successful after $t=3J^{-1}$. At lower potential energy, state 7 does not take more time than state 3 to decay and the other states do not take longer to show up.

From these experiments, I conclude that at high potential energies, there is no effective coupling between the paired and unpaired states but at low potential energies, the paired and unpaired states do couple with each other. This is because only states with similar energies communicate with each other. When the potential energy is set low, the difference between the two kinds of states is surmountable by the hopping parameter J and thus they couple with each other, but when the potential energy is set high, the difference in energy between the two states is too great and as such they cannot effectively couple.

Introduction of an impurity. If the energy difference is, in fact, the reason for this 'miscommunication' between the two kinds of states, it would seem this gap of energy could possibly be bridged by introducing an impurity into the system. The impurity I added is an excess of energy that is placed on one site and any particle that lands on this site obtains more energy in the value of the defect (ε). The defect was placed on site 1 and ε = 200 to match the value of the potential energy, U (which is now fixed at 200 for the remainder of the experiments). I also increased the size of the system to 6 sites in order to better understand the differences in the interactions. The basis vectors are shown in Fig.8.

	Basis for L=6
1	1 1 0 0 0 0
2	1 0 1 0 0 0
3	1 0 0 1 0 0
4	1 0 0 0 1 0
5	1 0 0 0 0 1
6	0 1 1 0 0 0
7	0 1 0 1 0 0
8	0 1 0 0 1 0
9	0 1 0 0 0 1
10	0 0 1 1 0 0
11	0 0 1 0 1 0
12	0 0 1 0 0 1
13	0 0 0 1 1 0

14	0 0 0 1 0 1
15	0 0 0 0 1 1
16	2 0 0 0 0 0
17	0 2 0 0 0 0
18	0 0 2 0 0 0
19	0 0 0 2 0 0
20	0 0 0 0 2 0
21	0 0 0 0 0 2

Figure 8: basis vectors of system with 6 sites and 2 particles

The new Hamiltonian for the larger dimension and including the impurity is shown in Fig.9.

$$\begin{pmatrix}
200. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & -\sqrt{2} & 0. & 0. & 0. & 0. \\
-1 & 200. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & -1 & 200. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & -1 & 200. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & -1 & 200. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & -\sqrt{2} \\
0. & -1 & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & -\sqrt{2} & 0. & 0. & 0. \\
0. & 0. & -1 & 0. & 0. & -1 & 0. & -1 & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & -1 & 0. & 0. & -1 & 0. & -1 & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
-1 & 0. & 0. & 0. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & -\sqrt{2} & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & -1 & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & -\sqrt{2} & 0. \\
0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -1 & -1 & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -1 & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & -\sqrt{2} & \\
-\sqrt{2} & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 600. & 0. & 0. & 0. & 0. & 0. \\
-\sqrt{2} & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 200. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 200. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 200. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 200. & 0. \\
0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -\sqrt{2} & 0. & 0. & 0. & 0. & 0. & 200.
\end{pmatrix}$$

Figure 9: Hamiltonian of system with L=6, 2 particles, and defect, $\varepsilon = 200$, on site 1

For this new system, I begin the experiment in the seventh state which is |010100>. This state is unaffected by the impurity because none of the particles occupy the first site which is where the impurity is placed.

