Second Quantization and Majorana Modes

Particles That are Their Own Antiparticles

Arnab Barman Ray

This article reviews the basic concepts of second quantization as used in condensed matter physics. The Kitaev chain was the first system shown to exhibit Majorana zero modes, which exhibit novel statistics and thus find enormous applications in topological quantum computation. Simple calculations of the band structure and density of states showing the presence of Majorana zero modes are presented.

Arnab Barman Ray is a graduate student at the Institute of Optics, University of Rochester. He completed his Integrated Masters in Physics from IIT Kharagpur in 2018. This article presents a part of the work carried out by him under Dr Saurabh Basu at IIT Guwahati in the summer of 2016.

1. Second Quantization

Second quantization presents an elegant way of representing the Schrödinger equation for multiple particles in terms of creation and annihilation operators. It is ubiquitous in modern theoretical research in condensed matter physics. As opposed to "first" quantization, where operators like momentum or energy act on a specific state, in second quantization, the states themselves can be said to be represented by operators which act on the fundamental vacuum state. Unlike the single-particle Schrödinger equation, Hamiltonians in this new formalism do not necessarily conserve particle number.

Second quantization is allowed by the remarkable fact that any multi-particle wavefunction of say N particles can be broken down into linear combinations of the tensorial product of the individual basis states for a particular Hermitian operator, which is usually the position operator or can even be the position or spin operator. This can be proved using the completeness relation of the single-particle basis states.

$$\Psi(r_1, .., r_i, .., r_j, .., r_n, t) = \sum_{v_1, v_2, .., v_n, t} A_{v_1, v_2, .., v_n}(t)\, \phi_{v_1} \phi_{v_2} ..... \phi_{v_n} \quad (1)$$

As we can see, the time dependence is carried by the coefficients,

Keywords
Second quantization, Majorana modes, bosons, fermions, antiparticle, quantum computation, Kitaev chain, topology.

while the single-particle wavefunctions are orthonormal eigenstates of some Hermitian operator. Sum is over all possible combinations of the eigenvalues.

Multi-particle wavefunctions are endowed with the property of indistinguishability, i.e. it is fundamentally impossible to tell one electron from another or a photon from another.

Multi-particle wavefunctions are endowed with the property of indistinguishability, i.e. it is fundamentally impossible to tell one electron from another or a photon from another. So, if we were to interchange the position coordinates x_i and x_j, the observable properties should not change. This implies that:

$$\begin{aligned} &|\Psi(r_1,..,r_i,..,r_j,..,r_n,t)|^2 = |\Psi(r_1,...r_j,..,r_i,..,r_n,t)|^2 \\ \implies &\Psi(r_1,..,r_i,..,r_j,..,r_n,t) = e^{i\phi}\Psi(r_1,...r_j,..,r_i,..,r_n,t)\,, \end{aligned} \tag{2}$$

where ϕ is some real number denoting the phase. Performing another exchange of the coordinates in (2), we get,

$$\Psi(r_1,..,r_i,..,r_j,..,r_n,t) = e^{i2\phi}\Psi(r_1,...r_i,..,r_j,..,r_n,t)\,.$$

So, to have a *single-valued* wavefunction, we see that 2ϕ must be equal to some integral multiple of 2π. We, therefore, get two possibilities, $\phi = 2\pi$ or π. These correspond to the conditions,

$$\Psi(r_1,..,r_i,..,r_j,..,r_n,t) = \pm\Psi(r_1,...r_j,..,r_i,..,r_n,t).$$

[1] See *Resonance*, Vol.22, No.3, 2013.

The plus and minus signs correspond respectively to bosons[1] and fermions.

Since all the particles involved are indistinguishable, it no more makes sense to talk about individual particles. Instead, we take the discussion to the number of states with a particular eigenvalue that is present in the wavefunction. In this sense, second quantization is also called the *occupation number formalism*. A state in this formalism exists in a mathematical structure called the Fock space F, which is defined differently for bosons and fermions. Mathematically, for bosons, the Fock space is the direct sum of the spaces formed from symmetric (in the sense that interchanging particle indices does not change the wavefunction) tensor products of n number of single particle Hilbert spaces, where n varies from 0 (vacuum) to infinity. For fermions, the definition remains the same except that it now involves the direct sum of the

anti-symmetric tensor products of states in the individual Hilbert spaces. Readers are referred to sources [1] and [2] (see Suggested Reading) to gain a fuller understanding of how this leads to the occupation number formalism.

$$F = \begin{cases} \bigoplus_{m=0}^{\infty} Sym(H^m) & \text{for bosons} \\ \bigoplus_{m=0}^{\infty} Antisym(H^m) & \text{for fermions.} \end{cases} \tag{3}$$

In the position space, the basis in occupation number formalism for N particles looks like:

$$\Phi_{n_1,n_2,\ldots} = \langle r_1, r_2, \ldots | n_1, n_2, \ldots \rangle$$
$$= \begin{cases} (\frac{n_1!n_2!\ldots.}{N!})^{1/2} \sum_\sigma \phi_1(r_{\sigma(1)})\phi_2(r_{\sigma(2)})\ldots & \text{for bosons} \\ (\frac{1}{N!})^{1/2} \sum_\sigma (-1)^\sigma \phi_1(r_{\sigma(1)})\phi_2(r_{\sigma(2)})..... & \text{for fermions,} \end{cases} \tag{4}$$

where $\sum_i n_1 = N.\sigma$ represents a permutation of the set $\{1, 2, ...\}$ which in this case indicates the particle indices. The sum is over all possible permutations of a set of N indices. The state basically says that there are n_1 particles in state ϕ_1, n_2 in state ϕ_2 and so on. The additional factor $(\frac{(n_1!n_2!\ldots.)}{N!})^{1/2}$ for the bosonic case is required for the basis vector to have unit norm. Similarly, for fermions, the normalization factor $(\frac{1}{N!})^{1/2}$ is used. Depending on the parity of the permutation, the factor $(-1)^\sigma$ introduces the condition (2) for the fermions.

