Dynamical and Quantum Phase Transitions with Tridiagonal Matrices

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I. INTRODUCTION

The purpose of this research is to better understand the static and dynamical properties of quantum systems. What makes a quantum system a metal, a material in which particles can move easily? What makes it an insulator, a material in which particles are trapped to confined regions of space? What triggers the transition from a metallic phase to an insulating phase? To answer these questions, we consider quantum systems described by Hamiltonian matrices that have a tridiagonal form. A tridiagonal matrix is a band matrix that has nonzero elements only on the main diagonal, the first diagonal below the main diagonal, and the first diagonal above the main diagonal. We study how the eigenvalues and eigenstates of these matrices depend on the parameters of the Hamiltonian and use these results to predict the dynamical behavior of the system.

The advantage of using tridiagonal matrices is that they are easy to study numerically and in some cases can even lead to analytical solutions. Despite their simplicity, they model realistic systems of nature and provide a pedagogical framework to learn about concepts and tools of quantum mechanics which include: quantum spins, quantum superposition, delocalization measures, the Schrödinger equation, and quantum phase transitions.

We study three spin models. They are known as the clean XX model, the disordered XX model, and the Lipkin-Meshkov-Glick model. The clean XX model is often referred to in literature as the tight-binding model. This is a model in which a particle can hop from one site to a neighboring site without any impediment. By this we mean that all sites are energetically equivalent, which justifies calling it a "clean" model. This model represents ideal crystals. In the disordered XX model case, energy barriers of random amplitudes make it more difficult for a particle to hop from one site to another. These barriers represent impurities that are in fact always present in real crystals. Ideal

crystals are perfect conductors (metals), where the particles can move freely. In the disordered XX model (real crystals), the connectivity decreases with the disorder strength. By increasing the disorder, one can then analyze the metal-insulator transition.

We use the Lipkin-Meshkov-Glick model to study a different kind of transition. This model was originally introduced in nuclear physics and has become a basic model to describe magnetic properties of a collective spin system with long-range interactions. Depending on the values of the parameters, the system exhibits a ferromagnetic phase, where the spins get aligned (ordered) in a single direction. With this model, one can study the transition from an unordered paramagnetic phase to the ferromagnetic one.

The identification of the different phases of matter is tightly associated with the development of new materials. They are critical components of emerging technologies, which may revolutionize how we use and produce energy, may lead to new electronic and spintronic devices, and may constitute the building blocks of digital and analog quantum simulators. The potential economical and social impact of the discovery of novel phases of matter is immense. Yet, one needs to know where to look to have a higher chance to find them. This is the crucial role played by applied and fundamental research.

II. LINEAR ALGEBRA

We will introduce this research with a background in linear algebra because it is the language used in quantum mechanics. Linear algebra is the branch of mathematics concerned with vector spaces and their properties. The equations that describe the properties of vector spaces are represented using matrices and vectors.

In quantum mechanics, the state of a particle is given by a vector and the physical variables, such as position, momentum, and energy, are represented by matrices. This section will help describe what vectors and matrices are in further detail.

II.1. Vectors

A vector space is made up of a set of vectors $(|a\rangle, |b\rangle, |c\rangle \ldots)$ with a set of scalars (*a, b, c, ...)* that is closed under two operations: vector addition and scalar multiplication. What this means is that these two operations are well-defined and using them will always keep the result inside the given vector space.

Vector addition: the sum of any two vectors is another vector. The property of addition for vectors is both commutative and associative.

Scalar multiplication: the product of a scalar with a vector will always be a vector and scalar multiplication is distributive with respect to vector addition and associative with other scalars that a vector is multiplied by.

A linear combination of vectors is an expression of the form $(a|a\rangle + b|b\rangle + c|c\rangle \ldots)$. A vector, $|\lambda\rangle$, is said to be linearly independent of a set of vectors if it cannot be written as a linear combination of any of the vectors in the set. Along the same lines, a set of vectors is called linearly independent if each of the vectors inside the set is independent of the others. If every vector in a collection of vectors can be written as a linear combination of the members of a set, that collection of vectors *spans* the space. A set of linearly independent vectors that spans the space is called a *basis* [1].

II.1.a Inner Product

Two vectors can be multiplied in two ways in three dimensional space. The way we will use in this thesis is called the dot product, or more generally, the *inner product*. It is calculated by multiplying the components with the same index *i* together and summing such that [2],

$$\overrightarrow{A} \cdot \overrightarrow{B} = A_1 B_1 + A_2 B_2 + A_3 B_3 ...$$

or

$$< \overrightarrow{A} | \overrightarrow{B} >= \sum_i A_i B_i$$

.

II.1.b. Normalized Vector

To normalize a vector, first one must find the magnitude of the vector. The magnitude is calculated by adding the square of each term together, and then taking the square root. For a vector with entries $(x_1, x_2, ...x_n)$, the magnitude (norm) would be equal to

$$\sqrt{x_1^2 + x_2^2 + ... + x_n^2}$$

.

The vector becomes normalized by dividing every entry in the vector by its magnitude to create a vector of length 1, known as the unit vector.

II.1.c. Orthogonal Vectors

Two vectors are said to be orthogonal if their dot product is 0. Orthogonal vectors are thought of as higher dimension perpendicular vectors.

II.1.d. Orthonormal Set

If all the vectors in a set are unit vectors (i.e. normalized) and are mutually orthogonal, the set is called an orthonormal set and is linearly independent. An orthonormal set which forms a basis, a set of vectors that spans a vector space, is called an orthonormal basis. In this research, we consider an orthonormal basis.

II.2. Matrices

Vectors can undergo linear transformations. For example, they can be multiplied by a scalar, reflected over the x axis, or rotated 90 degrees. Such transformations cause the vectors in a space to become other vectors. It is convenient to display the effect a linear transformation will have on a set of vectors in matrix form. Thus, linear transformations can be studied according to the theory of matrices [3].

II.3. Eigenvectors and Eigenvalues

Most vectors that undergo linear transformations in 3D space that consist of a rotation about a specified axis by an angle, θ, will change in a complicated way. But if the vector lies *along* the axis, its behavior is very simple. It will not change at all and $(\hat{T}|\alpha\rangle = \lambda|\alpha\rangle)$. In a complex vector space, every linear transformation has "special" vectors that lie along the axis and are transformed into scalar multiples of themselves. They are called eigenvectors of the transformation and the number λ is called their eigenvalue.

With respect to a specific basis, the eigenvector equation takes on the matrix form

$$Ta = \lambda a \qquad \text{or} \qquad (T - \lambda I)a = 0,$$

where a is nonzero and 0 is the zero matrix, the matrix whose elements are all 0. Because a is not zero, the matrix $(T - \lambda I)$ is singular and therefore, has a determinant of 0.

$$det(T - \lambda I) = \begin{bmatrix} T_{11} - \lambda & T_{12} & T_{13} \\ T_{21} & T_{22} - \lambda & T_{23} \\ T_{31} & T_{32} & T_{33} - \lambda \end{bmatrix} = 0$$

Expanding the determinant gives the *characteristic equation* for the matrix and the solutions to the characteristic equation give the eigenvalues. (Note: an n x n matrix, has between 1 and n distinct eigenvalues.)