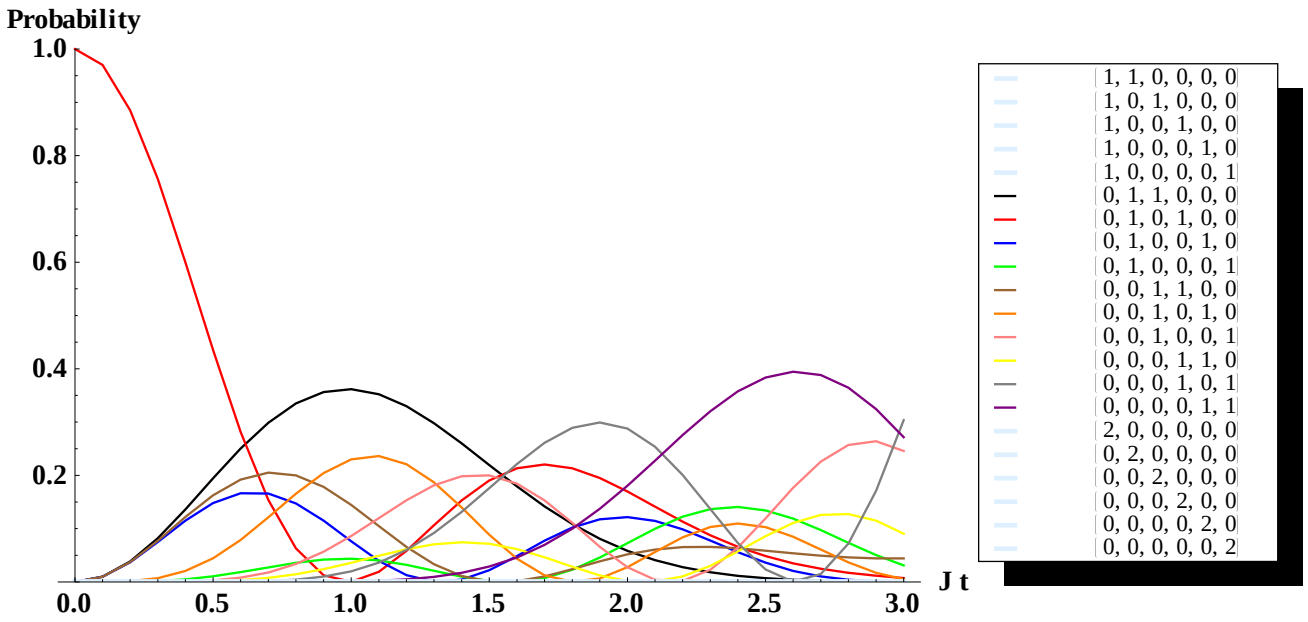

Figure 10: Probability of each basis vector in time.

L=6, 2 particles, U = 200, ε = 200 on site 1, *Initial state: Ψ(0) = |0 1 0 1 0 0>*

The result of this experiment is as I expected. The first five states, states with one particle on the site of the impurity, do not couple with the initial state because of the added energy from the impurity. Whereas, in the previous experiments all the unpaired states interacted with each other due to their similar energy levels, in this experiment, because of the added energy from the impurity, states one through five cannot couple effectively with the rest of the unpaired states. Again, as expected, states 16 through 21, the paired states, have no participation in the evolution of the initial state.

Another interesting initial state is state 16, |200000>. This state cannot couple with any other state as seen in Fig.11 because it has two particles in the site of the impurity. The energy level of state 16, ($E \sim 600$), is so much higher than any of the other states that it does not couple with any of them.

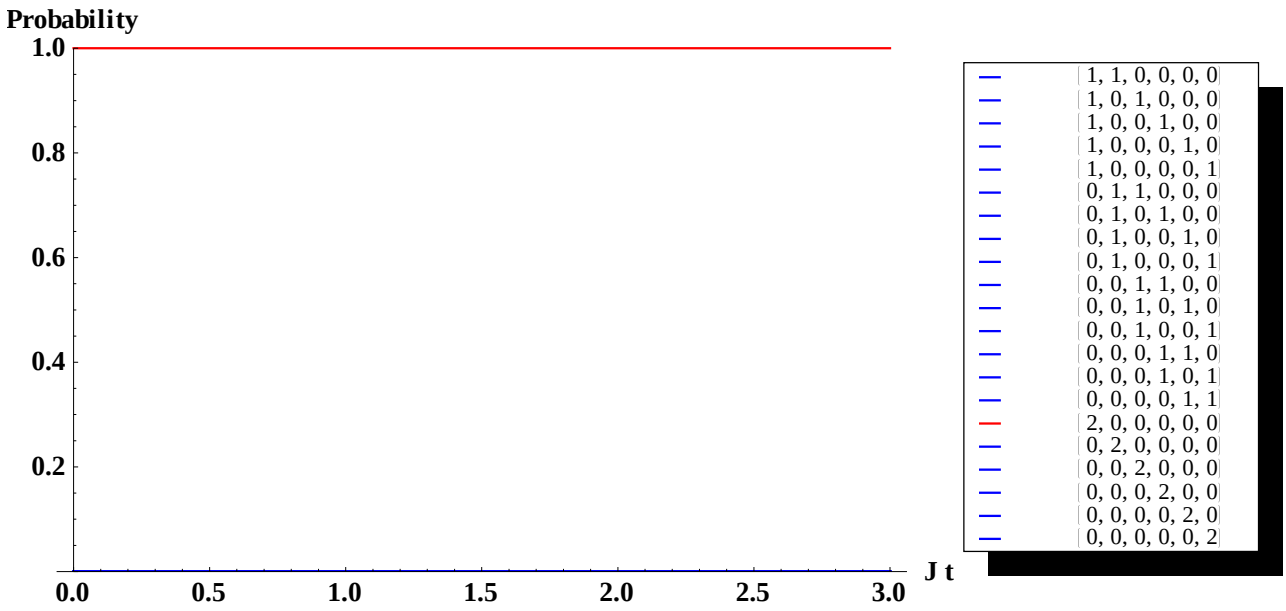

Figure 11: Probability of each basis vector in time.