The orthonormality condition is given by:

$$\langle n_1', n_2', ...|n_1, n_2, ...\rangle = \delta_{n_1' n_1} \delta_{n_2' n_2} ... \tag{5}$$

Equation (4) allows us to see how the Pauli exclusion principle is derived from (1) for the general case. A general fermionic wavefunction, from (4) can be represented in the form of a determinant called the *Slater determinant*:

A general fermionic wavefunction can be represented in the form of a determinant called the *Slater determinant*.

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \dots & \phi_1(r_N) \\ \phi_2(r_1) & \phi_2(r_2) & \dots & \phi_2(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(r_1) & \phi_N(r_2) & \dots & \phi_N(r_N) \end{vmatrix}$$

If two electrons were to occupy the same eigenstate, there would be at least one column with two equal elements, consequently giving a determinant value of 0.

So, we can see that if two electrons were to occupy the same eigenstate, there would be at least one column with two equal elements, consequently giving a determinant value of 0. So the wavefunction vanishes.

Having defined the space and the vectors we are going to work with, we now briefly introduce the creation and annihilation operators and their properties for bosons and fermions below.

1.1 *Bosons*

The bosonic creation and annihilation operators are defined through their actions on a general occupation state as follows:

$$b_i^\dagger |n_1, n_2, ...n_i, ..\rangle = \sqrt{n_{i+1}} |n_1, n_2, ...n_i + 1, ..\rangle \quad (6)$$

$$b_i |n_1, n_2, ...n_i, ..\rangle = \sqrt{n_i} |n_1, n_2, ...n_i - 1, ..\rangle. \quad (7)$$

The creation operator $b_i^\dagger$ creates a new particle in the state ϕ_i, while the annihilation operator b_i destroys one particle in the state ϕ_i. Their operation on the vacuum state (different from the number 0), is given as: $b_i^\dagger|0\rangle = |n_i = 1\rangle$. When the annihilation operator acts on the vacuum state, the resultant is simply zero: $b_i|0\rangle = 0$.

The above properties allow us to introduce the number operator $b_i^\dagger b_i$, which when acted upon a state can give us the number of particles in a particular eigenstate ϕ_i.

$$b_i^\dagger b_i |n_1, n_2, ...n_i, ..\rangle = n_i |n_1, n_2, ...n_i, ..\rangle. \quad (8)$$

One has to note that not all states in the Fock space are eigenstates of the number operator.

The above properties allow us to state the fundamental commutation relations followed by these operators in the Fock space:

$$[b_j, b_k] = 0 \qquad [b_j^\dagger, b_k^\dagger] = 0 \qquad [b_j, b_k^\dagger] = \delta_{jk}. \tag{9}$$

1.2 *Fermions*

A state for fermions in the occupation number representation may look like this: $|1, 0, 1, 1, 1, 0...1, ..\rangle$. Amusingly, this looks like a bunch of bits in machine language.

The fermion creation and annihilation operators have the properties:

$$f_i^\dagger |n_1, n_2, ... \underbrace{1}_{\text{ith state}}, ..\rangle = 0 \quad f_i^\dagger |n_1, n_2, ... \underbrace{0}_{\text{ith state}}, ..\rangle = (-1)^{\mu_i} |n_1, n_2, ... \underbrace{1}_{\text{ith state}}, ..\rangle$$
$$f_i |n_1, n_2, ... \underbrace{1}_{\text{ith state}}, ..\rangle = (-1)^{\mu_i} |n_1, n_2, ... \underbrace{0}_{\text{ith state}}, ..\rangle \quad f_i |n_1, n_2, ... \underbrace{0}_{\text{ith state}}, ..\rangle = 0 \tag{10}$$

where μ_i is equal to the number of particles in states whose indices are marked less than i,

$$\mu_i = \sum_{j=1}^{i} n_j.$$

We cannot create more than one particle in the same state. A number operator $f_i^\dagger f_i$ can be used, but unlike in the bosonic case, it can have eigenvalues of either 0 or 1.

These operators can be shown to obey the following anti-commutation relations:

$$\{f_j, f_k\} = 0, \qquad \{f_j^\dagger, f_k^\dagger\} = 0, \qquad \{f_j, f_k^\dagger\} = \delta_{jk}. \tag{11}$$

1.3 *Hamiltonian in Operator Language*

Here, we are briefly going to review how to represent general operators in second quantized language.

One body operators like kinetic energy and background potential can be written as:

$$T_{tot} = \sum_{i,j} \langle i|T + V_b|j\rangle a_i^\dagger a_j. \tag{12}$$

One of the conventional approaches in theoretical and computational investigation of condensed matter systems is to use the mean field theory to reduce quartic operators to quadratic operators, and then try and diagonalize the resulting matrix to obtain the single-particle energy eigenvalues, assuming that they exist.

This an example of a *quadratic* operator. The above term is often called the *hopping potential*.