Follow the following example for a clearer understanding of how eigenvectors and eigenvalues of a matrix are calculated.

Given the matrix, M, where

$$M = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}$$

Its characteristic equation would be calculated as follows:

$$\begin{bmatrix} (2 - \lambda) & 0 & -2 \\ -2i & (i - \lambda) & 2i \\ 1 & 0 & (-1 - \lambda) \end{bmatrix} = -\lambda^3 + (1 + i)\lambda^2 - i\lambda = 0$$

The solutions for λ, the eigenvalues, are 0, 1, and i.

To solve for the eigenvectors that correspond to each of these eigenvalues, solve for the product of the matrix and an eigenvector equal to the eigenvalue multiplied by that eigenvector. In this particular

case where the matrix has dimension 3x3, we get a set of three equations with 3 variables. For example, for the case where the eigenvalue is zero, $\lambda = 0$, we have,

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Which yields the following three equations,

$$\begin{aligned} &2a_1 - 2a_3 = 0, \\ &-2ia_1 + ia_2 + 2ia_3, \\ &a_1 - a_3 = 0 \end{aligned}$$

where $a_1 = a_3$ and $a_2 = 0$ which can yield any multiple of the vector $\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$. The same process is done to find the eigenvectors that correspond to the remaining two eigenvalues. $\begin{pmatrix} 2 \\ 1-i \\ 1 \end{pmatrix}$ for $\lambda = 1$ and $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ for $\lambda = i$. Notice that the eigenvectors obtained here are not normalized. To normalize, we need to follow the procedure described in Sec.II.1.b. In addition, the eigenvalues are not all real, because the matrix M is not Hermitian. Hermitian matrices are discussed in the Sec.II.5 below.

II.4. Diagonalization

The procedure of solving the characteristic equation to find the eigenvalues and eigenstates is known as diagonalization. This name refers to the fact that if we write the matrix of interest in the basis that corresponds to the eigenvectors of that matrix, the matrix will have a diagonal form, where the diagonal elements are its eigenvalues. When a matrix can be brought to such a diagonal form by changing the basis, it is said to be diagonalizable. (A matrix is only diagonalizable if and only if its vectors span the space) [3] .

In this research, in order to diagonalize a matrix numerically, we used Wolfram Mathematica, a software created for technical computing. We wrote a piece of code to generate the appropriate matrix elements, and then used the built-in commands (Eigenvalues[ ] and Eigenvectors[ ]) to find the eigenvalues and eigenvectors of the matrices. A similar process can be done in another programming language, such as python.

II.5. Hermitian Matrices

A Hermitian matrix is a complex square matrix that is equal to its own conjugate transpose i.e. the element in the i^{th} row and j^{th} column of the matrix is equal to the complex conjugate of the element in the j^{th} row and i^{th} column. Even though the matrix may have complex entries, its eigenvalues are real. Matrices that describe real systems of nature are Hermitian to guarantee that the eigenvalues, which represent the allowed energies of the system, are real.

If the matrix contains only real numbers and is Hermitian, then it is necessarily symmetric. This means the element in the i^{th} row and j^{th} column is equal to the element in the j^{th} row and i^{th} column. In this thesis, we deal with symmetric matrices [3].

III. INTRODUCTION TO QUANTUM MECHANICS

III.1. What is quantum mechanics?

Quantum mechanics is the branch of physics that relates to the very small. At the scale of atoms and electrons, many laws that describe how things of everyday sizes move do not hold true. Quantum mechanics is built on three revolutionary principles, developed and experimented with between 1900 and 1930, that are able to successfully describe the motion of very small particles.

The first principle is that there are quantized properties. Sometimes certain properties, like energy and position, can only exist in set amounts [4]. An example Richard Feynman gives in a lecture of his titled, "The Character of Physical Law," [5] is that in quantum physics, properties can be like children. Children only come whole. One cannot have two and a half children, s/he can only have two children or three children. So too, certain properties in quantum physics. They are not continuous, rather, they are quantized.

The second and third principle come hand in hand. The second is that light can behave as a particle, while the third is that matter can behave as a wave [4].

We will now compare these ideas with the prior beliefs of how the physical world works. How does quantum mechanics differ from classical mechanics?

III.2. Discrete levels of energy

In classical mechanics, when a system's energy increases, it does so in a uniform continuous manner. In quantum mechanics however, there are discrete energy levels. Electrons in atoms do not smoothly increase in energy. Rather, they make jumps from one energy level to another.

The one discrete energy that exists is directly proportional to the frequency of the radiation of a system such that,

$$E = \hbar \nu$$

where E is the energy of each quantum, ħ is Planck's constant divided by 2π, or approximately 1.05 x 10^{-34} J • s, and v is the frequency of radiation.

III.3. Probabilistic nature

While classical mechanics is intrinsically deterministic, because of the uncertainty relation, wave-particle duality, and the principle of superposition (all topics that will be discussed in this section), quantum mechanics is intrinsically probabilistic. The probability of quantum mechanics does not emerge from lack of knowledge, but it is built on the theory - we simply cannot have information about the system before measuring it.

III.4. Uncertainty relation

An aspect of how the predictability of classical vs. quantum mechanics differs is as follows. The position and velocity of a projectile that moves through space according to classical laws of physics can be determined at any point and time of its flight. However, the position and velocity of particles like electrons or photons of light, which behave according to quantum laws of physics, can never be determined simultaneously.

III.5. Wave-Particle Duality

Part of the probabilistic nature of quantum mechanics is based off of the complex behavior of particles that move according to the laws of quantum physics. Such particles, like electrons and photons, behave like both waves and particles at the same time.

Richard Feynman discusses this idea extensively in his lecture, “The Character of Physical Law” [5]. He explains that light was first believed to behave like a particle, like rain, or like bullets from a gun, Then, it was understood to move like water, in waves. With further research, namely, the photoelectric effect, light was again considered to act like particles, called photons.

A similar confusion existed with the behavior of electrons. First they were understood to behave like particles, but then, slit diffraction experiments showed they behaved like waves!

This growing back-and-forth confusion whether light and electrons behave as waves or particles came to an end with the introduction of quantum mechanics in 1925. Quantum mechanics clarified that they behave as both waves *and* particles. Depending on the experiment, one aspect or the other will be revealed. Feynman emphasizes that although this concept is hard to grasp, it is an essential characteristic of physical law.

III.6. Superposition

In classical mechanics, an object can only have one position, energy level, or speed at a time. But particles of matter that can be described using quantum mechanics can have more than one position, energy level, or speed at the same time. How does it make sense for a particle to be in more than one position at one point in time? The way this is thought of is that the particle exists across all possible positions simultaneously. This is because a quantum particle moves both like a particle, and like a wave. Although the idea of existing as a superposition of two states does not make intuitive sense, it is a characteristic of quantum physics [6].

One practical application of superposition is the quantum computer. Because a system can be in many states at the same time, the result of superposition, we can use each branch of the system to perform a different computation. This is known as quantum parallelism. Parallelism is applied in computer systems to generate a higher number of computations in a shorter amount of time by dividing the work needed to be done within different processors and often different computers. The idea of a

quantum computer is to make use of quantum parallelism to have an enormous amount of different computations being performed simultaneously in a single device.