L=6, 2 particles, U = 200, ε = 200 on site 1, *Initial state: Ψ(0) = |2 0 0 0 0 0>*

I want to see if the added impurity can allow communication at high potential energy between an unpaired state which has one particle on the site of the impurity and thus higher energy and a paired state that is not in the site of the impurity. In an attempt to discover this, I will present two graphs with paired initial states whose particles are not in the site of the impurity.

The first of these graphs is the graph of initial state 17, |020000>. The pair of particles in this state is in the site which is directly next to the defect site and because of the fact, as I have mentioned before, that the system is a ring the defect site neighbors both sites 2 and 6. As such, the graph for state 21, |000002>, whose paired particles are also in a site directly next to the defect site has a symmetric form to the graph of state 17 (Fig.12).

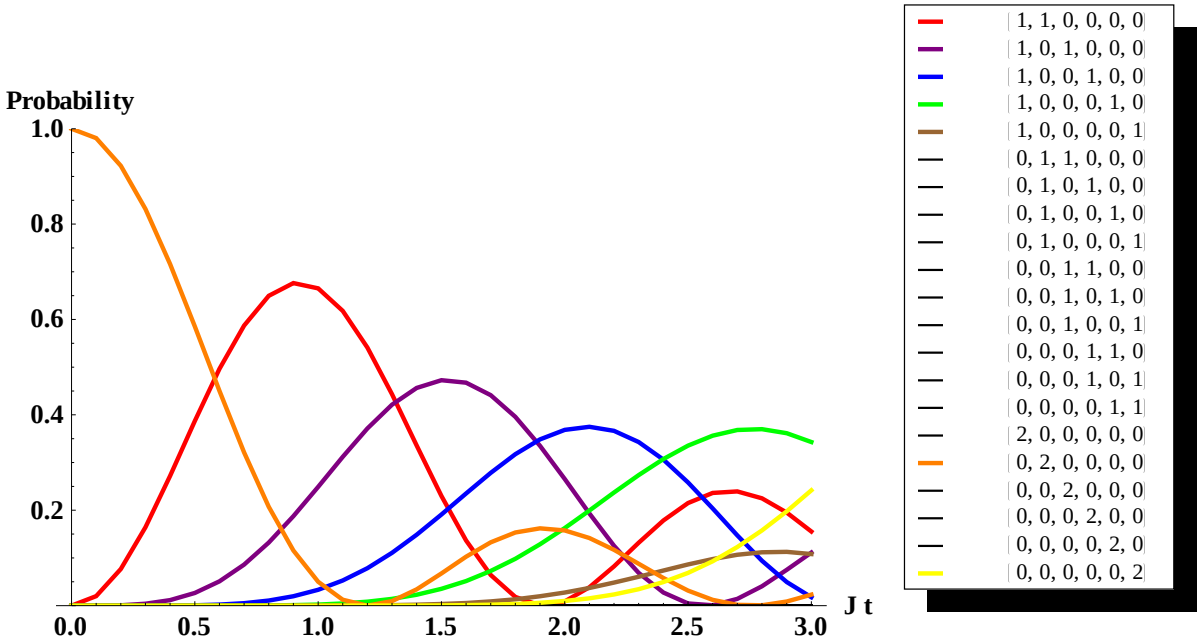

Figure 12: Probability of each basis vector in time.

L=6, 2 particles, U = 200, ε = 200 on site 1, *Initial state: Ψ(0) = |0 2 0 0 0 0>*

This result is very puzzling. The impurity seems to have worked: the initial paired state coupled with all the unpaired states that have one particle in the site of the impurity. What is puzzling is that this initial paired state, state 17, only coupled with one other paired state – state 21, which, as I stated previously, is the state symmetric with the initial state – but didn't couple with any of the other paired states.

The other graph that will help determine the effectiveness of the impurity is the graph whose initial state is state 18, |002000>. The pair in this state is not in the site directly next to the defect as was the pair in state 17.

