Prototypical Quantum Spin Hamiltonians in the Language of Jordan-Wigner Fermions

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Abstract

We present here the Jordan-Wigner solutions to three prototypical spin 1/2 Hamiltonians. In particular, we consider the 1D transverse Ising model, XY model, and Kitaev honeycomb model. After transforming the Hamiltonian to spinless fermions via Jordan-Wigner transformation, we employ Fourier transform then Bogoliubov transformation to diagonalize the Hamiltonian exactly. Moreover, the spectrum of elementary excitations as well as the ground-state energy are examined. In addition, some correlation functions of the solved models are covered briefly. Lastly, the research problem of an extension to the Kitaev model is introduced.

Contents

1 Introduction

Condensed matter physics is an area of physics that studies the physical properties of materials and their collective phenomena, such as magnetism, superconductivity. Of particular interest is the development of theoretical models and their solution. Methods to solve these models often make use of different transformations such as the Jordan-Wigner transformation that allows to study magnetic phenomena in fermionic language. The Jordan-Wigner transformation is a powerful tool for exploring quantum mechanical properties of many-body systems. In this research proposal, we will study three prototypical quantum spin Hamiltonians: the Ising, XY, and Kitaev honeycomb model. Then we will propose a study of an extended Kiteav honeycomb model.

2 Background

2.1 Second Quantization

Second quantization is a formalism that was developed to describe and analyze quantum many-body systems. It enforces identical particle's statistics in the form of creation and annihilation operators. Any state can be generated by acting with creation and annihilation operators on a many-body vacuum state $|0\rangle$.

Fermionic operators satisfy the following set of anti-commutation relations:

$$\{c_i, c_j^\dagger\} = \delta_{ij}; \quad \{c_i^\dagger, c_j^\dagger\} = 0; \quad \{c_i, c_j\} = 0 \tag{1}$$

The actions of fermionic operators on the vacuum are given as:

$$c_i |0\rangle = 0; \quad \langle 0| c_i^\dagger = 0 \tag{2}$$

For bosonic operators:

$$[a_i, a_j^\dagger] = \delta_{ij}; \quad [a_i^\dagger, a_j^\dagger] = 0; \quad [a_i, a_j] = 0 \tag{3}$$

The actions of bosonic operators on the vacuum are given as:

$$a_i |0\rangle = 0; \quad \langle 0| a_i^\dagger = 0 \tag{4}$$

2.2 Spin Hamiltonians

Spin Hamiltonians are mathematical models that describe the behavior of interacting spin systems. These Hamiltonians typically consist of sums of spin operators.

Spin operators are operators that satisfy the following commutation relations:

$$[S^i, S^j] = i\hbar\varepsilon_{ijk} S^k; \quad [\sigma^i, \sigma^j] = 2i\varepsilon_{ijk}\sigma^k \tag{5}$$

Where i, j and k can be spin labels x, y and z. Moreover, they fulfill this anti-commutation relation:

$$\{S^i, S^j\} = \hbar\delta_{ij} I; \quad \{\sigma^i, \sigma^j\} = 2\delta_{ij} I \tag{6}$$

Here σ_i's are spin 1/2 operators, and S_i's are general spin operators. For spin 1/2 they are related as follows:

$$S^i = \frac{\hbar}{2}\sigma^i \tag{7}$$

Three examples of spin Hamiltonians are given below:

$$H = -\sum_i \left[S_i^x + \bar{\lambda} S_i^z S_{i+1}^z\right]; \qquad \text{The Ising model} \tag{8}$$

$$H = \sum_i \left[(1+\gamma)\, S_i^x S_{i+1}^x + (1-\gamma)\, S_i^y S_{i+1}^y\right]; \qquad \text{The XY model} \tag{9}$$

$$H = -J_x \sum_{x-links} \sigma_j^x \sigma_k^x - J_y \sum_{y-links} \sigma_j^y \sigma_k^y - J_z \sum_{z-links} \sigma_j^z \sigma_k^z; \qquad \text{Kitaev Honeycomb Model} \tag{10}$$

Where $\bar{\lambda}$, γ, J_i are model parameters, which are typically related to magnetic couplings.