IV. SPINS ½

Another difference between classical and quantum mechanics is the way in which a concept called "spin" is characterized. The next section will go into detail on this topic.

In classical mechanics, an object has two kinds of angular momentum. The first one, orbital angular momentum measures the motion of the center of mass about the nucleus ($\mathbf{L} = \mathbf{r} \times \mathbf{p}$) . The second is spin which measures motion about the center of mass -- the spin of electrons around the nucleus ($\mathbf{S} = \mathbf{I}\ \omega$). S is ultimately the sum of the orbital angular momenta.

In quantum mechanics an object also has two kinds of angular momentum. The first one, orbital angular momentum, is defined the same way as it is in classical mechanics, as an extrinsic property that is determined by the motion of the particle in space. The second however, spin, is defined differently from the way it is in classical mechanics. In quantum mechanics, spin (**S**) is unrelated to motion in space. Rather, it is an intrinsic property of a particle. It is an individual, isolated characteristic that cannot be broken down into a sum of orbital angular momenta like in classical mechanics.

In quantum mechanics, every particle has a specific and immutable value of **S**. We call this value the spin of that species. Different particles have different spin values. For example, electrons have spin ½ and photons have spin 1. **S** is a fixed value for each of these particles.

The particles that make up ordinary matter, protons, neutrons, and electrons, all have spin of s = ½. These states of **S** have two eigenstates, spin up $(\uparrow)$, and spin down $(\downarrow)$ with respect to a specific chosen direction. Throughout this thesis we are referring to the z-direction.. We can describe the general state of a spin-1/2 particle using their spin up and spin down as basis vectors [3].

To describe a system with one single spin-½ particle, we use the spin operators $S^{x,y,z} = \hbar\frac{\sigma^{x,y,z}}{2}$.

We set ħ=1 and $\sigma^x, \sigma^y, \sigma^z$ are the Pauli matrices given by

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

A spinor is a two-component vector that represents the quantum state of the spin. This state can be written in terms of basis vectors that correspond to the eigenstates of S^z, denoted by $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ for spin-up in the *z*-direction and $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for spin-down in the *z*-direction. The eigenvalue associated with the first vector is +½ and with the second vector, -½. The Spin operators S^x and S^y flip the spin as follows:

$$\hat{S}^x|\uparrow\rangle = \frac{1}{2}|\downarrow\rangle, \quad \hat{S}^x|\downarrow\rangle = \frac{1}{2}|\uparrow\rangle;$$
$$\hat{S}^y|\uparrow\rangle = \frac{-i}{2}|\downarrow\rangle, \quad \hat{S}^y|\downarrow\rangle = \frac{i}{2}|\uparrow\rangle.$$

Since spins-1/2 can only have two states, they are examples of two-level systems [1].

V. LATTICE HAMILTONIAN

A solid with magnetic properties can be viewed as a lattice where on each site there is a spin. Here, we consider a one-dimensional lattice or chain. We therefore deal with a chain of two-level system sites. The Pauli matrices act on each site individually.

The different spins of the system can interact. How they interact is described mathematically by the so-called Hamiltonian. This is an operator that represents the total energy of the system. By diagonalizing the Hamiltonian matrix, we find the discrete energies of the system.

In a general one-dimensional spin-1/2 system with L sites, the Hamiltonian matrix has dimension 2^L x 2^L. This is because there may be 2^L different states. For example, suppose a chain with four sites. Each site can have either a spin up or spin down. Therefore, we can have 2^4 different states.

For our chain, we assume that only one spin is pointing up and all others are pointing down. This up-spin is referred to as the excitation of our system. It can move through the chain, but it cannot be annihilated. Excitations cannot be created either. So our system conserves the total number of excitations. The Hamiltonian matrix that describes this system has dimension L.

We also assume that the excitation can only hop between directly neighboring sites. That is, it can hop from site n to site n+1 or to site n-1, but it cannot hop to a more distant site, such as n+2, without first passing through site n+1. In this scenario, the Hamiltonian matrices that we consider are tridiagonal matrices.

Another aspect of the chain is its geometric structure. A chain can be round or it can be linear. Other terms exchangeable with “round chain” are a periodic chain, a ring, or a closed system. In such a chain, the excitation on site 1 can hop to site L (the last site in the chain) and vice versa, the excitation on site L can hop to site 1. In a linear chain, a chain with open boundaries, an excitation at site 1, can only hop to its neighboring site, site 2 and because the chain is linear, and not connected at its two ends, excitations are never able to hop between sites 1 and L.

VI. THREE SPIN-½ MODELS

We consider three different spin-1/2 models with a single excitation. They are the clean XX model, the disordered XX model, and the Lipkin-Meshkov-Glick Model.

VI.1. XX Model

The Hamiltonian that describes the XX model is,

$$H = \sum_{n} \frac{J}{4} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y]$$

where J is the coupling strength. Because the Hamiltonian for this matrix only couples a state with one up spin with another state that has only one up spin, the number of total excitations in the system is always conserved in the XX model.

Consider a system with four sites. Because this model has only one excitation, the excitation can be in any of four locations and therefore, the system has four possible states. They are |1000>, |0100>, |0010>, or |0001>, where 0 indicates a spin down and 1 indicates a spin up. These states constitute the orthonormal basis that we use to write the Hamiltonian matrix. We refer to this basis as the site-basis.

To illustrate how to obtain the Hamiltonian matrix, we will go through the steps for the state $|1000\rangle$.

Let us see what the term $\sum_n \sigma_n^x \sigma_{n+1}^x$ and the term $\sum_n \sigma_n^y \sigma_{n+1}^y$ do to this state. Since σ_x and σ_y flip the spin we find that,

$$\sum_n \sigma_n^x \sigma_{n+1}^x |1000 >= |0100\rangle + |1110\rangle + |1011\rangle + |0001\rangle$$

$$\sum_n \sigma_n^y \sigma_{n+1}^y |1000 >= |0100\rangle - |1110\rangle - |1011\rangle + |0001\rangle .$$

The last state on the right, |0001>, appears when we have a chain with periodic boundary conditions (a ring).

Combining the two equations above, we find that

$$H|1000 >= \sum_n \frac{J}{4}[\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y]|1000 >= \frac{J}{2}|0100 > + \frac{J}{2}|0001 >$$

The action of the Hamiltonian on the other three states can be calculated analogously.

The corresponding full Hamiltonian matrix can now be constructed using what we just calculated. We look at all the possible pairs that could be made, and place the corresponding matrix element in the Hamiltonian matrix.

Along the diagonal, all the values result to 0.