Two-body potentials, for example, the Coulomb potential can be written as follows:

$$V_{tot} = \frac{1}{2} \sum_{i,j,k,l} \langle ij|V_c|kl\rangle a_i^\dagger a_j^\dagger a_l a_k. \tag{13}$$

This is a *quartic* operator. One of the conventional approaches in theoretical and computational investigation of condensed matter systems is to use the mean field theory to reduce quartic operators to quadratic operators, and then try and diagonalize the resulting matrix to obtain the single-particle energy eigenvalues, assuming that they exist.

1.4 *Change of Basis*

The creation and annihilation operators are defined with respect to a particular basis, usually taken to be the eigenstates of a certain Hermitian operator, as is evident through the previous analysis. The following relations relate operators in one basis to another:

$$\tilde{a_j}^\dagger = \sum_k \langle k|j\rangle a_k^\dagger. \tag{14}$$

The Hermitian conjugate provides the corresponding relation for the annihilation operators.

2. The Kitaev Chain

The Kitaev chain, first introduced by Alexei Yu. Kitaev, was the first such system shown to exhibit Majorana zero modes (MZMs), which are *topologically protected* states, robust with respect to any local perturbations (impurities or defects). These MZMs exhibit exotic statistics which has recently given rise to the emerging field of topological quantum computation.

In his paper [3], Kitaev introduced a toy model which simulates the properties of a wire placed on the surface of a p-wave superconductor (where the spin of the fermions are paired). The wire

has n fermionic sites which can be occupied or unoccupied by spinless fermions. Kitaev introduces the tight-binding Hamiltonian, in the language of second quantization [3] as:

$$H = \sum_j (-w(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - \mu(a_j^\dagger a_j - \frac{1}{2}) + \Delta a_j a_{j+1} + \Delta^* a_{j+1}^\dagger a_j^\dagger) . \tag{15}$$

The summation in the Hamiltonian indicates that we consider only the nearest neighbor interactions in all the terms. It is noted that the Hamiltonian is Hermitian in nature as required by the general theory.

Here, a_j and $a_j^\dagger$ follows the usual fermionic anti-commutation relations,

$$\{a_j, a_k\} = 0, \qquad \{a_j^\dagger, a_k^\dagger\} = 0, \qquad \{a_j, a_k^\dagger\} = \delta_{jk} . \tag{16}$$

Here, w is the hopping amplitude between the neighboring fermions which involves the kinetic energy and background potential term. μ is the chemical potential, which as shown, is coupled with the number operator and describes the dependence of the energy of the system on the number of fermions present. The last two terms in the Hamiltonian are actually approximated versions of a quartic operator representing two-body potentials, in which two of the operators have been replaced by their average values. Δ is a complex number called the *superconducting gap*, which is an approximation for two operators obtained from the mean field theory. We absorb the phase of the superconducting gap while defining the Majorana operators:

$$c_{2j-1} = e^{i\theta/2} a_j + e^{-i\theta/2} a_j^\dagger, \qquad c_{2j} = -ie^{i\theta/2} a_j + ie^{-i\theta/2} a_j^\dagger , \tag{17}$$

where θ is obtained from the superconducting gap, $\Delta = |\Delta| e^{i\theta}$.

In terms of these Majorana operators, the Hamiltonian can be rewritten as:

$$H = i/2 \sum_{j=1}^{n-1} [-\mu c_{2j-1} c_{2j} + (w + |\Delta|) c_{2j} c_{2j+1} + (-w + |\Delta|) c_{2j-1} c_{2j+2}] . \tag{18}$$

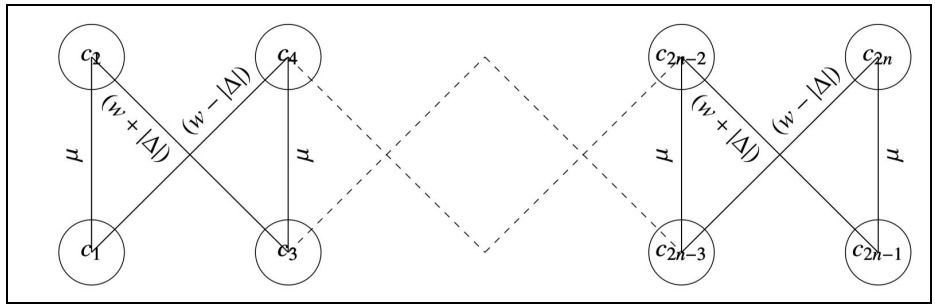

Figure 1. Coupling between the modes.

The coupling is graphically represented in *Figure* 1, where the nodes represent the two Majorana operators per fermionic site.

It is instructive to think of an electron to be made up of two Majorana quasi-particles. But one has to be careful because the MZMs themselves do not represent particles which could physically exist.

As we can clearly see from subsection (1.2), the transformation is orthogonal and each fermionic site gives rise to two Majorana operators which are Hermitian, i.e. $c_k^\dagger = c_k$ (this Hermiticity has given rise to the lore of *particles that are their own antiparticles*). The orthogonal transformation ensures the following properties for the modes:

$$\{c_j, c_k\} = 2\delta_{jk} \quad \text{and} \quad c_j^2 = 1\,.$$

It is instructive to think of an electron to be made up of two Majorana *quasi-particles*. But one has to be careful because the MZMs themselves do not represent particles which could physically exist because the number operator constructed as: $c_j^\dagger c_j = c_j^2 = 1$ makes no sense. In fact, these excitations are quite different from the theorized particles which are their own antiparticles – the Majorana fermions[2] – postulated by the great Italian physicist Ettore Majorana (see *Box* 1) in 1937. For example, Majorana fermions are still 'fermions', i.e. they follow Fermi–Dirac statistics (see *Box* 2) while the MZMs discussed here follow a kind of statistics different from both fermions and bosons.