2.3 Jordan-Wigner Transformation

The Jordan-Wigner (JW) transformation is a unitary transformation used to map a system of interacting spins to a system of non-interacting fermions. This transformation allows for the use of fermionic statistics, which in some cases make it easier to solve a spin Hamiltonian, and can make it easier to compute correlation functions.
The definition of the Jordan-Wigner includes a string of σ^z operators on different sites. This string must be defined such that it can thread all the sites up to the site of transformation. More generally, the objective is to define a convenient path for this string of σ^z operators that makes the model easily solvable.
For the Ising and XY models, or any 1-D chain model, the JW transformation is defined as follows:

$$S_i^+ = \prod_{j<i} \left[-S_j^z\right] c_i^\dagger; \quad S_i^- = c_i \prod_{j<i} \left[-S_j^z\right] \tag{11}$$

$$S_i^x = \frac{1}{2}\left(S_i^+ + S_i^-\right); \quad S_i^y = \frac{i}{2}\left(S_i^- - S_i^+\right) \tag{12}$$

$$S_i^z = 2c_i^\dagger c_i - 1. \tag{13}$$

Here, $c^\dagger$ and c are fermionic creation and annihilation operators.

For the Kitaev honeycomb model, which is two dimensional, the string of sigma σ^z operators is defined differently while maintaining the same condition: threading the whole lattice. In this case it is given as

$$\sigma_{ij}^+ = 2\left[\prod_{j'<j}\prod_{i'} \sigma_{i'j'}^z\right]\left[\prod_{i'<i}\sigma_{i'j}^z\right] c_{ij}^\dagger; \quad \sigma_{ij}^- = 2c_{ij}\left[\prod_{j'<j}\prod_{i'} \sigma_{i'j'}^z\right]\left[\prod_{i'<i}\sigma_{i'j}^z\right] \tag{14}$$

$$\sigma_{ij}^x = \frac{1}{2}\left(\sigma_{ij}^+ + \sigma_{ij}^-\right); \quad \sigma_{ij}^y = \frac{i}{2}\left(\sigma_{ij}^- - \sigma_{ij}^+\right) \tag{15}$$

$$\sigma_{ij}^z = 2c_{ij}^\dagger c_{ij} - 1 \tag{16}$$

2.4 Majorana Fermions

Majorana fermions are particles that are their own anti-particle, that can be described by a linear combination of creation and annihilation fermionic operators.

Majorana operators satisfy the relations below:

$$\{A_i, A_j\} = \delta_{ij}; \quad A^\dagger = A; \quad A^2 = 1 \tag{17}$$

Introducing Majorana quasi-particles can sometimes be useful in computing correlation functions as it will be shown in Sec. 3.1.3. In some cases it also makes it easier to identify conserved quantities such as is the case in honeycomb Kitaev-type Hamiltonians. This observation leads to much easier computations of physical properties.

2.5 Fourier Transformation of Fermionic Operators

Fourier transformations, can be used to transform the Hamiltonian into momentum space. For translation invariant Hamiltonians this has proven to be useful. After transforming the Hamiltonian into momentum space, due to transnational symmetry, one can find simplifications that lead to easier computations. The transformation is defined as follows:

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_q c_q^\dagger e^{iqj}; \quad c_j = \frac{1}{\sqrt{N}}\sum_q c_q e^{-iqj} \tag{18}$$

Here, $c_q^\dagger$ and c_q are fermionic creation and annihilation operators in momentum space, and N is the total number of sites. One important identity in dealing with Fourier transforms is the following:

$$\sum_j e^{i(q-q')j} = N\delta_{qq'} \tag{19}$$

2.6 Bogoliubov Diagonalization

A Hamiltonian is considered solved if it has been diagonalized. Some families of many-body Hamiltonian are especially easily diagonalizable. We consider here as an example the fermionic Bogoliubov type family of Hamiltonians in momentum space. This type of Hamiltonian can be written in the following form:

$$H = \sum_q \begin{bmatrix} \mathbf{c}_q^\dagger & \mathbf{c}_{-q} \end{bmatrix} \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} \mathbf{c}_q \\ \mathbf{c}_{-q}^\dagger \end{bmatrix} \tag{20}$$