H_{11} = < 1000 | H | 1000> = < 1000 | J/2 |0100> + < 1000 | J/2 |0001> = 0

H_{22} = < 0100 | H | 0100> = < 0100 | J/2 |1000> + < 0100 | J/2 |0010> = 0

H_{33} = < 0010 | H | 0010> = < 0010 | J/2 |0100> + < 0010 | J/2 |0001> = 0

Next to the diagonal:

$H_{12} = < 1000 \mid H \mid 0100> = < 1000 \mid J/2 \mid 1000> + < 1000 \mid J/2 \mid 0010> = J/2$

$H_{21} = < 0100 \mid H \mid 1000> = < 0100 \mid J/2 \mid 0100> + < 0100 \mid J/2 \mid 0001> = J/2$

$H_{23} = < 0100 \mid H \mid 0010> = < 0100 \mid J/2 \mid 0100> + < 0100 \mid J/2 \mid 0001> = J/2$

$H_{14} = < 1000 \mid H \mid 0001> = < 1000 \mid J/2 \mid 0010> + < 1000 \mid J/2 \mid 1000> = J/2$

Other:

$H_{13} = < 1000 \mid H \mid 0010> = < 1000 \mid J/2 \mid 0100> + < 1000 \mid J/2 \mid 0001> = 0$

$H_{24} = < 0100 \mid H \mid 0001> = < 0100 \mid J/2 \mid 0010> + < 0100 \mid J/2 \mid 1000> = 0$

Above, <1000|0100> represents the inner product between state |1000> and state |0100>. It can be written in a vector form as,

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

which is zero. Since these states form the orthonormal basis, only the product of a basis vector with itself gives 1. Once computing all these matrix elements, we can write the Hamiltonian in the following matrix form:

$$H = \begin{bmatrix} 0 & J/2 & 0 & J/2 \\ J/2 & 0 & J/2 & 0 \\ 0 & J/2 & 0 & J/2 \\ J/2 & 0 & J/2 & 0 \end{bmatrix}$$

The reason the top-right and bottom-left corner values are equal to J/2 is that this system is a closed system. This means that the term $\sigma_1^x \sigma_4^x + \sigma_1^y \sigma_4^y$ can be found in the Hamiltonian. This term indicates that the 4th site and 1st site couple with one another. In the case that the system had open-boundary conditions, and the 1st and 4th sites did not couple with each other, those corner values would be 0. If there are closed-boundary conditions, the matrix can still be called three-diagonal because along the center of the matrix, the pattern still stands. (Note: The Hamiltonian matrix that we obtained above has real elements and is symmetric.)

For this research, the Hamiltonian elements were computed using Wolfram Mathematica. Below is the piece of code used to generate the proper results. Before beginning to write the code for the Hamiltonian matrix, the proper parameters must be defined for L, the size of the system, and for J, the coupling strength.

First, we set the desired parameters. We then constructed a matrix with all the values on the sides of the main diagonal and the two corners (because we chose closed-boundary conditions) equal to J/2. We used the built in command to compute the eigenvalues - what determines the system's basis - and subsequently, the eigenvectors.

```
Clear[L, J];

L = 4;
J = 1;

Do[
  Do[
    elem[i, j] = 0;
    , {j, 1, L}];
  , {i, 1, L}];
Do[elem[i, i + 1] = J / 2;
  , {i, 1, L}];
Do[elem[i + 1, i] = J / 2;
  , {i, 1, L}];
Do[elem[L, 1] = J / 2;
  , {i, 1, L}];
Do[elem[1, L] = J / 2;
  , {i, 1, L}];
mat = Table[Table[elem[i, j], {j, 1, L}], {i, 1, L}];
MatrixForm[mat]

Ene = Eigenvalues[mat]
allvec = Eigenvectors[mat]
```

VI.1.a. Numerical & Analytical Results Agree

Above, we found the eigenvalues of the Hamiltonian matrix for the XX model numerically. However, there is an analytical approach to finding the same values. The values can be obtained from the equation [7],

$$E_k = J \cos\left(\frac{2\pi k}{N}\right)$$

and we confirmed that such values are equal to the ones we obtained from solving the XX model numerically.

VI.2. Disordered Model

The disordered model is very similar to the XX Model. Its Hamiltonian is calculated the same way albeit with an extra term added on to account for the on-site disorder.

$$H = \sum_n (\frac{h_n}{2})\sigma_n^z \ + \sum_n \frac{J}{4}[\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y]$$

What is on-site disorder? Within the system, each site has spin half and therefore, is a two level system, as explained earlier. The fact that there is disorder in the system means that each site has a different spacing between its two energies (whereas in the XX model, all sites have the same spacing). This splitting between the energy of the spin down and the energy of the spin up occurs when there is a magnetic field in the z direction acting on that site. If the magnetic fields acting on each site are all equal, we have the clean XX model. But if the magnetic fields acting on each site are different and randomly distributed, we have the disordered XX model, which we will call the "disordered model" for short.

Because of the addition of disorder to the system, the Hamiltonian of a disordered model differs from the Hamiltonian of the XX model. Along the diagonal, instead of the values being equal to zero (or equal to another fixed value), the values are non-zero and they depend on the state of the system and the strength of disorder. The rest of the elements in the Hamiltonian of the disordered model are calculated the same way they are in the XX model because the only difference is the disorder.

In this case, we control the strength of the magnetic field. Amplitudes of disorder are between 0 and *h*, where *h* is the strength of disorder. *h* can be very small or very large.

When constructing the matrix for the disordered model, the piece,

```
Do[elem[i, i] = h * (RandomReal[]);
  , {i, 1, L}];
```

is added to the code to account for the onsite disorder and is seen as the elements along the diagonal of the matrix.

An example of what a Hamiltonian for this model would like is as follows (obtained with an *h* value of 1 and a J value of J),

$$H = \begin{bmatrix} 0.363 & J/2 & 0 & J/2 \\ J/2 & 0.034 & J/2 & 0 \\ 0 & J/2 & 0.634 & J/2 \\ J/2 & 0 & J/2 & 0.492 \end{bmatrix}$$

with the diagonal terms varying with the strength of the disorder.

VI.3. Lipkin-Meshkov-Glick Model (LMG)

The third model to discuss is the Lipkin-Meshkov-Glick (LMG) Model. Its Hamiltonian is also a tridiagonal matrix, with all elements having the value of 0 aside from the diagonal and the lines directly above and below the diagonal. It is a symmetric matrix, similar to the ones previously discussed. Its elements are determined by the equation,

$$H_s = (1-\xi)\left(\frac{N}{2} + \mathcal{S}_z\right) - \frac{4\xi}{N}\mathcal{S}_x^2$$

where S_z is the total spin in the z direction and S_x is the total spin in the x direction.

The elements along the diagonal are calculated by

$$\langle s\, m_z | H_s | s\, m_z \rangle = \left(\frac{N}{2} + m_z\right)\left(1 - 2\xi + 2\frac{\xi m_z}{N}\right) - \xi$$

where m_z is the magnetization in the z direction (between -N/2 and N/2) and ξ is a value between 0 and 1.

The elements in the two lines alongside the diagonal can be calculated using

$$\langle s\, m_z + 2|H_s|s\, m_z\rangle = -\frac{\xi}{N}\sqrt{\left(\frac{N}{2}+m_z+2\right)} \times\sqrt{\left(\frac{N}{2}+m_z+1\right)\left(\frac{N}{2}-m_z\right)\left(\frac{N}{2}-m_z-1\right)}$$

This model is particularly interesting because it describes the change in energy of a quantum phase transition (QPT). A quantum phase transition is a change between two different phases of matter at zero temperature and is caused by the competition between the two interacting terms in the Hamiltonian equation.