[2] See A M Jayannavar and Arijit Saha, Emerging Trends in Topological Insulators and Topological Superconductors, *Resonance*, Vol.22, No.8, pp.787–800, 2017.

It is more correct to think in terms of combinations of Majorana modes which gives rise to fermionic excitations as seen from (17), $a_j^\dagger = \frac{1}{2}e^{i\theta/2}(c_{2j-1} - ic_{2j})$.

The fermionic number operator is: $a_j^\dagger a_j = \frac{(1+ic_{2j-1}c_{2j})}{2}$. Hence, $(ic_{2j-1}c_{2j}) = 1$ or -1 depending on whether the fermionic site

Box 1. Ettore Majorana

Ettore Majorana was an Italian theoretical physicist born in 1902. He worked initially on atomic spectroscopy. Later, he made important contributions in particle physics in the form of the Majorana equation, a variant of the Dirac equation for the electron, which uses a purely imaginary representation for the γ matrices, allowing real spinor solutions called Majorana fermions. Because the wavefunctions are real, the particles are their own antiparticles. At present, neutrinos are a major candidate for Majorana fermions. Majorana mysteriously disappeared off the coast of Palermo,while on a boat to Naples in 1932.

Box 2. Fermi–Dirac Statistics

Fermi–Dirac statistics – the law that governs the behaviour of fermions like electrons was discovered by Fermi and Dirac in 1926. Interestingly, Bose–Einstein statistics, which describes the behavior of bosons like photons, was first postulated by the Indian physicist S N Bose in a lecture class during an erroneous derivation of the Boltzmann statistics, which describes classical particles that are distinguishable.

is occupied or unoccupied. The parity operator is defined as: $P = \Pi_j(-ic_{2j-1}c_{2j})$. P commutes with the Hamiltonian $\mathbf{H}$ in (15). The eigenstates of $\mathbf{H}$ hence have definite parity, i.e. $P = -1$ or $+1$, depending on whether they have an odd or even number of fermions. A real orthogonal transformation of the Majorana operators given as $\vec{c'} = M\vec{c}$ where $MM^T = 1$, might or might not change the fermionic parity $P = (-i)^n\Pi_j c_j = det(M)(-i)^n\Pi_j c'_j$ of a state.

3. Two Special Cases

Now we look at two special cases of the Hamiltonian:

(a) The trivial case: $\Delta = w = 0$ and $\mu < 0$:

$$H_a = -\mu \sum_j (a_j^\dagger a_j - \frac{1}{2}) = \frac{i}{2}(-\mu) \sum_j c_{2j-1}c_{2j}\,. \qquad (19)$$

Here, the Majorana operators from a single site are paired to-

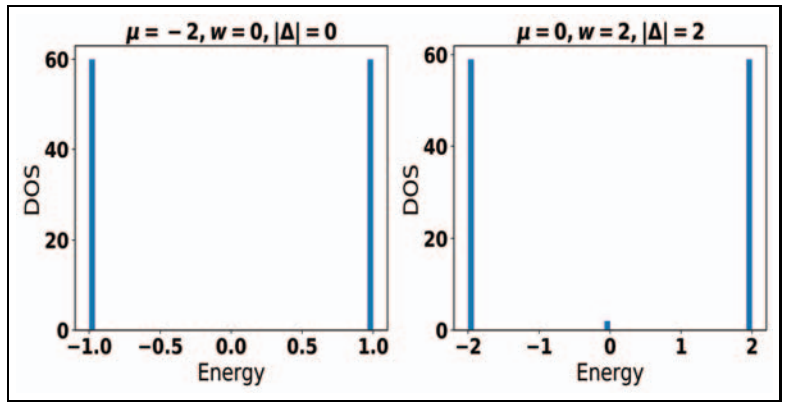

Figure 2. DOS for the trivial (left) and topological (right) case. Notice the peak at the zero energy in the topological case. These zero modes are the MZMs. Number of sites = 60.

gether to give rise to the original electrons. The ground state has occupation number 0.

(b) The topological case: $\Delta = w > 0$ and $\mu = 0$:

$$H_b = iw \sum_j c_{2j} c_{2j+1} = 2w \sum_{j=1}^{n-1} (\tilde{a}_j^\dagger \tilde{a}_j - \frac{1}{2}) . \qquad (20)$$

As we can see in *Figure* 2, the MZMs from neighbouring sites are coupled. The operators c_1 and c_{2n} do not appear in the Hamiltonian. New Fermionic modes constructed as $\tilde{a}_j = \frac{1}{2}(c_{2j} + ic_{2j+1})$ are the eigenmodes of this phase.

We can construct a non-local fermionic mode from the two Majorana operators that are left out from the Hamiltonian, $f^\dagger = \frac{1}{2}(c_1 - ic_{2n})$, a Fermionic eigenmode of the Hamiltonian with energy $-w$. The ground state of (20) must satisfy $\tilde{a}_j|\Phi_0\rangle = 0 \quad \forall \quad j$. Hence the parity operator P reduces to the form, $-ic_1c_{2n}$.