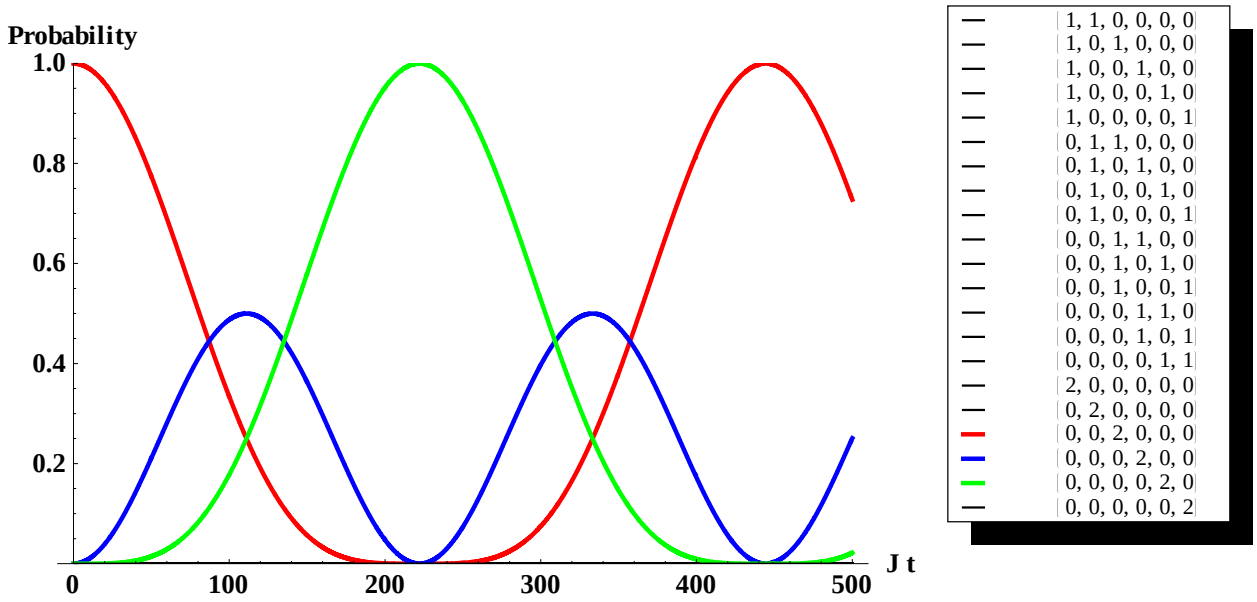

Figure 13: Probability of each basis vector in time.

L=6, 2 particles, U = 200, ε = 200 on site 1, *Initial state: Ψ(0) = |0 0 2 0 0 0>*

Here, the paired state does not couple with any of the unpaired states and only some of the other paired states. The results in Fig.12 and Fig.13 are baffling. Whereas, I had intended to discover whether the additional energy provided by the impurity would remedy the gap that exists between the paired and unpaired states, my experiments did not behave as I had expected. I expected that the results would indicate one way or the other – that the impurity did or did not bridge the gap between the two kinds of states – but my results are more complicated than that. It seems that the impurity did manage to bridge the energy gap when the paired particles were in the site directly next to the impurity but it did not bridge the energy gap when the paired particles were elsewhere.

There is, in fact, some additional energy provided to the paired state as a result of its proximity to the impurity, some sort of border effect. When the pair is near the impurity, it is

able to communicate with those unpaired states which have one particle occupying the impurity. However, when the pair is not near the impurity, it cannot communicate with any unpaired states even those with one particle on the site of the impurity.

I will show one more graph that may shed some light on these mysterious results. State 9, |010001>, is an unpaired state with both particles bordering the site of the impurity.