In the particular case of the LMG model, the control parameter ξ determines which term of the Hamiltonian dominates. When ξ is small, the first term is strong. It favors the alignment of the spins in the z-direction. As ξ approaches 1, the second term becomes stronger. It favors the alignment of the spins in the x-direction. As ξ increases from zero, the states of the system suffer a sudden change in their properties. The first to feel it is the ground state. It transitions from one symmetry to another when ξ=0.2. Higher excited states also transition from one symmetry to another, but for larger values of ξ. The transitions that occur at higher levels is known as excited state quantum phase transition (ESQPT).

If $\xi = 0$, the spins of the system stay the same and the first term of the equation is lost. Whereas if $\xi = 1$ or any other nonzero value, the spins of the system switch and the second term of the equation is lost [7].

VII. NUMERICAL RESULTS: STATIC PROPERTIES

Now that we have the Hamiltonian matrices and know how to diagonalize them, we proceed with the analysis of the eigenvalues and eigenstates of the three systems. First we study how the eigenvalues are distributed and next, we investigate how delocalized the eigenvectors are in the site-basis.

The eigenvectors are superpositions of basis vectors. It is as if the system could be in any of the basis states at the same time. The eigenvector is usually denoted with the greek letter ψ. For L=4, a certain eigenvector is given by

$$\psi = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = a_1|1000> + a_2|0100> + a_3|0010> + a_4|0001>$$

The number a_k in front of each basis vector is its probability amplitude. The absolute square of the probability amplitude, $|a_k|^2$, is the probability that after a measurement, the system will be found in the corresponding basis vector. For example, $|a_1|^2$ gives the probability that after a measurement, we find the system in the state |1000>, $|a_2|^2$ gives the probability to find the system in the state |0100> and it continues like this.

The elements of each basis vector can differ as follows. When the disorder is large, one vector element's value is close to 1 and the rest are close to 0. In this case, the system is most likely to be

found in the configuration with large probability amplitude and it is much less likely that it will be in any configuration otherwise.

If a system's basis vector element values are all dispersed, i.e. one is 0.567, another 0.435, another 0.511, the system is said to be delocalized. This happens when the disorder is weak and the particles can move without much impediment. In this case, the system is spread out between many different configurations.

As an illustration, we show below the eigenvector with lowest energy, known as ground state, for the disordered model with L=6, h=0.5, and J=1 (arbitrary units):

For one disorder realization, the lowest energy found was -0.843, which corresponds to the following eigenvector.

$$\begin{pmatrix} -0.512 \\ 0.405 \\ -0.343 \\ 0.341 \\ -0.328 \\ 0.483 \end{pmatrix} = -0.512|100000> +0.405|010000> -0.343|001000> \\ +0.341|000100> -0.328|000010> +0.482|000001>$$

This system is said to be delocalized because the a_k values vary, meaning there is significant participation from all the different basis vectors.

VII.1. Density of States

The density of states is the distribution of the many possible eigenvalues of a system. For each model, we graphed its density of states. The XX Model shows that its eigenvalues are mostly concentrated at the two ends. This disordered model has eigenvalues spread out mostly along the center values.

The LMG model's density of states is drastically different for ξ values above 0.2 and ξ values below 0.2. For ξ=0.2, the eigenvalues cluster around the ground state. This explains the peak of the density of states close to zero. As ξ increases, the peak moves to higher energies. This divergence in the density of states at high energies is the main characterization of what is known as ESQPT, or excited state quantum phase transitions. The energy where the peak occurs is the energy of the state that suddenly transitions from one symmetry to the other [7].

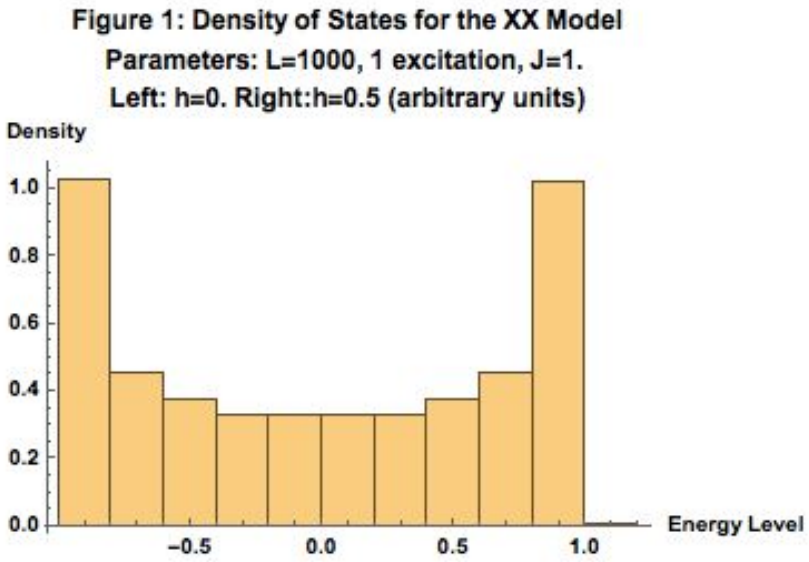


Figure 1: Density of States for the XX Model
Parameters: L=1000, 1 excitation, J=1.
Left: h=0. Right:h=0.5 (arbitrary units)

Figure 2: Density of States for the Disordered Model
Parameters: L=1000, 1 excitation, J=1.
Left: h=0. Right:h=0.5 (arbitrary units)

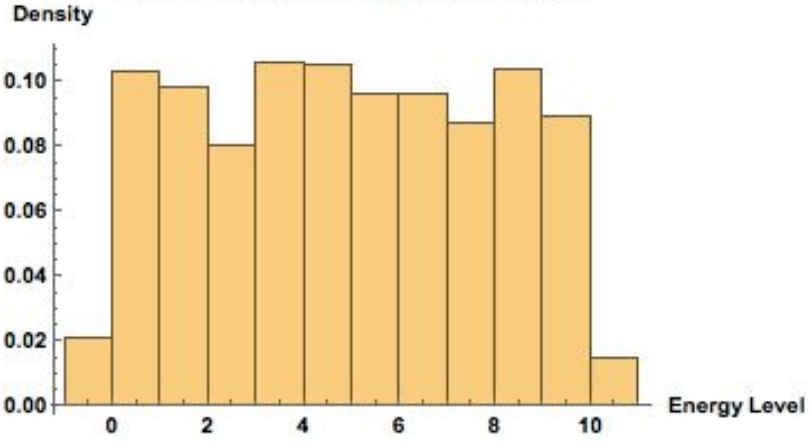


Figure 3: Density of States for the LMG Model
Parameters: L=1000, 1 excitation, J=1.
Left: h=0. Right: h=0.5. ξ = 0.15. (arbitrary units)