Now, both c_1 and c_{2n} commutes with H_b (this implies that the ground state of the Hamiltonian is an eigenstate of both these Majorana operators). Similar is the case for P. If $|\Phi_0\rangle$ is the ground state, it can be shown that both $c_1|\Phi_0\rangle$ and $c_{2n}|\Phi_0\rangle$ cannot be equal to $|\Phi_0\rangle$. The ground state therefore *must* be degenerate.

In fact, the two ground states $|\Phi_0\rangle$ and $|\Phi_1\rangle$ represent non-occupation and occupation of the non-local fermionic mode $f^\dagger$.

$$|\Phi_0\rangle = |0\rangle_f \Pi_{j=1}^{l-1} |0\rangle_j \text{ and } |\Phi_1\rangle = |1\rangle_f \Pi_{j=1}^{l-1} |0\rangle_j \,. \tag{21}$$

The two modes can be swapped between each other by an operation of c_1, c_{2n} or $f^\dagger$. Also, notice that $P|\Phi_0\rangle = +1$ and $P|\Phi_1\rangle = -1$, indicating the two states having odd (1) or even (0) fermions.

4. General Conditions for MZMs

The Hamiltonian in subsection (1.3) can be written in a matrix form in the Majorana matrix,

$$\mathrm{H} = \frac{i}{4} C^\dagger \mathbf{H} C \;\text{ and }\; \mathrm{C} = [\mathrm{c}_1, \mathrm{c}_2, \ldots, \mathrm{c}_{2\mathrm{n}}], \tag{22}$$

where the matrix $\mathbf{H}$ has the form:

$$\mathbf{H} = \begin{pmatrix} 0 & -\mu & 0 & (-w+|\Delta|) & 0 & 0\ldots \\ \mu & 0 & (w+|\Delta|) & 0 & 0 & 0\ldots \\ 0 & -(w+|\Delta|) & 0 & -\mu & 0 & (-w+|\Delta|)\ldots \\ (w-|\Delta|) & 0 & \mu & 0 & (w+|\Delta|) & 0\ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$\mathbf{H}$ is a skew-symmetric matrix. This means that it has purely imaginary eigenvalues of the form: $\pm i\epsilon_m$. We try to find solutions where one of the eigenvalues is zero.

$\mathbf{H}$ can be reduced to the block-diagonal form by a real orthogonal matrix W like:

$$A = W\mathbf{H}W^T = \begin{pmatrix} 0 & \epsilon_1 & 0 & 0\ldots & & \\ -\epsilon_1 & 0 & 0 & 0\ldots & & \\ 0 & 0 & 0 & \epsilon_2\ldots & & \\ 0 & 0 & -\epsilon_2 & 0\ldots & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{23}$$

Now, the Hamiltonian is of the form $H = \sum_m \epsilon_m b'_m b''_m$.

We try to find the conditions on W so that one of the eigenvalues is zero, Any skew-symmetric matrix $\mathbf{H}$ can be block-diagonalized by utilizing its eigenvectors.

$\mathbf{H}\vec{u_m} = +i\epsilon_m \implies \mathbf{H}\vec{u}^* = -i\epsilon_m$

We define new real vectors $\xi_m = i(u_m^* - u_m)/2$ and $\eta_m = (u_m + u_m^*)/2 \implies \mathbf{H}\xi_m = -\epsilon_m\eta_m$ and $\mathbf{H}\eta_m = \epsilon_m\xi_m$.

The transformation matrix W is defined as:

$$W_{2j-1} = [\eta_j^T] \text{ and } W_{2j} = [-\xi_j^T], \tag{24}$$

where W_i represents the i^{th} row of the matrix W.

It can be shown that W is orthogonal. In his paper, Kitaev employs an ansatz of the form:

$$b' = \sum_j (\alpha'_+ x_+^j + \alpha'_- x_-^j) c_{2j-1}, \quad b'' = \sum_j (\alpha''_+ x_+^{-j} + \alpha''_- x_-^{-j}) c_{2j}. \tag{25}$$

The motivation behind this is that we want the modes b and b' to be localized at different ends of the wire, and hence guess solutions that can have similar properties. The α coefficients are just constants used to parametrize the solutions. Seeking inspiration from the previous special case that exhibits MZMs, ultimately what we want is *both* $|x_+|$ and $|x_-|$ to be less than or greater than 1 so that b' and b'' are localized at the two opposite ends of the chain and decay exponentially towards the other end. Using the form of W, it can be shown in the limit $n \to \infty$, that the conditions are perfectly satisfied with $\epsilon_m = 0$ and $x_\pm = \frac{-\mu \pm \sqrt{\mu^2 - 4w^2 + 4|\Delta|^2}}{2(w+|\Delta|)}$, in the parameter space $2|w| > |\mu|$, $|\Delta| \neq 0$.

What we get in the end, are three distinct phases:

- *The trivial phase*: This rather boring phase enters into the picture when the zero modes are non-existent, i.e. when $\frac{2|w|}{\mu} < 1$.

- *The topological phase I*: Both $|x_+|, |x_-| < 1$ at $|\mu| < 2w$. This makes b' localized near $j = 1$ and b'' at $j = n$. The MM at $j = 1$ involves the c_1 mode, while that at n involves the c_{2n} mode.

- *The topological phase II*: Both $|x_+|, |x_-| > 1$ at $|\mu| < -2w$. In this case, b' is localized near $j = n$ and b'' at $j = 1$. Now the MM at $j = 1$ involves the c_2 mode, while that at n involves the c_{2n-1} mode.