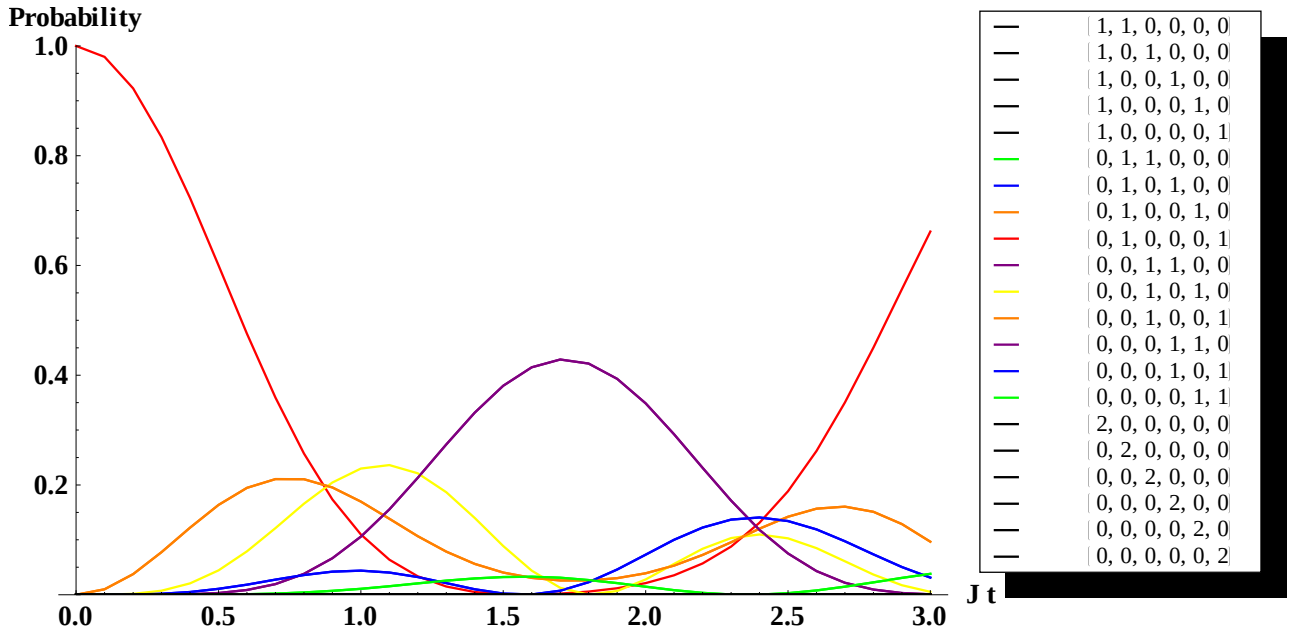

Figure 14: Probability of each basis vector in time.
L=6, 2 particles, U = 200, ε = 200 on site 1, *Initial state: Ψ(0) = |0 1 0 0 0 1>*

None of the paired states couple with this initial state and neither do any states with particles on the defect site. All the states that have symmetric positions with regard to the defect site are in the same color in this graph. For example, states 6, |011000> and 15, |000011>, are the green line. They have the same probability in this graph because they are symmetric around the defect site.

Although state 9, the initial state in Fig.14, has one particle in each of the sites next to the defect site, it does not couple with the unpaired states that have one particle in the site of the defect. In comparison, state 17, the initial state in Fig.12, also has two particles in the site next to the defect but these particles are paired and it does couple with the unpaired states containing one particle in the defect site. The only difference between states 9 and 17 is the fact that one is paired and one is not. The proximity of the particles to the defect site is exactly the same. And, yet, only the paired state couples with the unpaired states that have one particle in the site of the defect. In this way, at least, it is clear that the defect promotes coupling between the paired and unpaired states.

VII. Conclusions

These results lead me to conclude that there is some destructive quantum interference going on in these systems with defects [4]. It is not just conservation of energy that is dictating whether doublons will couple with states where the particles are on different sites.

Before we introduced the impurity, we saw that when the potential energy was very high, there existed an energy gap between the two kinds of states, paired and unpaired, and the gap was insurmountable such that the two kinds of states did not couple with each other at all. When the potential energy was lowered to a very small value, the gap was made small and so the two kinds of states were able to couple with each other.

After we introduced the impurity and the potential energy was still very high, the impurity should have bridged the energy gap that was preventing the two kinds of states from communicating. But what I saw was that there were other factors that were impeding the

effective coupling between these two kinds of states. I conclude that there are quantum interferences that are going on in these systems and it is not just the energy differences that are preventing the paired and unpaired states from coupling. In other words, the particles remain together due to quantum interference as well as energy differences.

VIII. Computer Code

Here I have included the full code for the Hamiltonian and graphs of the system. The parameters can easily be redefined to represent systems of different sizes, initial states, and energy constants.