Here, h_{ij}'s are matrix blocks of the same size, then the Hamiltonian is diagonalized in the following way (by employing a unitary transformation U):

$$H = \sum_q \underbrace{\begin{bmatrix} \mathbf{c}_q^\dagger & \mathbf{c}_{-q} \end{bmatrix} U^\dagger}_{\begin{bmatrix} \eta_q^\dagger & \eta_{-q} \end{bmatrix}} \underbrace{UhU^\dagger}_{D} \underbrace{U \begin{bmatrix} \mathbf{c}_q \\ \mathbf{c}_{-q}^\dagger \end{bmatrix}}_{\begin{bmatrix} \eta_q & \eta_{-q}^\dagger \end{bmatrix}^T} \tag{21}$$

Where $D = \begin{bmatrix} E_q & 0 \\ 0 & E_{-q} \end{bmatrix}$. Then, the Hamiltonian in diagonalized form has the form:

$$H = \sum_q E_q \eta_q^\dagger \eta_q + E_{-q} \eta_{-q} \eta_{-q}^\dagger \tag{22}$$

Where we may interpret E_q as particle energies and E_{-q} as hole energies.

2.6.1 Specific 2×2 Hamiltonian

We now consider a simple 2×2 Hamiltonian of the form

$$H = \sum_q \begin{bmatrix} c_q^\dagger & c_{-q} \end{bmatrix} \underbrace{\begin{bmatrix} \alpha & -i\beta \\ i\beta & -\alpha \end{bmatrix}}_{2\times 2} \begin{bmatrix} c_q \\ c_{-q}^\dagger \end{bmatrix} \tag{23}$$

Where α and β are real valued, and are elements of the 2×2 matrix. Then eigenvalues are given as:

$$\left| H - \omega_q \mathbb{I} \right| = \begin{vmatrix} \alpha - \omega_q & -i\beta \\ i\beta & -\alpha - \omega_q \end{vmatrix} = 0 \implies \omega_q = \pm\sqrt{\alpha^2 + \beta^2} \tag{24}$$

The unitary matrix U in (24) is:

$$U = \begin{bmatrix} | & | \\ V_1 & V_2 \\ | & | \end{bmatrix} = \begin{bmatrix} u_q & iv_q \\ iv_q & u_q \end{bmatrix}; \quad u_q = \frac{\alpha + \omega_q}{\sqrt{(\alpha + \omega_q)^2 + \beta^2}}; \quad v_q = \frac{\beta}{\sqrt{(\alpha + \omega_q)^2 + \beta^2}} \tag{25}$$

$$\begin{bmatrix} \eta_q^\dagger \\ \eta_{-q} \end{bmatrix} = \begin{bmatrix} u_q & iv_q \\ iv_q & u_q \end{bmatrix} \begin{bmatrix} c_q^\dagger \\ c_{-q} \end{bmatrix}; \quad \begin{bmatrix} \eta_q \\ \eta_{-q}^\dagger \end{bmatrix} = \begin{bmatrix} u_q & -iv_q \\ -iv_q & u_q \end{bmatrix} \begin{bmatrix} c_q \\ c_{-q}^\dagger \end{bmatrix} \tag{26}$$

Where V_1 & V_2 are the first and second eigenvectors of the matrix.

3 Spin Hamiltonians Solved in the Literature

3.1 1-D Chains: Ising and XY Models

3.1.1 Ising Model

If we apply a Jordan-Wigner (JW) transformation to the Ising model defined in (8) it will lead to quartic fermion terms when transforming $S_i^z S_{i+1}^z$. To avoid this issue we employ a canonical transformation:

$$S^x \to S^z; \quad S^z \to -S^x$$

After doing so, the Hamiltonian now reads:

$$H = -\sum_i \left[S_i^z - \bar{\lambda} S_i^x S_{i+1}^x\right] \tag{27}$$

Using (12) to rewrite spin operators as raising and lowering spin operators, we can rewrite the Hamiltonian as:

$$H = N - 2\sum_i S_i^+ S_i^- - \bar{\lambda}\sum_i \left[S_i^+ S_{i+1}^+ + S_i^+ S_{i+1}^- + S_{i+1}^+ S_i^- + S_i^- S_{i+1}^-\right] \tag{28}$$