Since the solutions are exact only in the limit of $n \to \infty$, for finite n, the two ground states are expected to have a small energy

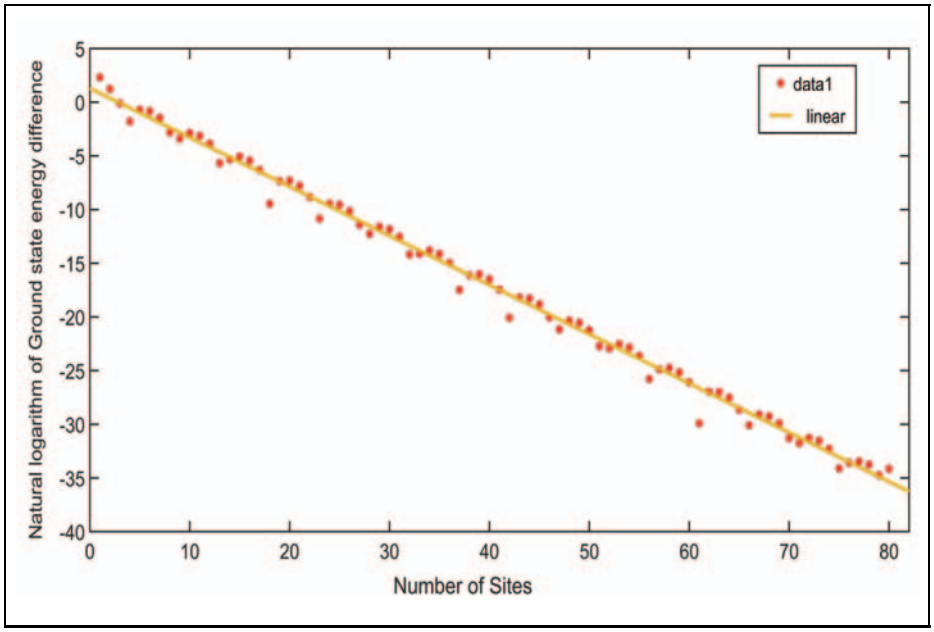

Figure 3. Exponential decay in energy difference between the two ground states for $\mu = 10$, $w = 7$ and $|\Delta| = 3$.

difference (and hence not perfectly degenerate) that decays exponentially with the increase in length of the chain. This has been verified for chains upto 80 sites long in *Figure* 3.

We verify the division between topological phase I and the trivial phase. We start with the values $\mu = 10$, $w = 4$ and $|\Delta| = 5$. We serially increase w by 0.5 and plot the resulting five histograms which depict the density of states.

As expected, for the first two cases (as shown in *Figure* 4), since $\mu > 2w$, there are no zero modes. Both the cases are gapped.

The critical point, where $2w = |\mu| = 10$ does exhibit zero modes but the spectrum is gapless and the states are not protected (*Figure* 5).

We can clearly see the zero modes for the next two cases in *Figure* 6. Both of these are gapped and support robust ground states.

To make the phase transition that is occurring here clearer and to depict the three different phases, we map out the spectrum of the system with respect to the hopping term in *Figure* 7. As we can see, the system essentially undergoes a phase transition from

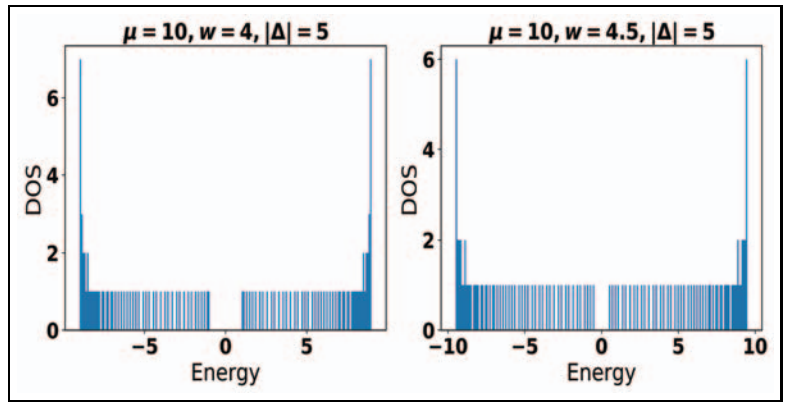

Figure 4. Trivial DOS for number of sites = 60.

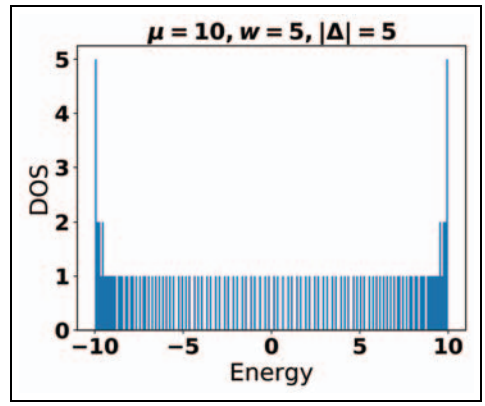

Figure 5. Critical point. Number of sites = 60.

the trivial phase into the topological phases at the points where $2w = \mu$ with the gap closing.