Notation:
L = number of sites in system.
dim = number of possible configurations of the system.
U = potential energy of system
Jhop = kinetic energy of system
defect = value of the defect
defectsite = site where the defect is placed
Initial = state that the system is initially in
tfinal = total amount of time for the experiment
Energies = eigenvalues of Hamiltonian
Vectors = eigenvectors of Hamiltonian
Psi = probabilistic wave function
Prob = absolute value squared of the wave function - probability that the system is in each state

Code for the Hamiltonian

```
(* PARAMETERS OF THE HAMILTONIAN *)
Clear[L, particles, dim];
L = 6;
particles = 2;
dim = L!/(particles! (L - particles)!) + L;

(* PARAMETERS *)
U = 200.;
Jhop = 1.00;
defect = 200.;
defectsite = 1;
Clear[time, Psi, Initial];
Initial = {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0};
tfinal = 31;

(* BASIS *)
Clear[onepersite, twopersite, basis];
onepersite = Flatten[{Table[1, {k, 1, particles}], Table[0, {k, 1, L - particles}]}];
twopersite = Flatten[{2, Table[0, {k, 1, L - 1}]}];
basis = Flatten[{Permutations[onepersite], Permutations[twopersite]}, 1];


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

(* Diagonal elements *)
Do[
  (*Impurity*)
  HH[i, i] = HH[i, i] + basis[[i, defectsite]] defect;
  (* Bose-Hubbard interaction: two particles per site *)
  Do[
    HH[i, i] = HH[i, i] + U basis[[i, j]] (basis[[i, j]] - 1)/2;
   , {j, 1, L}];
  , {i, 1, dim}];


(* Off-diagonal elements *)
Clear[howmany, site];
Do[
  Do[

    (* Initialization *)
    howmany = 0;
    SumParticles = 0;
    SumDifferenceOnSite = 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,
    SumDifferenceOnSite = SumDifferenceOnSite + Abs[basis[[i, k]] - basis[[j, k]]],
    SumParticles = SumParticles + basis[[i, k]] + basis[[j, 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 ||  site[2] - site[1] == L - 1,
  If[SumDifferenceOnSite == 2,
    {HH[i, j] = - Sqrt[SumParticles/2] Jhop,
     HH[j, i] = - Sqrt[SumParticles/2] Jhop}]]];

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

Diagonalizing the Hamiltonian

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

MatrixForm[Chop[Hamiltonian]];
Energies = Eigenvalues[Hamiltonian];
Vectors = Chop[Eigenvectors[Hamiltonian]];
```

Dynamics of the System and Graphs

```
Do[
time = 0.0 + (tt-1)0.1;
Psi[tt]=(MatrixExp[-I Hamiltonian time]).Initial;
,{tt,1,tfinal}]

Do[
Prob[k] = Table[{0.0 + (tt-1)0.1, Abs[Psi[tt][[k]]]^2}, {tt,1,tfinal}];
,{k,1,dim}];
```

- This is the code for Figure 12.

```
(*U =  200 ,  Initial State  { 0 2 0 0 0 0 }, defect on site 1*)
<<PlotLegends`
ListPlot[{Prob[1],Prob[2],Prob[3],Prob[4],Prob[5],
Prob[6],Prob[7],Prob[8],Prob[9],Prob[10],Prob[11],
Prob[12],Prob[13],Prob[14],Prob[15],Prob[16],Prob[17],
Prob[18],Prob[19],Prob[20],Prob[21]}
, Joined→True,
PlotStyle→{{Red,Thick},{Purple,Thick},{Blue,Thick},
{Green,Thick},{Brown,Thick},Black,Black,Black,Black,
Black,Black,Black,Black,Black,Black,Black,{Orange,Thick}
,Black,Black,Black,{Yellow,Thick}},
PlotRange → {0,1},AxesLabel → {"J t", "Probability"},
LabelStyle → Directive[ Black, Bold, Medium ] ,
PlotLegend → Table[basis[[k]],{k,1,21}],LegendPosition → {1,-.5},
LegendSize → {.6,1.3}]
```

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References

[1] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. Hecker Denschlag, A. J. Daley, A. Kantian, H. P. Büchler and P. Zoller, "Repulsively bound atom pairs in an optical lattice," *Nature* **441**, 853 (2006).

[2] R. Feynman, R. Leighton, and M. Sands, *The Feynman Lectures on Physics*, Pearson/Addison-Wesley (2006).

[3] P. A. Tipler, *Modern Physics*, Worth (1978).

[4] L. F. Santos and M. I. Dykman, "Quantum interference-induced stability of repulsively bound pairs of excitations", *New Journal of Physics* **14**, 095019 (2012).

[5] D. J. Griffiths, *Introduction to Quantum Mechanics,* Pearson Prentice Hall (2005).

[6] M. Karbach and G. Muller, "Introduction the Bethe Ansatz I," *Computers in Physics* **11**, 1 (1997).