An introduction to Kitaev model-I

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This pedagogical article is aimed to the beginning graduate students interested in broad field of frustrated magnetism. We introduce and present some of the exact results obtained in Kitaev model. The Kitaev model embodies an unusual two spin interactions yet exactly solvable model in two dimension. This exact solvability renders it to realize many emergent many body phenomena such as $Z_2$ gauge field, spin liquid states, spin fractionalization, topological order exactly. First we present the exact solution of Kitaev model using Majorana fermionisation and elaborate in detail the $Z_2$ gauge structure. Following this we discuss exact calculation of magnetization, spin-spin correlation function establishing its spin-liquid character. Spin fractionalization and de-confinement of Majorana fermion is explained in detail. Existence of long range multi-spin correlation function and topological degeneracy are discussed to elucidate the entangled and topological nature of any eigenstate. Some elementary questionnaires are provided in appropriate places for assimilation of the technical details.

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I. INTRODUCTION

With the advent of time, discoveries of various new states of matter continues to surprise and challenge the knowledge and understanding of mankind. For long time we were familiar with solid, liquid and gaseous states of matter. However, gradually we discovered that there are subtle differences in the microscopic organizations within various solid or liquid or gaseous states and this needs further classifications and characterizations. For example, a solid can be a crystal or amorphous, can be metal, insulator or semiconductor.

In this article we are going to understand quantum spin liquid states which for quite some time puzzled the present condensed matter community for its unique property and possible application for future technology. We would take some effort to understand the each term of the phrase “quantum spin liquid”. In ordinary liquid states like water we are concerned about the positions and orientations of each water molecule with respect to other neighbouring water molecule. In this context some preliminary idea like symmetry, long range order and other properties that constitute a particular materials may constitute a perfect crystals or ordered solid phases of matter. In that case what we are interested is the collective states of such large collection of spins shows diverse states having long range order or absence of it. Ferromagnetic state or paramagnetic states are example of that respectively. However there is a possibility of states of matter governed by the fundamental property of quantum mechanics which makes it possible to have states beyond simple ordered collinear states of paramagnetic states. The superposition principle enables this miracles due to which the system can be in a given time, probabilistically, in many states. For example $|\Psi_i\rangle$ is a many-body spin state for the system where spins at a given site $i$ is in a state $|i_p\rangle$. It is possible to have another many-body spin configuration given by state $|\Psi_j\rangle$ where spins at a given site $j$ is in a state $|j_p\rangle$. $|\Psi_i\rangle$ is said to be different then $|\Psi_j\rangle$ where $|i_p\rangle \neq |j_p\rangle$ for at least a given site $j$. One can easily construct different non-equivalent many-body spin configuration. The fundamental postulate of quantum mechanics says that it is possible for the system to be in state $|\Psi\rangle = \sum_i a_i |\Psi_i\rangle$ where $\sum_i |a_i|^2 = 1$. The possibility that such construction is possible is at the heart of quantum spin-liquid states. If an experiment is done on such system to investigate the many-body spin configurations of the collective spins, one finds different outcome at different times but with certain
probability. However all the $|\Psi_i\rangle$ that appears in the expressions of $|\Psi\rangle$ are not arbitrarily chosen. They are governed by the microscopic Hamiltonian or mutual interactions among the spins. There are specific relations among all the $|\Psi_i\rangle$ that appears in the expressions of $|\Psi\rangle$. Such relations can be of diverse nature and very different from model to model or system to system. This particular aspect is known as entanglement. In the present study, in view of the Kitaev model, we would like to explain some concepts and advanced idea of the modern condensed matter physics and give examples of other system in comparison with Kitaev model. We begin by introducing Kitaev model in section II. Here we describe in detail the exact solution of Kitaev model, its $Z_2$ gauge structure and ground state wave function explicitly. Various exercises are also given for beginning graduate students to assimilate technical details. Doing this would help appreciating the Kitaev model further. In section III, we evaluate various order parameter such as magnetization, two-spin correlation function to establish the spin-liquid character of Kitaev model. Multispin correlation function and topological degeneracy is also explained in a simple way to show the long range entanglement hidden in any eigenstate. We present a brief recapitulation and discuss some recent development for further reading in section IV.

II. KITAEV MODEL

At zero temperature, a quantum mechanical system minimizes its energy by occupying its ground states. Hamiltonian is the operator form of energy whose eigenvalues and eigenstates determines all the property of the system in principle. Let's consider a particular Hamiltonian that is of our interest in this article, so called Kitaev Hamiltonian. The system is defined on a honeycomb lattice and at each site of this lattice there is a spin-1/2 particle. The spin 1/2 particles interact with each other in a specific way. The origin of such interaction is beyond the scope of this pedagogical article and interested readers are requested to have a look at the recent progresses. We will only discuss few elementary reasons and consequences of the origin of interactions which involves spin-magnetic moments. Let's consider the situation where we bring in two hydrogen atoms close to each other from an initial position where they were at large separation. Hydrogen atom is made of one proton and one electron. The electron at ground state occupy the 1s state with orbital angular momentum $L = 0$ state. This happens because 1s state is spherically symmetric. However the intrinsic spin angular momentum of the electron could be quantized in $+\frac{1}{2}$ or $-\frac{1}{2}$ direction, this we represents as $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. When the two Hydrogen atoms are far apart the relative spin states of the two electrons can be shown to be arbitrary. However when the two hydrogen atoms come nearby then the electronic orbital of two electron overlaps which means that electrostatic potential energy increases. To minimise this electrostatic energy and also to maintain the two electronic wave function to be antisymmetric according to Pauli principle, one can show that the electronic spins forms a singlet, which can be shown to be an eigenstate of the operator $\vec{S}_1 \cdot \vec{S}_2$ where $\vec{S}_{1/2}$ represents the spin angular moments of the electrons. In a nutshell, the origin of magnetic interaction is due to the interplay of minimization of electrostatic energy due to overlapping orbitals in conjunction with the antisymmetrization of wave function according to Pauli principle. Extending this idea to complex condensed matter system composed of varieties of atoms/molecules, different complex spin Hamiltonian can emerge. The most well known of them is so called Heisenberg Hamiltonian $H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$. Here $|ij\rangle$ denotes a pair of sites which could be nearest neighbour or next nearest neighbour. The sign of $J_{ij}$ could be positive or negative depending on the relative orbital properties of the participating atoms/molecules. With this prelude we describe the Hamiltonian that is celebrated as Kitaev model. To understand that for a hexagonal lattice, there are three different kind of bond that can be grouped according to their alignment as show in Fig. 1. There are vertical bonds and lets call it $z$-bond. There are bonds with positive slope and lets call it $x$-bond and the bonds which are having negative slope are termed as $y$-bonds. Now it is clear that a given site is connected to three other sites by these three different type of bonds. The spin-spin interaction between two neighbouring spins depends on the kind of bonds they are connected with. For example, a given spin located at site ‘$i$’ interact with another spin located at site $i + \delta_x$ with $S_{i+x} \cdot S_{i+x+\delta_x}$, where as the same spin interact with its neighbouring site located at site $i + \delta_y$ and $i + \delta_x$ with $S_{i+y} \cdot S_{i+y+\delta_x}$ and $S_{i+y} \cdot S_{i+y+\delta_y}$ respectively. In the above $S_i^\alpha$, $\alpha = x,y,z$ denotes the spin component of the spin angular moment. With this in mind the Hamiltonian for the system can be written as follows,

$$H = \sum_{\langle ij \rangle_x} J_x S_i^x S_j^x + \sum_{\langle ij \rangle_y} J_y S_i^y S_j^y + \sum_{\langle ij \rangle_z} J_z S_i^z S_j^z \tag{1}$$

In the above equation the coupling parameter $J_x, J_y, J_z$ are taken positive. However the analysis we will follow and the details of the property that we will discuss remains unchanged for any combinations of signs of the coupling strength. This is another remarkable characteristics of Kitaev model.

In this pedagogical article we try to give a few exact results and exciting physics that this Hamiltonian contains. To get insight what does this innocently looking Hamiltonian as given in Eq. 1 contains, we take simple limits and readers are asked to find the answers themselves before proceeding further.

- Consider the spins as classical spins and find the classical configurations of spins that minimizes the
is special in the sense $B_1$. It can be represented as a problem it becomes the dimension of Hilbert space which is commonly available, one can solve a system of 30-40 spins. The system with such small number of spins often misses to capture the long range order and the true characteristics of the model developed only in the thermodynamic limit. For one dimensional system this might be enough. This fundamental limitation is the main challenge to modern condensed matter research. One commonly used technique to deal with the spin-Hamiltonian is that, we use suitable auxiliary variable to express the spins. Many times we use fermionic or bosonic field operators to express the spin-1/2 angular momentum algebra. This process is called fermionisation or bosonisation depending on the auxiliary field operator that are used. Below we provide two such very commonly used fermionisation process implemented for one dimensional spin problem and reader is asked to implement it themselves to understand the usefulness of it.

Exercise-1

- **Jordan-Wigner Fermionisation and its application to transverse field Ising Model**$^{3,14}$, 1d X-Y model$^{15}$
- **Spin-1/2 one dimensional Kitaev model**$^{16}$
- **Apply the Jordan-Wigner Fermionisation for 1d Heisenberg model and explain the differences with the transverse field Ising model, 1d X-Y model or 1d Kitaev model. Compare the results with the one dimensional antiferromagnetic Heisenberg chain**$^{17}$.