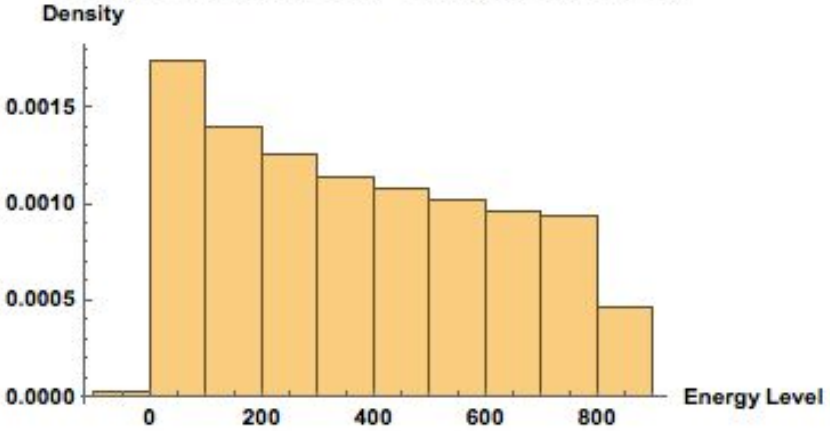
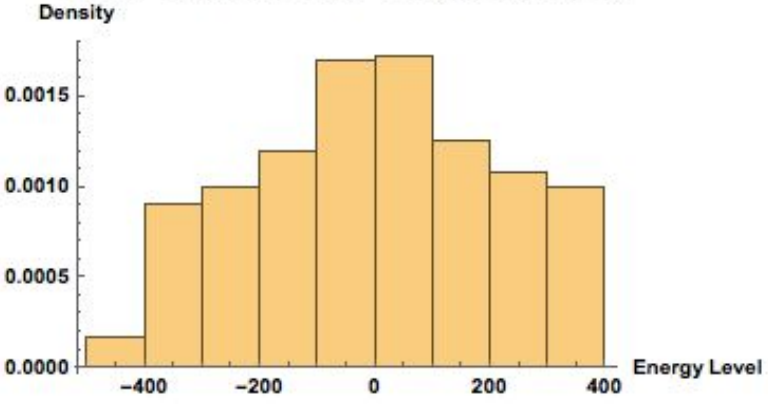


Figure 4: Density of States for the LMG Model
Parameters: L=1000, 1 excitation, J=1.
Left: h=0. Right: h=0.5. ξ = 0.6. (arbitrary units)



VII.2. Participation Ratio

The participation ratio is a quantity that measures the level of delocalization of a given state. It is defined as:

$$PR = \frac{1}{\Sigma(|a_k|^4)}.$$

The lower the value of the participation ratio, the less spread out the state is. And conversely, the larger the value of an *inverse* participation ratio, the more spread out the state is.

The participation ratio of a system can characterize the system as either a metal or an insulator. A metal is a material that has a high participation ratio - the excitation is spread out on many different sites, and therefore the material is a good conductor. An insulator is when the excitation is confined to fewer sites of the system and the system has a small participation ratio. If the excitation is confined to a single site, then the state coincides with the basis vector and its participation ratio has the minimum value of 1.

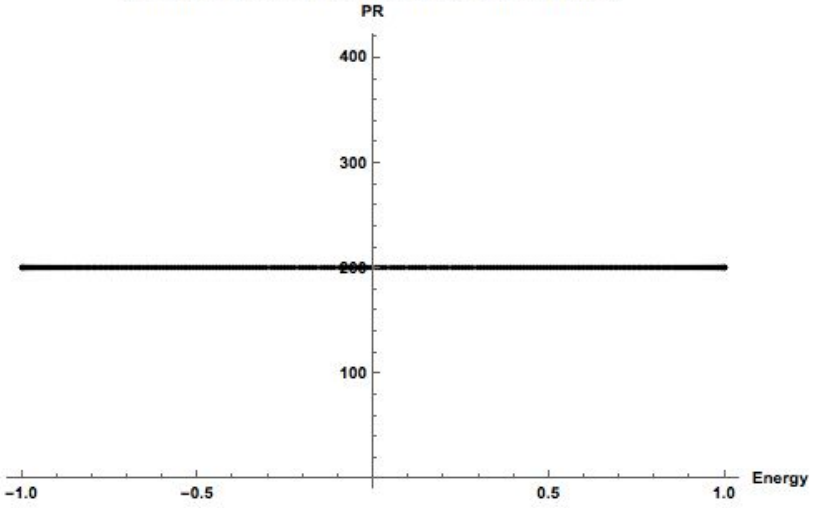
In the XX model, where all sites have the same level spacing, the excitation can be equally on any site, all sites are equivalent. In such a case, the participation ratio for any eigenvector is large. In the disordered model, the mismatch between the energies of different sites makes it more difficult for the excitation to spread through the chain. The participation ratio is smaller than in the XX model and it decreases as we increase the strength of disorder.

We will now look at how the participation ratio changes for each of the three models described in section VI.

VII.2.a. XX Model

For the XX ring model, the participation ratio for any eigenvector is the same and the value is large. This means that any eigenvectors is equally spread out. No basis vector has any advantage over another, they all participate equally, and all sites are equivalent.

Figure 5: Participation for the XX Model.
Parameters: L=300, 1 excitation, J=1 (arbitrary units)



VII.2.b. Disordered Model

The disordered model has two competing terms. When calculating its participation ratio, the question is, which of the competing terms will win?

If the first term is very large (h = 100), the graph of the participation ratio will look flat and will converge close to 1, like the first image below. This means that each eigenvector coincides with a single basis vector instead of being a superposition of more than one basis vector. Such a system is in a single configuration. It is only on the state |1000> or on the state |0100>, instead of having a probability of being in one or the other. In this extreme case where PR (participation ratio) = 1, we say that the system is onsite localized. The localization happens because the energy difference

between different sites is larger than the coupling parameter J. The term $\frac{J}{4}\sum_n \sigma_n^x \sigma_{n+1}^x$ cannot effectively couple different basis vectors. A system with this configuration would make a good insulator.

As the *h* value gets closer and closer to the value of J, the system starts to become more spread out, and its participation ratio increases (as you can see in the second image below where there is an *h* value of 10).

If the *h* is close to the value of J (i.e. if J is 1 and then *h* is 0.5, 0.1, or 0.2), like in the third image below, the distribution is the messiest. In this case, some states are delocalized and some are localized, but most of them have a large participation ratio. A system with this configuration would therefore make a good conductor.

Figure 6: Participation for the Disordered Model.
Parameters: L=300, 1 excitation, J=1.
h = 100. (arbitrary units)

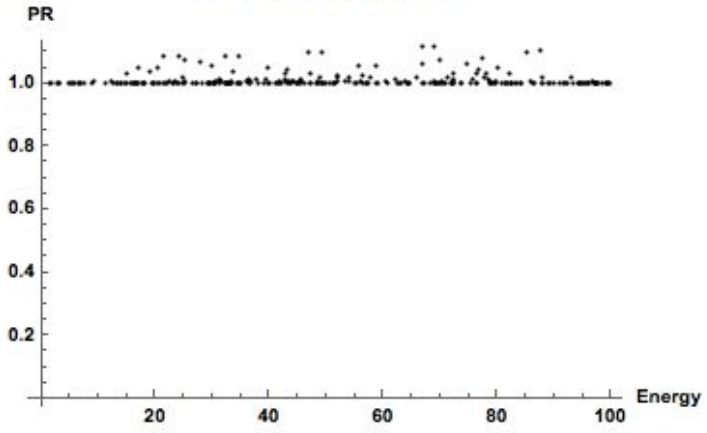


Figure 7: Participation for the Disordered Model.
Parameters: L=300, 1 excitation, J=1.
h = 10. (arbitrary units)