Now, we employ the JW transformation in (11) to obtain a fermionic Hamiltonian:

$$H = N - 2\sum_i c_i^\dagger c_i - \bar{\lambda}\sum_i \left[c_i^\dagger c_{i+1}^\dagger + c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger - c_i c_{i+1}\right] \tag{29}$$

The next step now is to apply a Fourier transform in (18) and (19), and rearranging our terms such that we are only summing over positive modes, we obtain the following Hamiltonian:

$$H = -2\sum_{q>0}(1 + \bar{\lambda}\cos q)(c_q^\dagger c_q - c_{-q}^\dagger c_{-q}) + 2i\bar{\lambda}\sum_{q>0}\sin q(c_q^\dagger c_{-q}^\dagger - c_q c_{-q}) \tag{30}$$

$$= -2\sum_{q>0}\begin{bmatrix} c_q^\dagger & c_{-q}\end{bmatrix}\begin{bmatrix} 1+\bar{\lambda}\cos q & -i\bar{\lambda}\sin q \\ i\bar{\lambda}\sin q & -1-\bar{\lambda}\cos q\end{bmatrix}\begin{bmatrix} c_q \\ c_{-q}^\dagger\end{bmatrix} \tag{31}$$

We can see that this Hamiltonian has the same form as (23), thus, we can diagonalize it using (24). The result is the following diagonal Hamiltonian :

$$H = 2\sum_q \omega_q \eta_q^\dagger \eta_q + E_0 \tag{32}$$

$$E_0 = -\sum_q \omega_q; \quad \omega_q = \sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2} \tag{33}$$

The ground state energy may be computed analytically by taking the continuum limit of the summations:

$$E_0 = -\sum_q \omega_q \to \frac{E_0}{N} = -\int_{-\pi}^{\pi}\frac{dq}{2\pi}\omega_q \tag{34}$$

$$\frac{E_0}{N} = -\int_{-\pi}^{\pi}\frac{dq}{2\pi}\omega_q = -\frac{1}{\pi}\int_0^{\pi}\sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2}\,dq = -\frac{2}{\pi}(1+\bar{\lambda})\mathbf{E}\left(\frac{\pi}{2}, \sqrt{\frac{4\bar{\lambda}}{(1+\bar{\lambda})^2}}\right) \tag{35}$$

Here, $\mathbf{E}(\frac{\pi}{2}, k)$ is the complete elliptic integral of the second kind.