The Hamiltonian in Eq. 1 is special in the sense that usually the spin-spin interaction between the spins have all the component involved with the expression $S_x^1S_x^2 + S_y^1S_y^2 + S_z^1S_z^2$. However for the Kitaev interaction only one component of spins is involved with a given spin. For this reason Kitaev interaction is also called an anisotropic Heisenberg interaction. Another key feature of this model is the presence of large number of conserved quantities. For each plaquette we can define an operator which commutes with the Hamiltonian. We call this plaquette operator as $B_p$ where the subscript ‘p’ stands for the plaquette index. Plaquette operators defined on different plaquettes commute among themselves. With reference to the Fig. 1 $B_p$ is defined as,

$$B_p = \sigma_p^x \sigma_p^y \sigma_p^z \sigma_p^4 \sigma_p^6.$$  

(2)

Thus for each plaquette ‘p’ we can define a $B_p$. It can be easily checked that,

$$[B_p, H] = 0, \quad [B_p, B_q] = 0, \quad p \neq q.$$  

(3)

In the above $p, q$ indicate different plaquette indices. This implies that $B_p$'s are conserved quantities for this model. It is easy to verify that $B_p^2 = 1$ which implies that eigenvalues of $B_p$ are ±1. We will see later that this conserved quantity plays a significant role in the dynamics of Kitaev model. We now present the formal solution of this spin model as obtained by Kitaev himself$^{7}$. He showed that this spin model can be solved exactly using a fermionisation procedure which expresses the spin 1/2 operators in terms of Majorana fermion operators. In the next we elaborate on this.

A. Exact Solution of Kitaev model

The Hamiltonian is an effective representation of how the constituent particles or spins in question interact and there are energy cost for each specific interaction. For interacting particles, there are varying degrees of interactions associated with different energy cost. The Hamiltonian is an operator form of energy and its spectrum or eigenstates of the Pauli matrix. If there are ' $\vec{a}_1$ ' and ' $\vec{a}_2$ ' are two basis vectors. In the lower right corner an elementary hexagonal plaquette is used to define the conserved quantity $\vec{a}_1 \cdot \vec{a}_2$ in the limits $a) J_x = J_y = 0, J_z \neq 0$, $b) J_x \neq 0, J_y \neq 0, J_z = 0$ and $c) J_x \neq 0, J_y \neq 0$. With $J_z = 0$.

For more on classical solution the reader is requested to have a look at the reference by $^{10}$.

**FIG. 1.** In the left we have shown a cartoon picture of honeycomb lattice. Black and green filled circles shows two sub lattices that honeycomb lattice is made of. The green, black and red bonds respectively contain $x$-type, $y$-type and $z$-type interactions respectively. ‘ $\vec{a}_1$ ‘ and ‘ $\vec{a}_2$ ‘ are two basis vectors.
B. Fermionisation of spin 1/2 operators

Apart from the Fermionisation procedure mentioned in the exercises in Sec. II B, here we outline another fermionisation procedure which was used by Kitaev himself. We again ask the reader to do the following exercise before proceeding further.

Exercise-2

- Define the operator, \( c = (c_1 + c_1^\dagger), c^x = \frac{i}{2}(c_1 - c_1^\dagger), \) \( c^y = (c_2 + c_2^\dagger), c^z = \frac{i}{2}(c_2 - c_2^\dagger). \) Verify that they satisfy usual anticommutation relation, they are self conjugate and when multiplied with itself gives unity.

- Define \( \sigma^x = ic^x, \sigma^y = ic^y, \sigma^z = ic^z. \) Verify that Pauli matrices satisfy usual commutation relation.

- Check whether the above definition reproduces \( \sigma^x \sigma^y \sigma^z = \pm i \) for the odd particle states and even particle states respectively.

- Find the physical Hilbert space corresponding to the definition. Remember that a spin-1/2 particle has a matrix representation by Pauli matrices and has a Hilbert space dimension two. However in the auxiliary variable when we express the spin variable by fermionic operators, we used two fermions. Now each fermions has a Hilbert space dimension two, thus two fermions together has Hilbert space dimension of four. Thus the initial physical Hilbert space of a given spin of dimension two has been mapped to a Hilbert space dimension of four. This causes enlargement of Hilbert space dimensions and accounts for unphysical states. The previous exercise is aimed at having an idea about sub-classification of this extended Hilbert space where \( \sigma_x \sigma_y \sigma_z = \pm i \) needs to be worked out.

C. Quadratic Hamiltonian

To proceed we write the Hamiltonian in terms of fermionic operators as discussed above. After inserting the relations given in Exercise-2 in Eq. 1(i.e \( \sigma^\alpha = ic^\alpha_i, \alpha = x, y, z \), it reduces to

\[
H = \sum_{x-\text{link}} J_x (ic^x_i c^x_j) i c_i a c_j + \sum_{y-\text{link}} J_y (ic^y_i c^y_j) i c_i a c_j + \sum_{z-\text{link}} J_z (ic^z_i c^z_j) i c_i a c_j,
\]

(4)

In the above equation ‘a’ and ‘b’ denotes the sublattice index. We observe that each term in the above Hamiltonian is quartic in Majorana fermion operators. Generally such quartic Hamiltonian is quite difficult to solve. However it can be easily noted that operators in the parenthesis of each term of the above Hamiltonian commute with the Hamiltonian and commute among themselves. Which means they follow the following commutation relation which the interested readers are requested to check before proceeding further.

\[
[ic^\alpha_{i,a} c^\beta_{i,a} c^\beta_{i,b}, ic^\alpha_{i,a} c^\beta_{i,b}] = 0, [ic^\alpha_{i,a} c^\beta_{i,b}, ic^\alpha_{i,a} c^\beta_{i,b}] = 0
\]

(5)

In the above equation \( \alpha, \beta = x, y, z \) and \( (i, j) \) denotes a pair of nearest neighbour sites joined by a \( \alpha \)-type bond. It means that they are conserved quantities as far as this fermionised Hamiltonian is concerned. This fact makes Eq. 4 to be effectively quadratic in Majorana fermions. Let us call, \( ic^\alpha_{i,a} c^\beta_{i,b} = u_{i,j}^\alpha \) for the \( x \)-link. Similarly we define \( u_{i,j}^y \) and \( u_{i,j}^z \) on \( y \) and \( z \) links respectively. It is obvious that, \( u_{i,j}^{\alpha\beta} = -u_{j,i}^{\alpha\beta} \) and its eigenvalues can take value \( \pm 1 \) given the fact \( (u_{i,j}^\alpha)^2 = 1 \). Here we follow the convention of keeping the indices of the site belonging to the ‘\( a \)’ sub lattice first and then for ‘\( b \)’ sub lattice in the expression of \( u_{i,j} \) (for brevity many times explicit mention of \( \alpha \) in the expression of \( u_{i,j}^\alpha \) will be avoided.).

Exercise-3

- Using the definition of fermionization in Exercise-2 and definition of \( B_p \) as in Eq. 2 show that

\[
B_p = \prod_{(j,k)\text{boundary}(p)} u_{j,k}^\alpha.
\]

Using the above replacements for the conserved quantities on each bond, the Hamiltonian takes the following form,

\[
H = \sum_{<ij>_x} J_x u_{i,j}^x ic_i a c_j + \sum_{<ij>_y} J_y u_{i,j}^y ic_i a c_j + \sum_{<ij>_z} J_z u_{i,j}^z ic_i a c_j
\]

\[
\Psi^\dagger H(\Psi) = \Psi^\dagger \Psi
\]

where \( \Psi^\dagger = (c_1, c_2, ..., c_N) \) is an one dimensional row matrix of length ‘\( N \)’ and \( H(\Psi) \) is a \( N \times N \) matrix which depends on the values of \( u_{i,j} \) on each link. Now we see that above Hamiltonian describes a tight binding Majorana fermion hopping interactions but the hopping matrix elements are coupled with conserved operator or fields \( u_{i,j}^\alpha \) on each bonds. As we mentioned that this operators have eigenvalues \( \pm 1 \). These \( u_{i,j}^\alpha \) are called \( Z_2 \) gauge fields because of the eigenvalue to be \( \pm 1 \). Depending upon the values of these \( Z_2 \) gauge fields the eigenvalues of the system will change. Physically one way to visualise is that initially we had quartic Majorana fermion interaction of the form \( ic^\alpha_{i,a} c^\beta_{i,j} ic_i a c_j \). This process can be visualise in many ways. For example this can be
thought as two Majorana fermion hopping process happening simultaneously such as $c_{\alpha}^{\dagger} \rightarrow c_{\beta}^{\dagger}$, $c_{\alpha} \rightarrow c_{\beta}$ or $c_{\alpha}^{\dagger} \rightarrow c_{\beta}$, $c_{\alpha} \rightarrow c_{\beta}$ or similar processes. Alternatively it can be thought of as two on site interactions happening simultaneously yielding an energy cost. This on sight interaction involves the Majorana fermions at a given site only. All possible equivalent explanation exists for such four body interactions and they all are true. However the fact that the combination $ic_{\alpha}^{\dagger} \rightarrow c_{\beta}$ is a conserve quantity signify that once eigenvalue of $ic_{\alpha}^{\dagger} \rightarrow c_{\beta}$ is fixed to either +1 or -1 (like an initial condition) it remains same with time. Lets assume that the eigenvalue is fixed at +1 (or -1) then the hopping process $c_{\alpha} \rightarrow c_{\beta}$ with an phase +1 (or -1). This also signify that the process $c_{\alpha}^{\dagger} \rightarrow c_{\beta}$, $c_{\alpha} \rightarrow c_{\beta}$ or other possible processes are not allowed by the system. Further in Eq. 8, if we transform $c_{\alpha} \rightarrow \lambda i c_{\alpha}$, we observe that to keep the Hamiltonian invariant under such transformation $u_{ij}$ must change according to $u_{ij} \rightarrow \lambda i u_{ij} \lambda i$, where the allowed value of $\lambda$ is again ±1. Th us the Hamiltonian given in Eq. 8 has a underlying $Z_2$ symmetry 18.