To see that the zero-modes in the two topological phases are different, the reader is encouraged to plot something called the linear density of states (LDOS), which is obtainable from the retarded Green's function associated with the Hamiltonian. One has to take the site-trace of the matrix, $G^R(\omega) = \frac{1}{\omega - i\delta - H}$, in the basis of the MZMs, to find the weight contributed by that site to the eigenstate at energy ω. Doing so, one would find that in topological phase I, the major contribution at $\omega = 0$ comes from the c_1 and c_{2n} modes, while in the topological phase II, the same role is played by c_2 and c_{2n-1}.

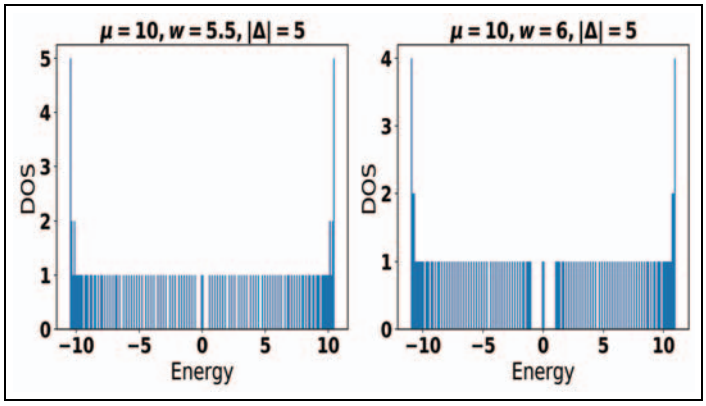

Figure 6. Topological DOS. Number of sizes = 60.

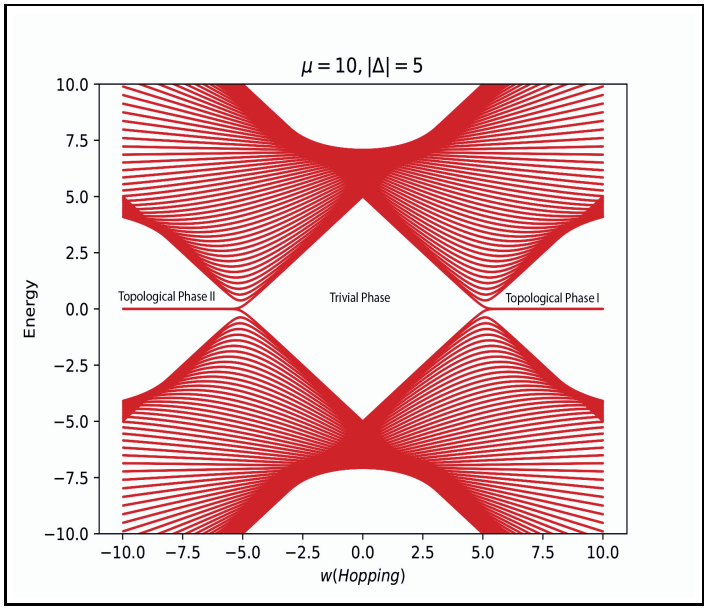

Figure 7. Energy spectrum. Number of sites = 60.

5. The Bulk Spectrum

In this section, we investigate the properties of the bulk spectrum for the chain. We write the original fermionic position operators in terms of the creation operators, $a_k^\dagger$ of the momentum states $\frac{1}{\sqrt{n}}e^{ikx}$. The site-wavefunctions can be thought of as localized

delta functions.

$$a_j^\dagger = \frac{1}{\sqrt{n}} \sum_{k \in FBZ} \langle k|\delta(x-j)\rangle a_k^\dagger . \tag{26}$$

The Hamiltonian in subsection(1.1) is then rewritten in the Bogoliubov–deGennes form using contributions from both $+k$ and $-k$ operators as:

$$H = \begin{bmatrix} a_k^\dagger & a_{-k} \end{bmatrix} \begin{bmatrix} -2w\cos k - \mu & -2\Delta i \sin k \\ 2\Delta^* i \sin k & 2w\cos k + \mu \end{bmatrix} \begin{bmatrix} a_k \\ a_{-k}^\dagger \end{bmatrix} \tag{27}$$

Diagonalizing this we end up with the spectrum:

$$\epsilon(k) = \pm \sqrt{(2w\cos k + \mu)^2 + 4|\Delta|^2 \sin^2 k} . \tag{28}$$

The diagonalized Hamiltonian is: $H = \sum_k \epsilon_k \tilde{a}_k^\dagger \tilde{a}_k +$ constant, where the operators $\tilde{a}_k^\dagger = u_k a_k + v_k a_{-k}^\dagger$ and

$$u_k = \frac{\Delta_k}{|\Delta_k|}\left(\frac{\epsilon_k + (2w\cos k + \mu)}{2\epsilon_k}\right)^{1/2} \text{ and } v_k = \left(\frac{\epsilon_k - (2w\cos k + \mu)}{\Delta_k^*}\right) u_k \tag{29}$$

where $\Delta_k = -2\Delta^* i \sin k$.

The spectrum is shown below for different values of the parameters. we see the phase is gapless at the critical point: $\mu = 2w$.

Equation (28) allows us to characterize the bands by analytically calculating the *topological numbers* associated with the curve $\epsilon(k)$.

6. Topology and Quantum Computation

Certain symmetries that the Hamiltonian possesses ensures a band gap that protects the MZMs. The fact that these modes lie at zero energy in the middle of the gap makes these modes delocalized at the ends of the wire.