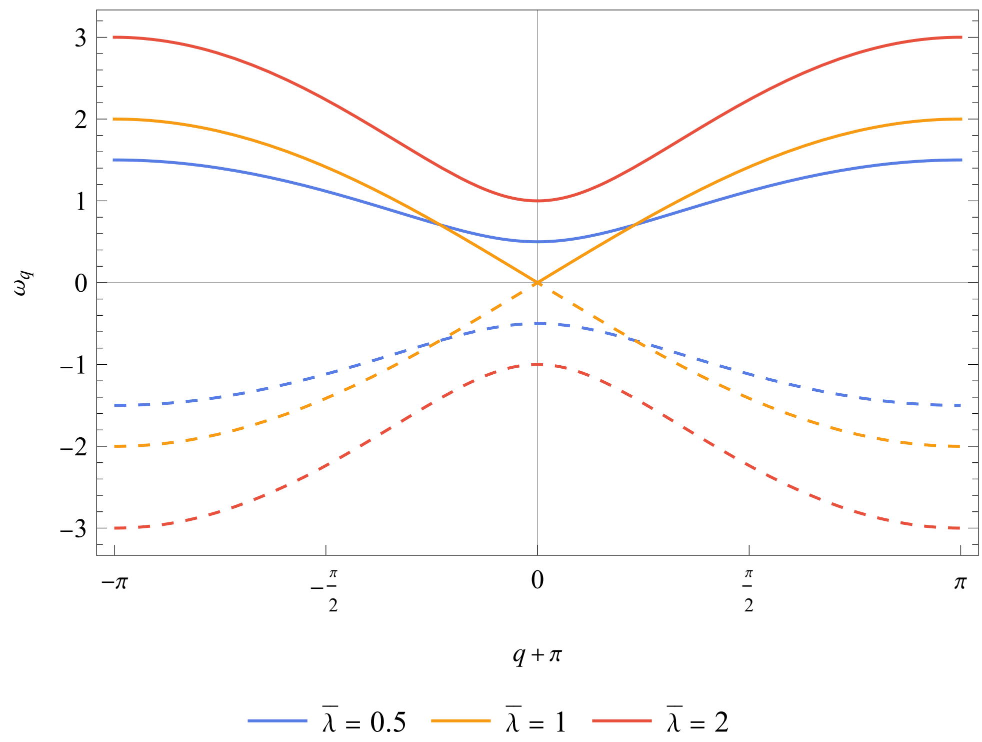

Figure 1: Energy of elementary excitations for different $\bar{\lambda}$. Dashed lines are hole energy.

3.1.2 XY Model

The XY model Hamiltonian (9) does not need any canonical transformations before employing a Jordan-Wigner transformation. This is because when we rewrite it in fermionic language it is quadratic already. We start by using (12) to rewrite spin operators as raising and lowering spin operators. We may then rewrite the Hamiltonian as:

$$H = 2\sum_i \left[S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \gamma\left(S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-\right)\right] \tag{36}$$

Now, we employ the JW transformation in (11) to obtain a fermionic Hamiltonian that is given below:

$$H = 2\sum_i \left[c_i^+ c_{i+1} - c_i c_{i+1}^+ + \gamma\left(c_i^+ c_{i+1}^+ - c_i c_{i+1}\right)\right] \tag{37}$$

The next step now is to apply a Fourier transform in (18) and (19), and rearranging terms in the Hamiltonian we are left with a sum over positive modes as shown below:

$$H = 4\sum_{q>0} \left[\cos q\left(c_q^+ c_q - c_{-q} c_{-q}^+\right) + \gamma i \sin q\left(c_{-q} c_q - c_q^+ c_{-q}^+\right)\right] \tag{38}$$

$$= 4\sum_{q>0} \begin{bmatrix} c_q^\dagger & c_{-q} \end{bmatrix} \begin{bmatrix} \cos q & -i\gamma\sin q \\ i\gamma\sin q & -\cos q \end{bmatrix} \begin{bmatrix} c_q \\ c_{-q}^\dagger \end{bmatrix} \tag{39}$$

We can also see that this Hamiltonian has the same form as (23), thus, we can diagonalize it using (24). The result is this following Hamiltonian in its eigenspace:

$$H = 4\sum_q \omega_q \eta_q^\dagger \eta_q + E_0 \tag{40}$$

$$E_0 = -2\sum_q \omega_q; \quad \omega_q = \sqrt{1-(1-\gamma^2)\sin^2 q} \tag{41}$$

Similar to (35), the ground state energy is:

$$\frac{E_0}{N} = -2\int_{-\pi}^{\pi} \frac{dq}{2\pi}\omega_q = -\frac{1}{2\pi}\int_0^{\pi/2} \sqrt{1-(1-\gamma^2)\sin^2 q}\,dq = -\frac{2}{\pi}\mathbf{E}\left(\frac{\pi}{2}, \sqrt{1-\gamma^2}\right) \tag{42}$$

Where $\mathbf{E}(\frac{\pi}{2}, k)$ is the complete elliptic integral of the second kind.