**Exercise-4**

- Derive the Hamiltonian as in Eq. 8
- Prove that $[H, u_{ij}^{\alpha}] = 0$, $[u_{ij}^{\alpha}, u_{kl}^{\beta}]$, $\alpha, \beta = x, y, z$
- Derive the Heisenberg equation of motion for the operator $ic_{\alpha,i} c_{\beta,j}$ and $ic_{\alpha,i}^{\dagger} c_{\beta,j}^{\dagger}$ and try to explain it with your own understanding.

It is to be noted that the new conserved quantities, $u_{ij}$, were absent in the original spin Hamiltonian. In the original spin Hamiltonian as given in Eq. 1, there is no conserve quantity associated with a bonds. Earlier we found that there was only one type of conserve quantity associated with each hexagonal plaquette only and it is given in Eq. 2. Also from exercise 3 (Eq. 6), we found that the $B_p$ is a product of six conserved quantities ($u_{ij}$’s) defined on each bond. Initially our physical degrees were the spins represented by a product of two Majorana fermions. The bond conserved quantity $u_{ij}$ is also product of two Majorana fermions but each Majorana fermion is taken from the two spins attached at the end of a particular bond. And one can verify that a $u_{ij}$ can not be expressed in terms of spins. It is the product of $u_{ij}$ over the links of a hexagonal plaquette which can be expressed as a product of six spin operators and called $B_p$. One can easily verify that the square of $B_p$ is one indicating that the eigenvalue of the operator $B_p$ is ±1. We have also seen that eigenvalue of the bond-conserve quantity $u_{ij}$ is also ±1. As $B_p$ is expressed as a product of six $u_{ij}$ we can understand that for a given eigenvalue of $B_p$ there are many choices for the eigenvalues of the participating $u_{ij}$’s. Among the total 2$^6$ configurations that six $u_{ij}$ provide, half of them yields $B_p = 1$ and other half yields −1. For a given eigenvalue of $B_p$ say +1, among the various combinations, we will observe that a given $u_{ij}$ changes its eigenvalue from +1 to −1 though value of $B_p$ is fixed to 1. For this reason $u_{ij}$’s are called gauge fields analogous to magnetic vector potential and $B_p$’s are physical observable analogous to Magnetic field. Physically $u_{ij}$ can not be measured and its expectation value or outcome in experiment will be zero because of gauge averaging over many combinations that one $u_{ij}$ takes. However eigenvalue of $B_p$ is a physical observable. Thus we will use the phrase that $B_p$ is gauge invariant and $u_{ij}$ are not gauge invariant.

**Technicallity**

Before proceeding further we elaborate on the Hamiltonian represented in Eq. 8. The motivation is that physics is not always a story telling. Many truth of a given physical system can be understood by an intelligent mind without going into the details of mathematics. But very often, the situations become so complex for a many body system that one needs to rely on mathematicises. In Kitaev model such mathematics become exact beautifully and this motivates us to explain in detail the consequences of mapping of original spin problem into a Majorana fermion hopping problem coupled with $Z_2$ conserved gauge field. Such an exact description may happen for other system approximately and we believe that a thorough understanding of it in the context of Kitaev model will help the reader to extend their imagination easily to explore the intricacies of other complex system. Let consider a finite Honeycomb lattice such that it has $N_1$ dimer or $z$-bond in the $\vec{a}_1$ direction and $N_2$ dimer or $z$-bonds in $\vec{a}_2$ direction. Thus we have a system of $N$ spins with $N = 2N_1N_2$. Because there are two spins in a given $z$-bonds. Total number of bonds of a particular type say $x$, $y$, $z$ are equal and they are $N_1N_2$. Thus we have a total number of bonds $N_b = 3N_1N_2 = 3N/2$. The original spin Hamiltonian of $N$ spins is defined in $2^N = \mathcal{N}$ dimensional Hilbert space. This means that we are to solve a $M \times \mathcal{N}$ matrix with $M$ real eigenvalues and eigenstates. Now while we had employed a fermionization procedure where at each site there are two fermions implying that each site is associated with a Hilbert space dimension of four yielding total Hilbert space of $4^N = (2^2)^N = 2^N 2^N = M_1 = 2^M$ which means we have now enlarged Hilbert space yielding $M_1$ number of eigenstates/eigenvalue which is much more than the original Hilbert space. Thus though the original problem in spin-space was dimension $2^N$, after fermionisation now we have a problem of dimension $2^N \times 2^N$. This situation is depicted in Fig. 2.

Let us try to find another connection which will explain the relations between the eigenstates of the original spin problem given by Eq. 1 or Eq. 8 and Majorana fermion hopping problem given by Eq. 4. In the spin space we
that Hamiltonian is functional where the dimension of the outer big
and what is the
consequences of enlargement of Hilbert space dimension.

M
must have
N one gauge copy to another.
identical up to an gauge transformations which would connect
fermionisation using four Majorana fermions at a given site.

inal Hilbert space is shown. This happens due to Majorana
matrix is shown by the small coloured matrix. For a given
on the Majorana fermion and its relation to complex fermions
2
states can be written as
\begin{align*}
\lambda_{ij} = \sum_m \left( \frac{2}{m} \right),
\end{align*}

However we remember that such description is true for a given distribution of conserved quantities on every bonds. This situation is depicted in Fig. 3 where the dimension of the outer big matrix is \( \frac{N}{2} \times \frac{N}{2} = \frac{N^2}{4} \). Inside this big matrix the smaller diagonal matrix represent a certain distribution of conserved gauge field and the dimension of this smaller matrix is \( N \) yielding \( \frac{N}{2} \) complex single particle complex fermionic eigenstate which in turn yield \( 2^{\frac{N}{2}} \) many body state. Now we already mentioned there are in total \( N_b = 3N/2 \) number of bonds yielding in total \( 2^{3N/2} \) such combinations. This means, in reference to Fig. 3, we have \( 2^{3N/2} \) such small diagonal matrix. Each of this smaller matrix yields an eigenstates of \( 2^{N/2} \) number. Thus the total number of eigenstates is \( 2^{N/2}2^{3N/2} = 2^N \) which matches with our earlier counting.

Earlier we mentioned that \( u_{ij} \)'s are not gauge invariant quantities and they are not physical observable. The gauge invariant physical observables are the plaquette conserve quantity \( B_p \). There are many combinations of \( u_{ij} \) which yields a configurations of \( B_p \) for each plaquette. And it is important to note that the energy eigenvalue only depends on the distribution of \( B_p \) not \( u_{ij} \). If two configurations of \( u_{ij} \) yields same distributions of \( B_p \), they should have identical eigenvalues. In reference to Fig. 3, this means that there are many gauge equivalent smaller matrix which gives identical distributions of \( B_p \) and have identical energy eigenvalues. We leave it to the interested reader to check themselves with the following exercise.

Exercise-5

- Calculate the number of ways in which one can have \( B_p = 1 \) for all the plaquette. Is this number same for having a random configuration of \( B_p \) for all the plaquette.

- In Fig. 4, A and B we have given two configurations for \( B_p = 1 \) for all the plaquette. Following the procedures of Ref. 3, Sec-5, construct the eigenvalues and check that they yields identical spectrum. Construct similar distributions of gauge field such that it gives \( B_p = -1 \) for all the plaquette. Calculate the spectrum as done for \( B_p = 1 \) and find which configuration has minimum ground state energy. Explain your finding.

Lieb Theorem

We observe from Eq. 8 that Hamiltonian is functional of configurations of conserve quantity \( u_{ij} \) defined on each bonds. Such Hamiltonian can be represented by block diagonal form in the eigenstate of \( u_{ij} \) as represented by the small square matrix in Fig. 3. Each sub-block refer to
a certain distribution of \( u_{ij} \) and we also explained before that each block corresponds to a certain distribution of gauge invariant conserve quantity \( B_p \) for each plaquette. There are many distinct configurations of \( u_{ij} \) which yields a unique configurations of \( B_p \). We also know that eigenvalue of \( B_p \) is \( \pm 1 \). Now the important question is the following. Does the ground state obtained from each sub-square block in Fig. 3 yields same energy or does it depends on the distribution of \( u_{ij} \) or does it depends on the distribution of \( B_p \). As the \( u_{ij} \) is not a gauge invariant object and physically not observable, the energy is not directly dependent on the distribution of \( u_{ij} \) rather it depends on the distribution of \( B_p \). The next question is which distribution of \( B_p \) yields the absolute minima. From a very remarkable theorem\(^{20} \) by E. Lieb. we know that uniform configuration of \( B_p = 1 \) for each hexagonal plaquette yields the global minima. This is obtained by fixing \( u_{ij} = 1 \) for every link (there are many other configurations which yields \( B_p = 1 \), however each of them would yield identical ground state energy). This has also been confirmed by Kitaev numerically\(^7 \). For the uniform choices of \( u_{ij} \) (which corresponds to global minima) we can easily diagonalise the Hamiltonian and get the ground state wave function.