The bands that we encountered can be characterized with a so-called winding number (which is an integer, denoted by Z). In this case, the modulus of the winding number turns out to be equal to the number of zero modes. Thus, the trivial phase would be characterized with $Z = 0$ while the topological phases would have $Z = \pm 1$ (there is of course, a specific formula to calculate Z, pertaining to the famous Gauss–Bonnet theorem but we omit it here for considerations of space). The point of all of this is to identify distinct phases that are *adiabatically* cut off from one

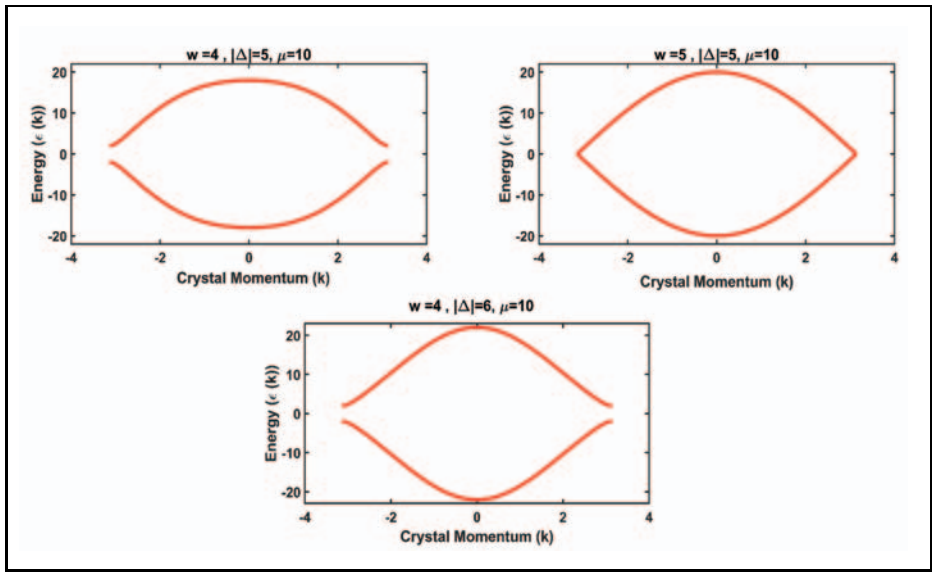

Figure 8. Bulk spectra at different parameter values.

another. In simple words, what we mean is that no matter in what way you continuously deform the parameters of the Hamiltonian (e.g the hopping or the order parameter), it would be impossible to reach one phase from the other without suffering a gap closure (phase transition).

Certain symmetries that the Hamiltonian possesses ensures a band gap that protects the MZMs. The fact that these modes lie at zero energy in the middle of the gap makes these modes delocalized at the ends of the wire. Non-locality (a consequence of the gap) of the resulting Fermionic mode (by fusing the two MZMs) ensures that it is not destroyed by local impurities or defects in the system.

Besides the role we have discussed just now, *topology* also plays a significant role in the process of quantum computation[3] that uses MZMs (hence the name *topological quantum computation*). Like we have hinted before, MZMs are *not* fermions but are in fact a class of particles called the *non-abelian anyons* (that exist in dimensions lower than 3). These exotic particles have different statistics from fermions in the sense that when we exchange these, instead of suffering a simple change in phase, the wavefunction

[3] See Apoorva Patel, Quantum Computation – Particle and Wave Aspects of Algorithms, *Resonance*, Vol.6, No.9, pp.821–835, 2011.

undergoes a highly non-trivial change. The process of *computation* involves exchanging multiple MZMs in a system, fusing them to form regular fermions and then measuring them. The process of exchange is called *braiding*, and the result depends on the topology of how these exchanges are carried out.

7. Conclusion

The computations of the density of states and related properties was carried out in Python or Matlab using inbuilt functions for matrix diagonalization.

The article shows the existence of MZMs for a particular part of the parameter space for the Kitaev chain and provides some basic explanations regarding topological protection and computation. Motivated students can find out that the ultimate fermionic mode is non-local by plotting something called the linear density of states (LDOS). Such an endeavor would include calculating the Green's function associated with the Hamiltonian. A small exercise might include adding noise to the Hamiltonian and checking the robustness of these modes.

The rapidly growing field of topological quantum computation presents new possibilities every day. The interested reader is invited to read [4] to gain a bird's eye view of the applications of MZMs and the experimental endeavors that have detected signatures consistent with these excitations.

Acknowledgements

This article would not have been possible without the fruitful discussions with Dr Saurabh Basu, who has guided the study from the start. The author would like to express his gratitude to the anonymous reviewer(s) who have helped in enriching this manuscript. The author would also like to thank IIT Guwahati and IIT Kharagpur.

References

[1] **Valery Shchesnovich, The Second Quantization Method for Indistinguishable Particles, *Lecture Notes in Physics*, UFABC 2010, arXiv:1308.3275.**

[2] **A Fetter, J D Walecka, *Quantum Theory of Many-particle Systems*, Dover Books on Physics, 2003.**

[3] **A Yu Kitaev, Unpaired Majorana Fermions in Quantum Wires, *Phys. Usp.*, Vol.44, pp.131–136, 2001.**

[4] **S D Sarma, M Freedman, C Nayak, Majorana Zero Modes and Topological Quantum Computation, *npj Quantum Information 1*, Article number: 15001, 2015. DOI: https://doi.org/10.1038/npjqi.2015.1**

Address for Correspondence
Arnab Barman Ray
The Institute of Optics
480 Intercampus Drive
River Campus
Rochester, NY 14627
Email:
abarmanr@ur.rochester.edu