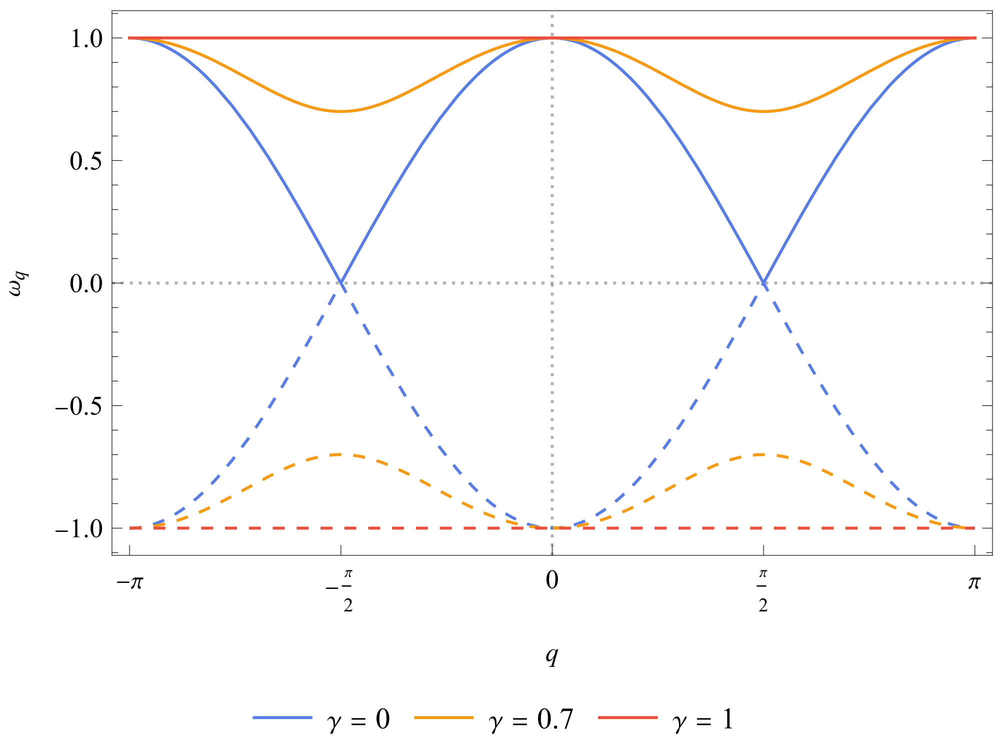

Figure 2: Energy of elementary excitations for different γ. Dashed lines are hole energy.

3.1.3 Correlation Functions

Correlation functions in condensed matter theory are related to physical observables that can be measured experimentally. Such as conductivity, magnetization, and spin-spin correlation functions. They can also be used to study the behavior of a system under external perturbations, such as an applied electric field or a magnetic field. The correlation functions we are interested in are defined as:

$$C^x_{ij} = \langle 0| S^x_i S^x_j |0\rangle \,; \quad C^y_{ij} = \langle 0| S^y_i S^y_j |0\rangle \,; \quad C^z_{ij} = \langle 0| S^z_i S^z_j |0\rangle \tag{43}$$

In order to calculate these correlation function we will use (12) as well as the JW transformation (11). The calculations are demonstrated in detail below for C^x_{ij}:

$$C^x_{ij} = \langle 0| S^x_i S^x_j |0\rangle = \langle 0| \left(c^\dagger_i + c_i\right) \prod_{i\le k<j} [-S^z_k] \left(c^\dagger_j + c_j\right) |0\rangle \tag{44}$$

However, we can simplify the string of $\prod_{i\le k<j}[-S^z_k]$ by introducing Majorana fermions:

$$A_i \equiv c^\dagger_i + c_i; \quad B_i \equiv c^\dagger_i - c_i; \quad A_i^2 = 1; \quad B_i^2 = -1; \quad \{A_i, B_j\} = 0 \tag{45}$$

$$S^z_k = 2c^\dagger_k c_k - 1 = \left(c^\dagger_k + c_k\right)\left(c^\dagger_k - c_k\right) = A_k B_k \tag{46}$$

$$\therefore C^x_{ij} = \langle 0| S^x_i S^x_j |0\rangle = \langle 0| A_i \prod_{i\le k<j} [A_k B_k] A_j |0\rangle = \langle 0| \prod_{i\le k<j} [B_k A_{k+1}] |0\rangle \tag{47}$$

Therefore, the correlation functions will yield:

$$C^x_{ij} = \langle 0| \prod_{i\le k<j} B_k A_{k+1} |0\rangle \,; \quad C^y_{ij} = \langle 0| \prod_{i\le k<j} B_{k+1} A_k |0\rangle \,; \quad C^z_{ij} = \langle 0| B_i A_i B_j A_j |0\rangle \,; \tag{48}$$