**Physical wave function and projection operator**

With the discussion of the foregoing paragraph, let us call the wave function obtained by diagonalizing Eq. 8 with uniform configuration of \( u_{ij} = 1 \text{ (yielding } B_p = 1 \text{ for each hexagonal plaquette)} \) as \( |\psi\rangle_{ext} \). We have deliberately added the subscript ‘\( ext \)’ to remind the fact that the above wave function is obtained in the extended Hilbert space. One may question whether the ground state energy obtained in such a way is the true ground state energy which should have been obtained in the physical Hilbert space. Moreover what about the wave function itself? Because to calculate other physical observable we need the true ground state belonging to the physical Hilbert space. Otherwise \( |\psi\rangle_{ext} \) is not of much useful. Now it is time to discuss this issue. Whenever we make an operation which takes us from an Hilbert space \( H^> \) with more number of states to another Hilbert space \( H^< \) with less number of states such that some states are excluded in \( H^< \), we need an projection operator. If any states \( \Psi^> \) belongs to \( H^> \), the corresponding states in \( H^<\) after projection is obtained as \( \Psi^< = P\Psi^> \) where \( P \) is the projection operator. The job of the projection operator is to remove the unphysical states and keep only the physical states in the expansion of \( \Psi^> = \gamma_i|\psi\rangle \). Now the important question is which distribution of \( B_p \) yields the absolute minima. From a very remarkable theorem\(^{20} \) by E. Lieb. we know that uniform configuration of \( B_p = 1 \) for each hexagonal plaquette yields the global minima. This is obtained by fixing \( u_{ij} = 1 \) for every link (there are many other configurations which yields \( B_p = 1 \), however each of them would yield identical ground state energy). This has also been confirmed by Kitaev numerically\(^7 \). For the uniform choices of \( u_{ij} \) (which corresponds to global minima) we can easily diagonalise the Hamiltonian and get the ground state wave function.

\[
|\psi\rangle_{phy} = P|\psi\rangle_{ext} \tag{9}
\]

Now we try to understand the projection operator and its expression in the context of Majorana fermionisation in a little depth and we find a useful connection among the various copies of the Hilbert space that we mentioned earlier. Let \(|\uparrow\rangle\) and \(|\downarrow\rangle\) be the eigenstates of \( \sigma_z \) with eigenvalue \( \pm 1 \). The action of \( \sigma_x \) and \( \sigma_y \) on these two states are defined as \( \sigma_x|\psi\rangle = |\psi\rangle \) and \( \sigma_y|\psi\rangle = i|\psi\rangle \). Now the complex fermion \( \alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6 \) that has been used to define the Majorana fermionisation of spin operators has the states \(|00\rangle, |10\rangle = c_{\uparrow}|0\rangle, |01\rangle = c_{\downarrow}|0\rangle, |11\rangle = c_{\uparrow}c_{\downarrow}|0\rangle \). It is clear that the original spin states needs to be mapped to these four states and there is an enlargement of states. To understand the mapping let us recall that \( D = \sigma_x\sigma_y\sigma_z = i \) is an identity which must be hold for any states. If we calculate \( D \) according to the definition given in Exercise-2 one finds \( D = i(1 - 2c_{\uparrow}c_{\downarrow})(1 - 2c_{\downarrow}c_{\uparrow}) \). Now we see that \( D = i \) holds true only for the states \(|00\rangle \) and \(|11\rangle \). Thus any physical states should have the general representation \( \Psi_{ph} = a_{00}|00\rangle + a_{11}|11\rangle \). But while working on the extended Hilbert space we encounter states \( \Psi_{ext} = a_{00}|00\rangle + a_{11}|11\rangle + a_{01}|01\rangle + a_{10}|10\rangle \). How do we get rid of the unphysical states \(|01\rangle \) and \(|10\rangle \). Note that the operator \( P = (1 + D)/2 \) acting on this unphysical states yields zero and keeps the physical states as it is. Thus it is straightforward to check that \( P\Psi_{ext} = \Psi_{ph} \). Now this is about a given site and we call this projection operator \( P_l = (1 + D_l)/2 \). The above explanation can be extended to all the sites of the entire system and the total projection operator is defined as,

\[
\hat{P} = \prod_{\text{all sites}} \frac{(1 + D_i)}{2} \tag{10}
\]

Before we go for a formal solution we advise the reader to go through the following exercise which will strengthen their familiarity with the concept of Majorana fermioni-
Exercise-6

- Find the eigenstates of the operator $c_i, c_i^\dagger, \sigma^y, \sigma^z$ defined in Exercise 2.
- Find the eigenstates of the operator $\sigma^x, \sigma^y, \sigma^z$ in the Fock space of four states described above and see the consequences of projection operators on them.

D. The ground state

We have already argued that it is the uniform configuration of $B \mu = 1$, which contains the global minima of the spectrum. Here we consider the choice $u_{ij} = 1$ for each link which is one of the realizations of $B \mu = 1$ for each plaquette. After doing that the Majorana fermion hopping Hamiltonian given in Eq. 1 reduces to a translational invariant Hamiltonian facilitating easy solution using Fourier transformations. The translational invariant Hamiltonian is given by,

$$H = \sum_{\vec{r}} J_x i c_{i,a} c_{j,b} + \sum_{\vec{r}} J_y i c_{i,a} c_{j,b} + \sum_{\vec{r}} J_z i c_{i,a} c_{j,b}$$

To solve the above Hamiltonian we define the following Fourier transformations for the Majorana fermions,

$$c_{i,a(b)} = \sum_{\vec{k}} \frac{1}{\sqrt{MN}} e^{i\vec{k} \cdot \vec{r}} c_{k,a(b)}$$

Here we have taken a lattice with $M$ and $N$ unit cells in the directions of $\vec{a}_1$ and $\vec{a}_2$ respectively as shown in Fig. 1. Here $\vec{r} = m\vec{a}_1 + n\vec{a}_2$ and $\vec{k} = \frac{2\pi}{a}\vec{b}_1 + \frac{2\pi}{b}\vec{b}_2$, where $\vec{b}_{1,2}$ are the reciprocal lattice vectors.

$$\vec{b}_1 = \frac{4\pi}{3\sqrt{3}} \left( \frac{1}{2} e_x + \frac{1}{2} e_y \right); \quad \vec{b}_2 = \frac{4\pi}{3} e_y$$

Here ‘$x$’ and ‘$y$’ varies from $-M/2$ to $M/2$ and $-N/2$ to $N/2$ respectively. The above discussion defines the Brillouin zone. We notice that the property $c_k^\dagger = c_i$ implies $c_k = c_{-k}^\dagger$. After performing the Fourier transformation, we get the Hamiltonian in k-space as follows,

$$H = \sum_{\vec{k} \in \text{HBZ}} (c_{k,a}^\dagger c_{k,b}) \left( \begin{array}{cc} 0 & i f_k^* \\ -i f_k & 0 \end{array} \right) (c_{k,a} c_{k,b})$$

In the above equation ‘HBZ’ stands for half Brillouin zone. Note that for the condition $c_k = c_{-k}^\dagger$, all the Majorana modes are not independent. Their is a specific way a Majorana fermion with positive momentum is related with a Majorana fermion with a negative momentum with the same magnitude. Equivalently the $c_k = c_{-k}$ implies that annihilating a Majorana fermion with momentum $k$ is same as creating a Majorana fermion with momentum $-k$. The spectral function $f_k$ is given by,

$$f_k = J_z + J_x e^{-ik_1} + J_y e^{-ik_2}$$

In above expression $k_1$ and $k_2$ are the components of $\vec{k}$ along ‘$x$’ bond and ‘$y$’ bond respectively. They are given by,

$$k_1 = \vec{k} \cdot \hat{n}_1; \quad k_2 = \vec{k} \cdot \hat{n}_2$$

Here $\hat{n}_1$ and $\hat{n}_2$ are the unit vector along the ‘$x$’ and ‘$y$’ bond respectively. The Hamiltonian given in Eq. 14 can be diagonalised easily with the following unitary transformation given below,

$$\left( \begin{array}{c} c_{k,a} \\ c_{k,b} \end{array} \right) = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} v_k & -i f_k^* \\ i f_k & v_k \end{array} \right) \left( \begin{array}{c} \eta_k \\ \xi_k \end{array} \right)$$

with $v_k = if_k^* / |f_k|$. The diagonalised Hamiltonian is given by,

$$H = \sum_k E_k (\eta_k^* \xi_k - \xi_k^* \eta_k)$$

where $E_k = |f_k|$ is the quasi particle energy associated with new field operators $\alpha_k$ and $\beta_k$. The ground state is obtained by filling up all the negative energy states of $\beta_k$ quasi particles and can be written as,

$$|G\rangle = \Pi_k \text{HBZ} \beta_k^\dagger |0\rangle$$

where $|0\rangle$ represents the vacuum state such that $\alpha_k |0\rangle = \beta_k |0\rangle = 0$. Here the summation is over the half Brillouin zone as explained before. At this point it is important whether the spectrum is gapped or not which implies that if we want to create an excitation over the ground state do we require finite energy or not. If $E_k = 0$
for some values of ‘k’ we need no finite energy to create an excitation over the ground state and the system is called gapless system. Whether a system is gapless or not has much bearing to the thermodynamic quantities of the system as it determines how the one part of the system responses due to disturbances at some other part. To find whether the spectrum is gapless or not we solve for $E_k = 0$ which implies $k_f = 0$. It turns out that the, $f_k = 0$ has solutions if and only if $|J_x|, |J_y|, |J_z|$ satisfy the following triangle inequalities:

$$|J_z| \leq |J_y| + |J_z|, \quad |J_y| \leq |J_x| + |J_z|, \quad |J_z| \leq |J_x| + |J_y|$$

(21)

The above inequalities as given in Eq. 21 can be represented as a point inside a equilateral triangle which has been shown in Fig. 6.