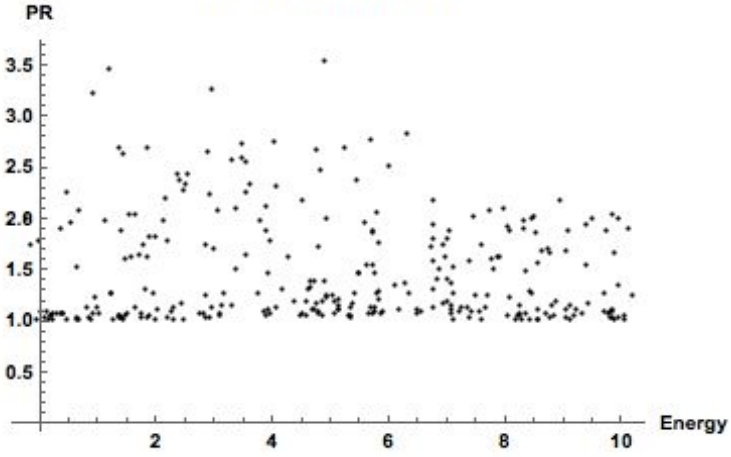
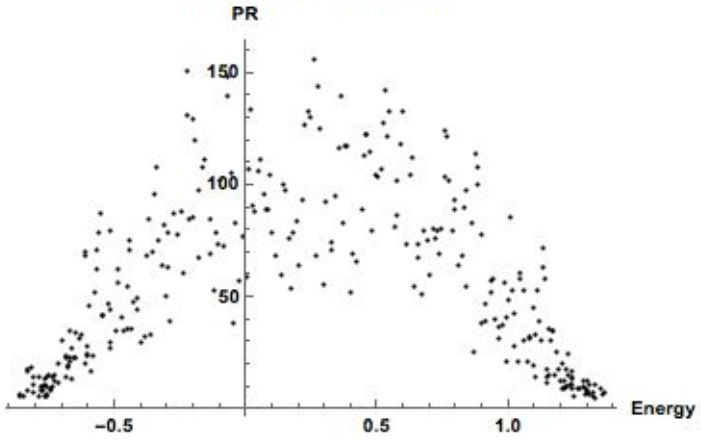


Figure 8: Participation for the Disordered Model.
Parameters: L=300, 1 excitation, J=1.
h = 0.5. (arbitrary units)



VII.2.c. LMG Model (ξ =0.2, 0.4, 0.6, 0.8)

The last model we studied has a varying participation ratio as well. When ξ = 0.2, the participation ratio graph has no dip in it. When ξ = 0.4, 0.6 or 0.8, the graph does have a dip in it. This dip in the value of the participation ratio occurs at the same energy where the peak for the density of states

happens. The dip shows that there is an abrupt change in the system properties at that energy level. Such features signal the excited state quantum phase transition.

Anywhere on the graph to the left or the right of the dip, i.e. at energies below or above the dip, the system will be a good metal (the states are delocalized). The states at the dip are localized (bad metal).

Figure 9: Participation for the LMG Model.
Parameters: L=600, 1 excitation, J=1.
ξ = 0.2 (arbitrary units)

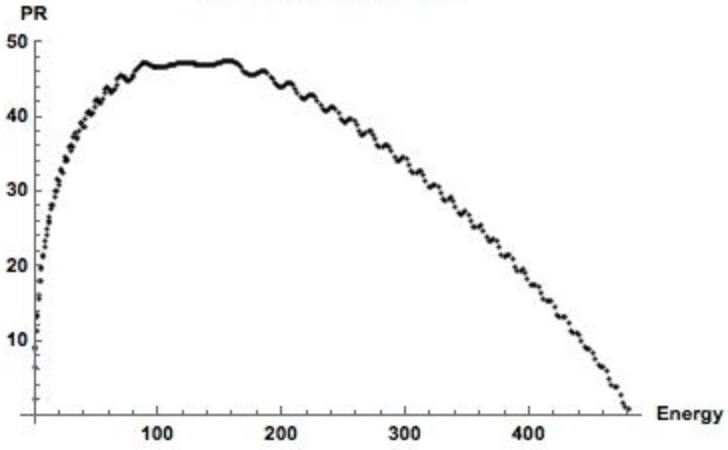


Figure 10: Participation for the LMG Model.
Parameters: L=600, 1 excitation, J=1.
ξ = 0.4 (arbitrary units)

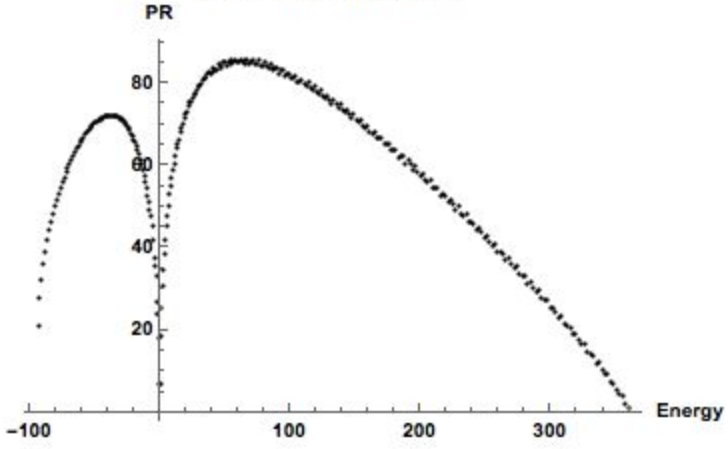


Figure 11: Participation for the LMG Model.
Parameters: L=600, 1 excitation, J=1.
ξ = 0.6 (arbitrary units)

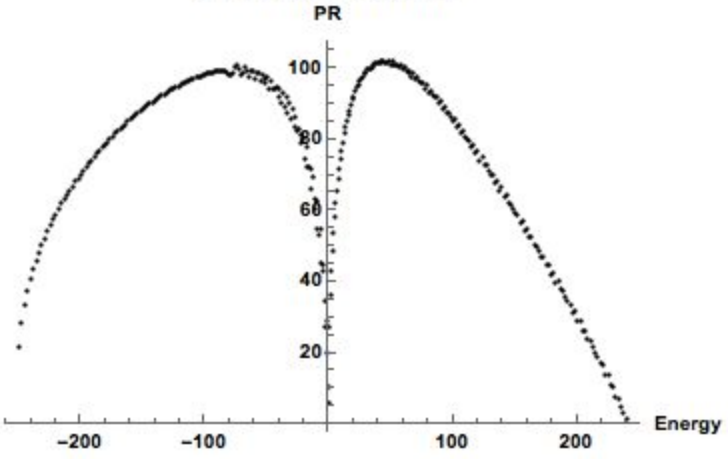
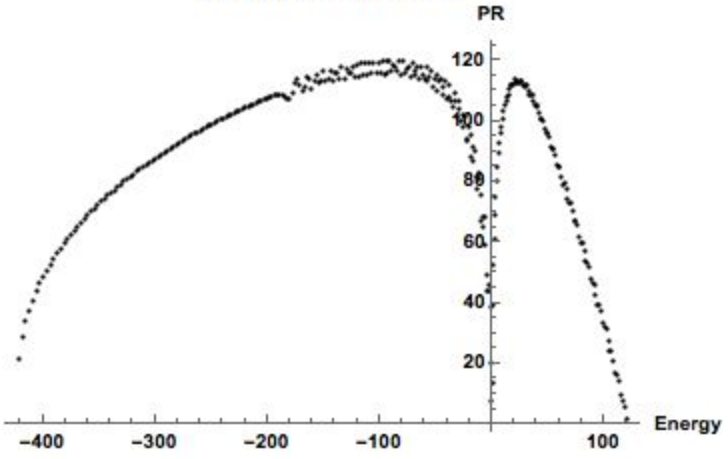


Figure 12: Participation for the LMG Model.
Parameters: L=600, 1 excitation, J=1.
ξ = 0.8 (arbitrary units)



VIII. NUMERICAL RESULTS: DYNAMIC PROPERTIES

Before describing the results, we need to explain how we study the dynamics of quantum systems.