Now we will employ Wick's theorem to calculate the Vacuum Expectation Values (VEVs). For two operators $\hat{A}$ and $\hat{B}$, their contraction is defined as:

$$\langle AB\rangle \equiv \hat{A}\hat{B} - {:}\hat{A}\hat{B}{:} \tag{49}$$

Where $:\hat{O}:$ is the normal order which is defined with creation operators left of annihilation operators. The first simplification occur when considering Wick's theorem for VEVs for fermions: all terms involving normal orders vanish, leaving only full contractions:

$$\langle 0|ABCDEF\ldots|0\rangle = \sum_\sigma \operatorname{sgn}(\sigma) \prod_{\text{all pairs}} \text{contraction pair}$$

For our strings in C^x, C^y, C^z described in A and B operators, only $\langle A_i B_j\rangle$, and $\langle B_i A_j\rangle$ are nonzero. $\langle A_i A_j\rangle = \delta_{ij}$ and $\langle B_i B_j\rangle = -\delta_{ij}$. Since $A's$ and $B's$ anti-commute, then $\langle B_i A_j\rangle = -\langle A_j B_i\rangle$. The correlation functions can be expressed as the following determinants:

$$G_{ij} \equiv \langle B_i A_j\rangle \,; \quad G_r \equiv G_{ii+r} = \langle B_i A_{i+r}\rangle = -\langle A_{i+r} B_i\rangle = G_{-r} \tag{50}$$

$$C^x_r = \begin{vmatrix} G_1 & G_2 & \ldots & G_r \\ G_0 & G_1 & \ldots & G_{r-1} \\ \ldots & \ldots & \ldots & \ldots \\ G_{2-r} & G_2 & \ldots & G_1 \end{vmatrix} \qquad C^y_r = \begin{vmatrix} G_{-1} & G_0 & \ldots & G_{r-2} \\ G_{-2} & G_{-1} & \ldots & G_{r-1} \\ \ldots & \ldots & \ldots & \ldots \\ G_{-r} & G_{1-r} & \ldots & G_{-1} \end{vmatrix} \qquad C^z_r = \begin{vmatrix} G_0 & G_r \\ G_{-r} & G_0 \end{vmatrix} \tag{51}$$

$$\text{With transverse field: } C^z_r \equiv C^z_r - (m^z)^2\,; \quad m^z = \langle B_i A_i\rangle = G_0 \implies C^z_r = -G_r G_{-r} = -G_r^2 \tag{52}$$

To evaluate these Green's functions, we need to evaluate the VEVs in terms of the diagonalized operators. Therefore we will apply Fourier transform (18), then Bogoliubov diagonalization by using the definition (26) for each model. After a short computation we find that in the continuum limit:

$$G_r = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \frac{u_q}{\omega_q} \cos qr - \frac{v_q}{\omega_q} \sin qr \tag{53}$$

For the transverse Ising model specifically, we may use the appropriate expressions for u_q, v_q and ω_q to find:

$$G_r = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\lambda \cos[q(r+1)] + \cos qr}{\sqrt{1 + \lambda^2 + 2\lambda \cos q}}\, dq \tag{54}$$

One can now evaluate the following values G_r for some special values of relative Ising coupling strength $\bar{\lambda}$:

$$G_r = \begin{cases} \frac{2}{\pi}\frac{(-1)^r}{2r+1} & \text{For } \bar{\lambda}=1 \\ \frac{1}{\Gamma(-r)\Gamma(r+2)} \equiv \delta_{r,-1} & \text{For } \bar{\lambda}=\infty \\ \frac{1}{\Gamma(1-r)\Gamma(r+1)} \equiv \delta_{r,0} & \text{For } \bar{\lambda}=0 \end{cases} \tag{55}$$

For the XY model employing similar steps we find:

$$G_r = \begin{cases} \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\cos q\cos qr - \gamma\sin q\sin qr}{\sqrt{1+(\gamma^2-1)\sin^2(q)}}\,dq & \text{For } r \textit{ odd} \\ 0 & \text{For } r \textit{ even} \end{cases} \tag{56}$$

One can now evaluate the following values G_r for some special values of anisotropy parameter γ:

$$G_r = \begin{cases} -\frac{1}{\pi}\frac{\sin\pi r}{r+1} \equiv \delta_{r,-1} & \text{For } \gamma=1 \\ \frac{2(-1)^{1/2(r+1)}}{\pi r} & \text{For } \gamma=0 \end{cases} \tag{57}$$