In Fig. 7 and Fig. 8, we plotted how the spectrum looks like for gapless and gapped phase respectively.

If the inequalities are strict, there are exactly two solutions: $k = \pm q_x$, one in each HBZ. The region defined by inequalities in Eq. 21 is the shaded region B in Fig. 6; this phase is gapless. The region marked by A is gapped. The low energy excitations are different in these two phases. In the gapless phase the low energy excitations are the Majorana fermions but in the gapped phases the low energy excitations corresponds to the vertex excitations which corresponds to the excitations of $B_p$, the conserved quantities. In the presence of magnetic field the phase B acquires a gap. These two regions are topologically distinct as indicated by spectral Chern number which is zero for phase A and one for the phase B$^7$. We have argued that as the projection operator $\hat{P}$ commutes with the Hamiltonian, the solution obtained

![Phase Diagram](image)

**FIG. 6.** Phase diagram for Kitaev model in the parameter space. A point in the above triangle describes relative magnitudes of $J_x, J_y, J_z$. Three sides of the triangle describe $J_z = 0, J_y = 0$ and $J_x = 0$ as given in the figure. The region ‘A’ is gapped and the region ‘B’ is gapless. The gapless region acquires a gap in the presence of Magnetic field.

![Spectrum](image)

**FIG. 7.** Spectrum $E_k$ as defined in Eq. 19 has been plotted above for $J_x = J_y = J_z = 1$. We observe that there are six points in the Brillouine zone where $E_k$ vanishes resulting a gapless spectrum. The dispersion near this gapless points are also linear.

![Spectrum](image)

**FIG. 8.** In the above $E_k$ has been plotted for $J_x = J_y = 1, J_z = 2.2$. We note that there is a gap between valence band and conduction band. The spectrum near the minimum for conduction band is quadratic.

in the extended Hilbert space is exact. One can indeed show that there exist a non zero projections. But this method of solving gives eigenstates of the Hamiltonian as well as the eigenstates of the conserved quantities in terms of Majorana fermions whose occupation number is not well defined. In the next section, we would extend the Majorana fermionisation in an useful way such that eigenfunctions of the Hamiltonian as well as $u_{ij}^\alpha$ is represented by the usual occupation number representation of complex fermions$^9$.  

### III. ORDER PARAMETER

We have seen that the initial spin-Hamiltonian given in Eq. 1 is reduced to an effective quadratic fermionic Hamiltonian as given in Eq. 4. The initial physical object was spin 1/2 magnetic moment. For a two spins belonging to two different sites, spin-angular momentum commute with each other if we express them by suitable representation. For spin-1/2 particle, the Pauli matrices are a faithful representations. However, the effective Fermionic Hamiltonian consists of Majorana fermions which anticommutes. This conversion of effective degrees of freedom is known as emergent degrees of freedom due to interactions. However there is a definite connections between them. The eigenstates either obtained by
diagonalizing the original spin-Hamiltonian or the effective Majorana Hamiltonian has one to one correspondence and they have identical eigenvalue spectrum. In dealing with physical systems, generally one is interested with the ground state wave functions at low temperature. Now we must ask what characterizes the ground states, what is the properties of the ground states of different phases, that will differentiate one phases from another. various order parameters are used to determine a certain phases and distinguish from other. The magnetization or spin-spin correlation between the effective degrees of freedom is such a measure. In many occasion such correlation functions can only be calculated approximately. However the beauty of Kitaev model renders us to compute the correlation functions exactly. Mathematically the correlation between two observables or operators \( \hat{O}_1 \) and \( \hat{O}_2 \) is expressed as \( \langle \hat{O}_1 \hat{O}_2 \rangle \) where \( \langle ... \rangle \) denotes ground state expectation value at zero temperature. At finite temperature it means a thermal average. Physically it means what is joint probability that if the operator \( \hat{O}_1 \) takes value \( \hat{O}_1 \) and the operator \( \hat{O}_2 \) takes value \( \hat{O}_2 \). Apart from correlation function magnetization is also used to characterizes phases of magnetic and interacting spin systems. Magnetization is defined as the average value of magnetic moment in a system and at low temperature for quantum mechanical system it is defined as \( \langle M \rangle \) where \( M = \frac{1}{2} \sum \langle \vec{m}_i \rangle \) and the angular bracket implies expectation with respect to ground state. Here \( \vec{m} \) is the magnetic moment at a given site. Now we follow an exact calculation of magnetization and two spin correlation function to find out what kind of order is exhibited by the ground state wave function. To do that we first discuss an extension of Kitaev’s Majorana fermionisation such that the mathematical steps to calculate the spin-spin correlation function or magnetization is very straightforward.

A. Bond fermion formalism

We have seen in Sec. II B that two complex fermions yield four Majorana fermions. Each complex fermion can be rewritten into two Majorana fermions. Now to facilitate the easy computation of spin-spin correlations we invert the above procedure by regrouping two different Majorana fermions to define a complex fermion. We have seen that at every link there has been one conserve quantity named \( u_{ij}^{\alpha} \), made out of the Majorana fermion \( c_{i,\alpha} \) and \( \tilde{c}_{j,\alpha} \). Here ‘i’ and ‘j’ denote the two sites of a bond, ‘a’ and ‘b’ denotes sub-lattice indices and ‘\( \alpha \)’ denotes a specific bond(\( \alpha = x, y, z \)). We regroup these two Majorana fermions to define a complex fermion named \( \chi_{(ij)_{\alpha}} \) which lives on the bond joining sites ‘i’ and ‘j’. We call this procedure as bond fermion formalism. From now on we follow the convention that the site ‘i’ in the bond \( (ij)_{\alpha} \) belongs to \( a \) sub-lattice and the site ‘j’ belongs to \( b \) sub-lattice. Also from now on we do not mention the sub-lattice index ‘a’ and ‘b’ explicitly. We define complex fermions on each bond as,

\[
\chi_{(ij)_{\alpha}} = \frac{1}{2} \left( c_{i}^{\alpha} + ic_{j}^{\alpha} \right) 
\]

\[
\chi_{(ij)_{\alpha}}^\dagger = \frac{1}{2} \left( c_{i}^{\alpha} - ic_{j}^{\alpha} \right) 
\]

For example with reference to the Fig. 9, for the z-bond joining site 2 and site 3, and for the y-bond joining site 1 and site 2, we define,

\[
\chi_{(23)_x} = (c_{2}^{y} + ic_{3}^{y}) 
\]

\[
\chi_{(12)_y} = (c_{1}^{y} + ic_{2}^{y}) 
\]

Then it follows that for the site ‘2’ and ‘3’ the \( \sigma^x \) operator becomes,

\[
\sigma^x_{2} = i c_{2}(\chi_{(23)_x} + \chi_{(23)_x}^\dagger) 
\]

\[
\sigma^x_{3} = i c_{2}(\chi_{(23)_x} - \chi_{(23)_x}^\dagger) 
\]

Below we write the result of this re-fermionisation for a bond of type ‘a’ joining site ‘i’ and ‘j’,

\[
\chi_{(ij)_{\alpha}} = \frac{1}{2} \left( c_{i}^{\alpha} + ic_{j}^{\alpha} \right) 
\]

\[
\sigma^a_{i} = ic_{i}(\chi_{(ij)_{\alpha}} + \chi_{(ij)_{\alpha}}^\dagger) 
\]

\[
\sigma^a_{j} = ic_{j}(\chi_{(ij)_{\alpha}} - \chi_{(ij)_{\alpha}}^\dagger) 
\]