Classical mechanics uses Newtonian laws to find the position of a particle in space at each instant of time t. In quantum mechanics, we use Schrödinger's wave equation to determine the state of the system at each instant of time. This equation is given by,

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

where i is the square root of -1 and ħ is Planck's constant divided by 2π, a value mentioned previously.

The solution of Schrödinger's equation is the wave function $\Psi(x,t)$. The wave function contains all the information we can have about the system. According to Born's statistical interpretation,

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

This interpretation says that the state of a particle is the probability of finding that particle at point x, at time t. Quantum mechanics is an intrinsically probabilistic theory. Before measuring the position of the particle, we cannot know with certainty where it is. We can only give the probability $|\Psi(x,t)|^2$ for finding it in a certain position. After we perform a measurement, the wave function collapses to a single point, and we suddenly find exactly where the particle is. But if we stop looking at this particle, the wave function spreads out again, and the uncertainty about the position of the particle comes back into the picture [3].

To solve Schrödinger's equation, we can separate the wave function into two functions. One is a function only of time and the other, only of position:

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

This method can only be used when the potential V does not depend on time.

The first step is to evaluate the first half of the equation. $\psi(x)$ is calculated from the eigenvectors that result from the diagonalization of the matrix.

The second step is to add the time-dependent term of the equation. It is with this step that we can observe changes in a system over time. The term that accounts for this is,

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

In the case of the specific lattice systems considered here, position is not continuous, so instead of writing $\psi(x)$, we write $|\psi_k>$. The solutions of the Schrödinger equation are given by the stationary states

$$|\Psi_k(t)>=|\psi_k> e^{-iE_k t}.$$

We prepare our system in a certain initial state. We choose the basis vector where the excitation is on site 1 as the initial state:

$$|\Psi(0)>=|1000>$$

This state will change in time as

$$|\Psi(t)>=\sum_n a_n|\psi_n> e^{-iE_n t}$$

where

$$a_n =<\psi_n|1000>$$

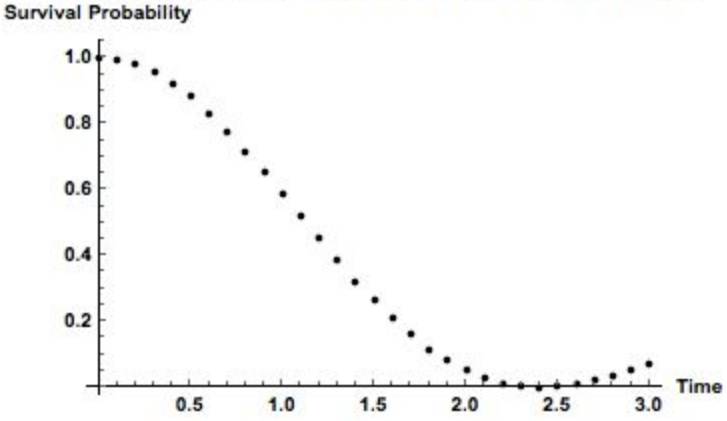
VIII.1. Survival Probability

Survival probability is defined as

$$SP(t) = | < \Psi(0)|\Psi(t) > |^2$$

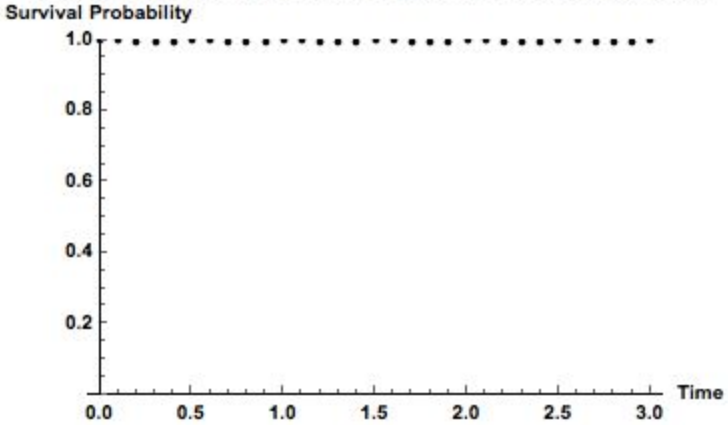
and described as the likelihood to find a system in the same state after a certain amount of time passes. We used the disordered model to graph the survival probability of $\psi(0)$ over time. When the disorder is small and the system is not very localized yet, we have a metal, a good conductor. As time passes, the excitation that was initially on site 1, can hop to other sites and spread out. As a result, the probability to find the system in its initial state decays.

Figure 13: Survival probability for the XX model.
Parameters: L=100, 1 excitation, h=1, J=1 (arbitrary units)



When the disorder is large and the system is localized (the material is an insulator), excitation cannot hop easily. If the disorder is very large, the excitation will be onsite localized, as in the graph below.

Figure 14: Survival probability for the Disordered model.
Parameters: L=100, 1 excitation, h=100, J=1 (arbitrary units)



It has been shown that one dimensional systems with a single excitation and random onsite disorder are insulators. In this thesis, we compared the level of localization of these finite systems for different strengths of disorder even though we know that the systems are localized. It is only in two dimensions or higher that there is a threshold above which the system becomes truly localized.

IX. CONCLUSION

In this research, we studied three system models, their static properties, their eigenvalues and corresponding eigenstates, and their dynamic properties. Just by studying the static properties of the systems, we were able to predict their dynamic properties. In systems with localized eigenstates, we could tell the dynamics would be slow and in delocalized systems, we could tell their dynamics would be fast.

We went on to analyze two different kinds of transitions using tridiagonal Hamiltonians. The first was the transition from metal to insulator. This kind of transition is know as a dynamical transition because it is associated with changes in the dynamics of a system. By changing the strength of the disorder, systems transition from localized to delocalized and we studied the differences between the systems in these cases. The second kind of transition was an example of a quantum phase transition. In the particular case studied here, the system changed from the ferromagnetic phase (where the spins are aligned in a single direction) to the paramagnetic phase (where the spins are not aligned). We used the LMG model to analyze this transition.

Using tridiagonal matrices to study these systems provided an uncomplicated way to learn a lot about quantum mechanics. There is much further research to be done in this area. Perhaps a good place to begin would be to study systems that have two or three dimensions instead of just one, as considered

here, or systems that contain more than a single excitation. Studying and analyzing such cases would reveal more about the nature of quantum mechanics and help us better understand the static and dynamical properties of more advanced quantum systems.

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XI. REFERENCES

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