It is clear that three components of a spin operator at a given site gets connected to three different \( \chi \) fermions defined on the three different bonds emanating from it. The bond variables are related to the number operators of these fermions, \( \hat{u}_{(ij)_{\alpha}} \equiv ic_{i}^{\alpha}c_{j}^{\alpha} = 2\chi_{(ij)_{\alpha}}^\dagger \chi_{(ij)_{\alpha}} - 1 \). Thus the effective picture is understood easily from the Fig. 9. We identify a \( \chi \) fermion on every bond whose occupation number can be zero or one. This occupation number determines the value of \( u_{(ij)} \) on that bond. But these fermions are conserved and serve as an effective \( Z_2 \) gauge potential for hopping ‘c’ fermions. As \( \chi \) fermions are conserved, all eigenstates can therefore be chosen to have a definite \( \chi \) fermion occupation number. The Hamiltonian is then block diagonal in occupation number representation, each block corresponding to a distinct set of \( \chi \)
fermion occupation numbers for every bonds. Thus all eigenstates in the extended Hilbert space take the following factorised form,

$$|\tilde{\Psi}\rangle = |M_G\rangle |G\rangle \equiv |M_G\rangle |G\rangle$$ (31) with

$$\chi_{(ij)_\alpha}^\dagger \chi_{(ij)_\alpha} |G\rangle = n_{(ij)_\alpha} |G\rangle$$ (32)

where $n_{(ij)_\alpha} = \frac{(u_{(ij)_\alpha} + 1)}{2}$ and $|M_G\rangle$ is a many body eigenstate in the matter sector determined by its fermions, corresponding to a given $Z_2$ field configuration determined by $|G\rangle$.

\[\sigma_i^\alpha = ic_i \left( \chi_{(ij)_\alpha} + \chi_{(ij)_\alpha}^\dagger \right) \rightarrow ic_i \hat{\sigma}_{1(ij)_\alpha} \hat{\sigma}_{2(ij)_\alpha} \] (33)

FIG. 10. How a spin fractionalises into two static $\pi$ fluxes and a dynamic Majorana fermion is shown. $|\psi\rangle$ is a state with zero flux. We apply $\sigma_i^\alpha$ where site ‘$i$’ is connected with site ‘$j$’. As a result we get a state $|\psi'\rangle$ with two static $\pi$ fluxes at the plaquette sharing bond $\langle ij \rangle$ and a dynamic Majorana fermion represented by black circle.

Now we discuss the results of the above transformations and find that it brings an immediate visualization of the spin-operators. We observe form Eq. 28 that the effect of $\sigma_i^\alpha$ on any eigenstate becomes very clear. When the spin-operator acts on any eigenstate, in addition to adding a Majorana fermion at site ‘$i$‘, it changes the bond fermion number from zero to one and vice versa (equivalently, $u_{(ij)_\alpha} \rightarrow -u_{(ij)_\alpha}$). The end result is that one $\pi$ flux is added to each of the two plaquettes that are shared by the bond $\langle ij \rangle$. Mathematically the action of any spin-operator on any eigenstate can thus be written as,

mathematically this implies that,

$$\langle G|G'\rangle = \delta_{n_G,n_{G'}}$$ (34)

where $n_G$ and $n_{G'}$ represent the distribution of $\chi$ fermions for the state $|G\rangle$ and $|G'\rangle$ respectively. This observation will be extremely helpful to compute spin-spin correlations exactly. Not only two-spin correlation function, magnetization can also be calculated exactly. Apart from two spin correlation functions other multi spin correlations can be calculated with straight forward generalisations of this fact that for any spin-spin correlator to be non-zero the first necessary conditions is that the simultaneous action of all the spin operators on the ground state must not change the flux configurations or equivalently must not alter the gauge fermion occupation number of the bonds. This fact can be extended to all the eigenstates of the Kitaev model as well which is remarkable for Kitaev model.

B. Magnetisation

Magnetization $\mathbf{\tilde{M}}$ is an important physical quantity which is easily measurable and can be controlled experimentally as well. A particular component of magnetisation is defined as below,

$$\mathbf{M}_\alpha = \frac{1}{N} \sum_i \langle \sigma_i^\alpha \rangle$$ (35)

In the above $\langle \sigma_i^\alpha \rangle$ denotes the expectation value with respect to ground state. For ferromagnetic state it can be found that at least one component of $\langle \sigma_i^\alpha \rangle$ is non-zero at every site and it is identical for every site. On the other hand for anti-ferromagnetic state $\langle \sigma_i^\alpha \rangle$ are also non-zero at every site however their value is opposite at different sites and makes some pattern depending on the underlying structure. In Fig. 11 we have shown such ferromagnetic and anti-ferromagnetic structure in square and honeycomb lattice. We can see easily that for anti-ferromagnetic state $\mathbf{M}_\alpha$ is zero though for all the sites having red spins are having opposite magnetization of blue spins. At a given site the average value of spin momentum is not zero. In the lower panel we have shown a different state where at each shaded green region defined on a pair of sites has the following singlet state $|s\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. For such a state average value of $\langle \sigma_i^\alpha \rangle$ is 0 at any site as $\hat{\sigma}_i^\alpha$ is not zero. Now let us see what is the value of $\langle \sigma_i^\alpha \rangle$ for the ground state of the Kitaev model. From the definition of spin-operator as expressed in Eq. 33 we see that action of a spin on the ground state creates two additional flux in the ground state as shown in Fig. 10, in addition it also adds a Majorana fermion to the ground state. Mathematically this
is expressed as
\[ \sigma_i^z |\bar{G}\rangle |M_G\rangle = c_i |G^{\alpha}\rangle |M_G\rangle \] (36)

Now as the different flux configuration state is mutually orthogonal due to different occupation number of the conserved \( \chi \) fermion, we obtain,
\[ \langle G | \langle M_G | \sigma_i^\alpha | G\rangle = \langle G | \langle M_G | c_i | G^{\alpha}\rangle = 0 \] (37)
because \( |G^{\alpha}\rangle = 0 \) following Eq. 34. Thus we see that the magnetization is zero for Kitaev model. It is zero for every site unlike the AFM state where the magnetization at a given site is not zero but when averaged over the system it is zero. For singlet singlet also the magnetization is zero at a given site. However there is an important difference between the AFM state, and the spin-singlet state shown in Fig. 11. For AFM state \( \langle \sigma_i^x \sigma_j^x \rangle = \pm 1 \) depending on whether the site \('i' and \)'j' are both aligned in the same direction or in opposite direction. Note that it does not depends on the distance between the two sites. It is said that the state has a long range correlation but short range nearest neighbour correlation exist which bears similarity with Kitaev model. However there are important differences between the singlet state and Kitaev model. In the below we have shown a dimer state configurations on square and honeycomb lattice where the green ellipses represents a dimer. The particular arrangement of dimers to cover the every site of the lattice is not unique and there exist alternative arrangement as well. The alternative arrangements often are topologically different.

Exercise-7

Consider a spin-singlet state formed between site 1 and site 2 as expressed by \( |s\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\rangle |\downarrow_2\rangle - |\downarrow_1\rangle |\uparrow_2\rangle) \) where \( |\uparrow_i\rangle \) and \( |\downarrow_i\rangle \) refers the spin at a site \('i' oriented along positive and negative \( z \) axis respectively. Do the following questions.

- Calculate \( \langle s | \sigma_1^x \sigma_2^x | s \rangle \)
- Using the transformation \( \frac{1}{\sqrt{2}} (|\rightarrow_i\rangle + |\leftarrow_i\rangle) \) and \( |\downarrow_i\rangle = \frac{1}{\sqrt{2}} (|\rightarrow_i\rangle - |\leftarrow_i\rangle) \) where \( |\rightarrow_i\rangle \) and \( |\leftarrow_i\rangle \) denotes the spin-oriented along \( x \)-axis, express \( |s\rangle \) in terms of \( |\rightarrow_i\rangle \) and \( |\leftarrow_i\rangle \)

From the above exercise it must be clear that spin-singlet product state is an unique state with no long range correlation but short range nearest neighbour correlation exist with \( \langle \sigma_i^x \sigma_j^x \rangle \) non-zero if \('i' and \)'j' are nearest neighbour and they belong to a given dimer.

FIG. 11. In the top panel we have shown anti-ferromagnetic spin configurations in square lattice and in honeycomb lattice. In the below we have shown a dimer state configurations on square and honeycomb lattice where the green ellipses represents a dimer. The particular arrangement of dimers to cover the every site of the lattice is not unique and there exist alternative arrangement as well. The alternative arrangements often are topologically different.

C. Two-spin correlations, fractionalization, de-confinement

Here we give an outline of computation of spin-spin correlation functions in Kitaev model which is valid for any region of the phase diagram. The derivation here is given in the extended Hilbert space but can be easily extended without any difficulties to physical Hilbert space. This happens because after the implementation of projection operator to ground state wave function obtained in extended Hilbert space one obtains many daughter states differed with respect each other only in gauge sector by fermion occupation number in certain manner so that action of two spins on any of them still creates orthogonal states and mutual overlap between such states are again vanishes. The above fact is expressed technically as the following. Because the spin operators are gauge invariant (commute with the projection operator) the result of computation of spin-spin correlation function in the extended Hilbert space yields no problem at all. First to begin with, we consider the two spin dynamical correlation functions, in an arbitrary eigenstate of the Kitaev Hamiltonian in some fixed gauge field configuration \( \mathcal{G} \),
\[ S_{ij}^{x\beta}(t) = \langle M_G | |\mathcal{G} \rangle (G) \langle \sigma_i^\alpha(t) \sigma_j^\beta(0) | \mathcal{G} \rangle |M_G\rangle \] (38)

Here \( A(t) \equiv e^{iHt} A e^{-iHt} \) is the Heisenberg representation of an operator \( A \), keeping \( h = 1 \). Physically the quantity \( S_{ij}^{x\beta}(t) \) in Eq. 38 gives the joint probability amplitude of finding a spin at \('j' \) (at time zero) along \('x' axis and of finding another spin at \('i' \) to be along \('\beta' \) axis. As
discussed before we write the action of spin operator on any eigenstate as,
\[ \sigma_j^{(0)}(G) |M_G\rangle = c_j(0)|G^{j}\beta)|M_G\rangle \]
\[ \sigma_i^{(t)}(G) |M_G\rangle = e^{(H-E)t}c_j(0)|G^{j}\alpha)|M_G\rangle \]
where, $|G^{j}\alpha(\beta)\rangle$ denote the states with extra $\pi$ fluxes added to $G$ on the two plaquette adjoining the bond in $\alpha$ or $\beta$ directions. It means that if $\alpha = x$, then the two plaquettes are created adjoining the site ‘$i’$ to another site ‘$k’$ joined by $x$-bonds. Similar explanation goes for the $\beta$ indices as well. In the above equation $E$ is the energy eigenvalue of the eigenstate $|G\rangle|M_G\rangle$.

Since the $Z_2$ fluxes on each plaquette is a conserved quantity due to the fact the it is determined by the occupation number of gauge fermions ($\chi$ fermions) on the links, it is obvious that the correlation function in Eq. 38 which is the overlap of the two states in equations 39, 40 is zero unless the spins are on neighbouring sites indicating that for non-vanishing values of correlation function we must have $j'$ as the nearest neighbour site of the site ‘i’.

Also note that the components $\alpha$ and $\beta$ must be identical so that the effect of $\sigma_i^{(}\alpha$ and $\sigma_j^{(}\beta$ is to create a pair of flux and then annihilate it bringing the flux configuration same as before. The above simple observations says that the dynamical spin-spin correlation has the form,
\[ S_{ij}^{\alpha\beta}(t) = g_{ij,\alpha}(t)\delta_{\alpha,\beta}, \text{ for } i,j \text{ nearest neighbours} \]
\[ = 0 \quad \text{otherwise.} \quad (41) \]

Computation of $g_{ij}(0)$ is straightforward in any eigenstate $|M_G\rangle$. For the ground state where conserved $Z_2$ charges are unity at all plaquette, we have an analytical expressions of the ground state wave functions as given in Eq. 20. For simplicity we provide the expression for equal-time correlation by having $t = 0$ without loss of generality. For correlation function at different time interested readers are requested to consult the original article\(^2\). Using Eq. 39 and Eq. 40, the equal time 2-spin correlation function for the bond $(ij)\alpha$ reduces to the following simple expectation value :

\[ \langle \sigma_i^{(}\alpha}\sigma_j^{(}\beta\rangle \equiv S_{ij}^{\alpha\beta}(0) = \langle M_G|G|c_i,c_j,G|M_G\rangle \quad (43) \]

In the above equation we have omitted the time index for $c_i$ and $c_j$ operator for simplicity. One can simplify the expressions in Eq. 43 by using the Fourier transformations of $c_i$ and $c_j$ operators and then employing the orthogonal transformations for $c_k$ operators as given in Eq. 18, we obtain the following final expressions for the two-spin equal time correlation function,

\[ \langle \sigma_i^{(}\alpha}\sigma_j^{(}\beta\rangle \equiv S_{ij}^{\alpha\beta}(0) = \frac{\sqrt{3}}{16\pi^2} \int_{BZ} \cos\theta(k_1,k_2)dk_1dk_2 \]

Where $\cos\theta(k_1,k_2) = \frac{\delta_{\alpha\beta}}{E_k}$, $E_k = \sqrt{(t_k^2 + \Delta_k^2)}$, in the Brillouin zone. $t_k = 2(J_x\cos k_1 + J_y\cos k_2 + J_z)$, $\Delta_k = 2(J_x\sin k_1 + J_y\sin k_2)$, $k_1 = k.n_1$, $k_2 = k.n_2$ and $n_{1,2} = \frac{1}{2}e_x \pm \frac{1}{2}e_y$ are unit vectors along $x$ and $y$ bonds. At the point, $J_x = J_y = J_z$, we get $S_{ij}^{\alpha\beta}(0) = -0.52$. It is of interest to examine how this non-vanishing two spin correlation depends on the parameters of the Hamiltonian mainly on $J_x, J_y, J_z$. The Fig. 12 shows how the nearest neighbour $z-z$ correlations varies in the parameter space. As we have calculated the above two spin-correlation function for two spins connected by a $z$-bond, we observe that as we increase the magnitude of $J_z$, the value of correlation also increases. In particular two limiting cases in the parameter values is worth examining. Consider the case $J_z = 0$. Looking at the Fig. 1 we observe that on this limit, the honeycomb lattice reduces as collection of decoupled chains. Thus the two spins which have been joined by an interaction are now without any interaction between them, though the spins maintain their original interactions with nearest neighbour spins in the respective chains. As there is no interaction between these two spins, we expect that there will be no correlation between them and from Fig. 13, we do find that indeed the correlation between them is zero. The other limiting cases is $J_z = \infty$ or $J_x = J_y = 0$, in this limiting case the two spins connected by a ‘$z’$ bonds does not interact with any other spins except the one connected by $J_z$ bonds. Thus one expect that the correlation will be stronger and reach the saturation value one as shown in Fig. 13. Another interesting fact to note that there is little change in slope as we increase from gapped region to gapless region.

\[ \frac{\sqrt{3}}{16\pi^2} \int_{BZ} \cos\theta(k_1,k_2)dk_1dk_2 \]

Fractionalization and De-confinement: We note
that here we have only discussed the derivation of equal time correlation function which means that in Eq. 38 both $\sigma$’s have identical argument for time. We found that the spin-spin correlation function is short-range and also bond dependent. This property of short-range and bond dependent nature of correlation function remains unchanged for different time correlation function as well. However the derivation and the exact expression requires a little mathematical digression and for that we do not present that in this article. Instead we discuss the issue without going into technical details to meet the inquisitiveness of the reader. Let us try to understand the physical consequences of Eq. 38, Eq. 39 and Eq. 40. The r.h.s of Eq. 38 involves inner product of two parts which are $\sigma_i^{(0)}(t)|G\rangle|M_G\rangle$ and $\langle M_G\rangle|\sigma_i^{(0)}(t)$ which are shown in Eq. 39 and Eq. 40. The meaning of Eq. 39 is easy to understand which tells what happens when a given spin acts on an eigenstate. It creates two fluxes in the gauge sector $|G\rangle$ of the eigenstate and also adds a Majorana fermion in the matter sector $|M_G\rangle$. Let us try to expand the meaning of Eq. 40 which represents how the action of a given spin on an eigenfunction evolves as function of time. To this end we yield the intermediate steps reaching Eq. 40 as follows.

$$\begin{align*}
\sigma_i^{(0)}(t)|G\rangle|M_G\rangle & = e^{iHt} \sigma_i^{(0)}(0)e^{-iHt}|G\rangle|M_G\rangle \\
& = e^{iHt} \sigma_i^{(0)}(0)e^{-iEt}|\sigma_i^{(0)}|M_G\rangle \\
& = e^{i(\bar{H}-E)t} \sigma_i^{(0)}|G\rangle|M_G\rangle \\
& = e^{i(\bar{H}-E)t} c_i(0)|G^{i,\alpha}\rangle|M_G\rangle.
\end{align*} \tag{44}$$

In the first and second steps we have used the definition of time evolution of an operator and applied eigenstate condition with energy $E$ respectively. The third step is a simple rearrangement and fourth step implements the effect of spin $\sigma_i^{(0)}$ which is equivalent to create two fluxes in the $|G\rangle$ (to have $|G^{i,\alpha}\rangle$) and also adding a Majorana fermion $c_i$ in the matter sector $|M_G\rangle$. Now we need to consider the effect of the exponential operator $e^{i(\bar{H}-E)t}$ on this. Remember that from Eq. 36 that $c_i(0)|G^{i,\alpha}\rangle|M_G\rangle$ is not an eigenstate of $H$. The situation is complicated for two reason. Firstly $|G^{i,\alpha}\rangle$ makes all the conserved quantity ‘u’ to be 1 except on a bond connecting site ‘i’. Secondly $c_i(0)|M_G\rangle$ is not an eigenstate for such distribution of u’s in Eq. 8. In general if a state is not an eigenstate of a Hamiltonian then the action of Hamiltonian on it results into superposition of many other eigenstates. Thus the action $\sigma_i^{(0)}(t)|G\rangle|M_G\rangle$ can be mathematically represented as follows,

$$\begin{align*}
\sigma_i^{(0)}(t)|G\rangle|M_G\rangle & = e^{-iEt} \left( \sum_j A_{ij} |M_G\rangle_j \right) |G_{i,\alpha}\rangle, \tag{45}
\end{align*}$$

where $|M_G\rangle_j$ represents ‘j’ the eigenstate in the presence of two fluxes. In each of these $|M_G\rangle_j$, the fluxes are in identical position, they are static but the Majorana fermion added to each of this eigenstate $|M_G\rangle_j$ are in different position in general. This effect is a remarkable effect and signifies that in essence a given spin is composed of two objects, a Majorana fermion and a two flux. While the fluxes do not move, the Majorana fermion moves as time evolves and it is not confined in a given region unlike static flux pairs. This implies that physically a spin is fractionalized into two objects. The fact that Majorana fermion is moving gives rise to a de-confinement phenomena. In Fig. 14, we depict pictorially the phenomena of fractionalization and de-confinement. The exact formula for $\sigma_i^{(0)}(t)|G\rangle|M_G\rangle$ can be seen in the original manuscript.

Now in comparison with the singlet state we discussed before we find a number of differences. The similarity between the two is that in both the cases the two spin correlation function is short range i.e it exists only for nearest neighbour bonds only. However there are a number of important differences. For example for singlet state, the correlation function is non-zero if the two sites belong to a singlet only and for a given singlet $\langle \sigma_i^\alpha \sigma_j^\alpha \rangle$ exist for $\alpha = x, y, z$. However for Kitaev model for any two nearest neighbour correlation function is non-zero but they are anisotropic in the sense that for a ‘$\alpha$’ type bonds only $\langle \sigma_i^\alpha \sigma_j^\alpha \rangle$ is non-zero and for other component the spin-spin correlation function is zero.

D. Multispin Correlation function, topological degeneracy

We have seen that for Kitaev model magnetization is zero at every site. Also two spin correlation function is

![](Fig14.png)

FIG. 14. Time evolution and fractionisation of a spin flip at $t = 0$ at site ‘i’, into a $\pi$-flux pair and a propagating Majorana fermion.

![](Fig15.png)

FIG. 15. Multispin correlation function exist for Kitaev model. For the sites 1 to 6, $\langle \sigma_1^\alpha \sigma_2^\alpha \sigma_3^\alpha \sigma_4^\alpha \sigma_5^\alpha \sigma_6^\alpha \rangle$ is non-zero. For detail see text below.
FIG. 16. A cartoon picture of torus geometry for a $4 \times 4$ hexagon has drawn. The numerics show the specific way the boundaries are connected with each other. The above geometry is not unique and different geometry of lattice exist for torus realization.

extremely short range such that it does not extend beyond nearest neighbour. It is natural to ask then what is the difference between a normal paramagnetic or other disordered magnetic state for which long range two spin correlation is zero. We will now discuss that. Though the two spin correlation exists only for nearest neighbour spins there is underlying long range correlation between spins such that spins at long distances are entangled unlike paramagnetic or other disordered magnetic state where such long range correlation does not exist. We will also compare it with the singlet state described before where such long range correlation does not exist. We will now explain this fact for Kitaev model defined on torus of honeycomb lattice. Torus means two dimensional lattice such that it is periodically connected in both the direction. In Fig. 16, we have shown such periodic boundary condition applied to a $4 \times 4$ arrangement of hexagons. As can be seen that the lower and upper sides are connected as well as the left and the right sides. Note that each one dimensional edges are periodically connected. Now we evaluate some numbers which the reader are requested to cross-check of this $4 \times 4$ arrangement of hexagon having 32 sites. For a general $N \times N$ hexagons, there are total number of sites $M = 2N^2$. Total number of hexagon is also $M$. We know that associated with each hexagon there is a conserve quantity called $B_p$. Thus there are in total $M$ number of $B_p$. Now one can check that for torus geometry once all the $B_p$ are multiplied together it becomes unity such that,

$$\prod_{p=1}^{M} B_p = 1 \quad (47)$$

This tells that all the $B_p$ is not independent and there are in total $M - 1$ independent $B_p$. It can be shown that there is a conserve quantity associated with every closed loop, but they are not independent as they can be constructed by a product of certain $B_p$'s. However there two global loop operator which extends from one end to another which can not be expressed as a product of $B_p$ and there are two such loop operators which we call $W_1$ and $W_2$. These are analogous to Wilson loop operator in quantum field theory\textsuperscript{26,27}. For example take a horizontal zig-zag line constituted out of alternating $x$ and $y$ bonds. the product of $\sigma_z$ for all the sites on that line is a conserved quantity.

$$W_1 = \prod_{x-y \ chain} \sigma_z^x \quad (48)$$

Similarly for a $x-z$ chain extending from one end to another end, we can construct $W_2$ which is conserved. Thus total number of conserved quantity becomes $M + 1$. Now
it can be checked that $W_i^2 = 1$ implying that eigenvalues of $W_i$ is $\pm 1$. The presence of these two additional independent conserved quantities imply that there will be four different eigenstates of certain identical configurations of $B_p$, but with different eigenvalues of $W_i$. These four eigenfunctions can be represented as,

$$|\Psi_1\rangle = |M_G\rangle |G(B_p); W_1 = 1, W_2 = 1\rangle$$

$$|\Psi_2\rangle = |M_G\rangle |G(B_p); W_1 = -1, W_2 = 1\rangle$$

$$|\Psi_3\rangle = |M_G\rangle |G(B_p); W_1 = 1, W_2 = -1\rangle$$

$$|\Psi_4\rangle = |M_G\rangle |G(B_p); W_1 = -1, W_2 = -1\rangle$$

These $W_i$ manifests a hidden topological order which we will try to understand by considering how many ways $W_1$ defined in Eq. 48 can be made one for one dimensional arrangement of spins. In Fig. 17, we have shown by red line the states for which even number of spins are aligned in positive $z$-direction. For a one dimensional chain of $N$ sites there are $2^{N-1}$ such states. Similarly by blue line, we represents states with odd number of spins oriented along negative $z$-axis. All the red states in a given $x-y$ line contribute to the wave function to make $W_1 = 1$ and such states can not be converted to an eigenfunction with $W_1 = -1$ by local flipping of a given spin or a number of spins. For that we need to convert all the red states to the blue one. It is non-local transformation in the Hilbert space and thus topological. However the energy does not depends on the eigenvalues of $W_i$, it only depends on the flux configurations $B_p$. Thus all the states $|\Psi_i\rangle, i = 1,4$ has identical energy in the thermodynamic limit. This is a manifestation of topological degeneracy.

**IV. DISCUSSION**

In this pedagogical paper, we have tried to explain few aspects of Kitaev model. We have explained in detail how the Majorana fermionisation is used to solve the model. By solving we mean finding the eigenvalue and eigenvectors. All the eigenvectors and eigenvalues of the Kitaev model can be found in principle. This is a distinct feature which makes it stand apart from other exactly solvable model where in some cases we have only the ground state. It may be noted that Kitaev model can be defined in any lattices with co-ordination number of three and exact solution can be obtained. The Kitaev model is reduced to a $Z_2$ gauge theory and in the ground state sector all the $Z_2$ gauge fields are such that their product over a plaquette becomes unity. Uniform choice of $Z_2$ gauge fields for every link is convenient choice for such configuration. The spectrum, phase diagram and calculation of correlation function has been shown explicitly and elaborately. Notable feature of the phase diagram is that it consists of gapless and gapped phase both. In the gapless phase near the region where the spectrum becomes zero, the energy varies linearly with momentum. On the hand where the spectrum is gapped, the energy varies as quadratically with momentum. The correlation function calculation shows that two spin correlation function is short range and bond dependent. This property of correlation function is true for both static and dynamic correlation function. The short range nature of correlation function indicates that Kitaev model is an example of quantum spin liquid state where there is no long range order between two spins as well there is no average magnetization i.e average value of any spin operator is zero. We have shown that the action of a spin operator on any eigenstate is two fold. Firstly it changes the occupation number of a $Z_2$ gauge field on a particular bond by changing the value of $B_p$ in the adjacent plaquette. Secondly it also adds a Majorana fermion at a given site the spin belongs to. However the time evolution of the state shows that the pair of flux created does not move but the Majorana fermion added can move and is not confined or attached to that site only. This phenomena is called fractionalization of spins into static fluxes and dynamic Majorana fermion. The moving Majorana fermion defines a de-confinement phase which is gapless one with linear spectrum at low energy.

Moving further we have shown how the long range or multispin entanglement exist in an eigenfunction by showing non-zero multispin correlation function and explained how it is different than other magnetic state with short range two-spin correlation. Existence of topological degeneracy of eigenfunction in thermodynamic limit has been explained schematically. Historically Kitaev model was conceived mainly with the aim of implementation to quantum computations due to the existence of topological order and non-trivial topological excitations called anyons. It may be noted that the gapped phase of Kitaev model realizes abelian anyons and gapless phase realizes non-abelian anyons. The braiding properties of these anyons in relation to realizing quantum gates has been discussed in detail. Historically Kitaev model is exactly solvable in the sense that all the eigenfunction and eigenvalues can be obtained formally. The exact solvability is lost once other more conventional spin-spin interaction such as Ising or Heisenberg interaction is added to Kitaev model. In this case the $Z_2$ gauge field defined on each bond is no longer remains conserved. The flux operator $B_p$ also does not commute with the Hamiltonian any more. Physically this means that the fractionali-
sation of spins into Majorana fermion and static fluxes are not possible no longer. Because the fluxes also move along with the Majorana fermions though their dynamics may be at different scale. Though the Kitaev model was proposed with a theoretical foundation for quantum computations, it was rather surprising that this unusual interactions happens to exist in certain materials such as Iridiate and $\text{RuCl}_3$ etc\textsuperscript{35-37}. Unfortunately along with Kitaev interaction, there exists some other interactions such as Heisenberg type interactions. Presently intense research is underway to explore various aspects Kitaev model such as fractionalisation, de-confinement to confinement transition, detection of spin-liquid state etc. Interested reader are requested to go through some of the recent developments\textsuperscript{38} and the references there in.

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