3.2 Kitaev Honeycomb Model

The Kitaev honeycomb model is defined on a 2D honeycomb lattice by the Hamiltonian introduced in (10). The honeycomb lattice is defined by two triangular Bravais lattices, and consequently, we have two sub-lattices which we will denote by white (w) and black (b) as seen in Figure 3:

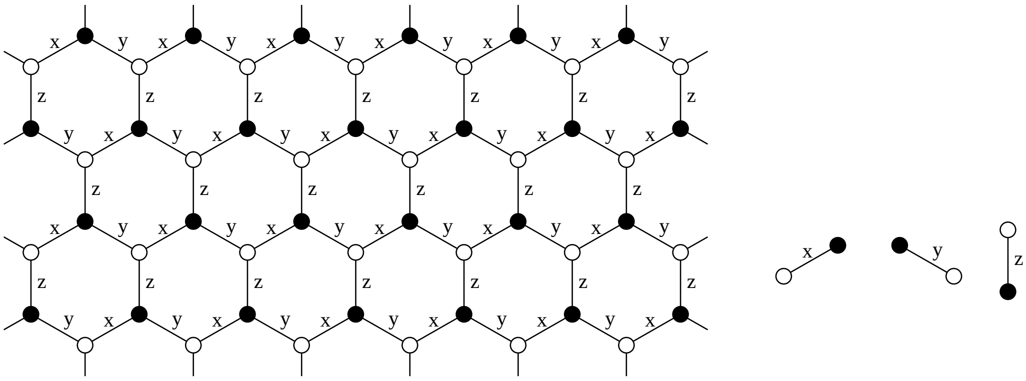

Figure 3: Kitaev's honeycomb lattice, with sub-lattices denoted by (w) & (b)

First, we will deform the honeycomb lattice into a topologically equivalent brick-wall lattice:

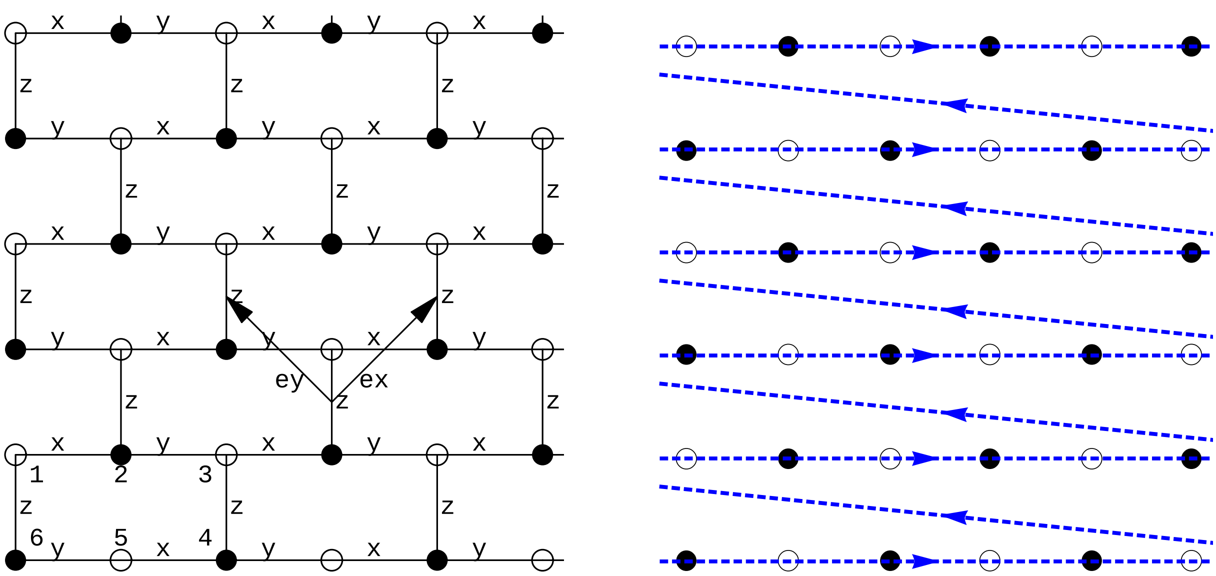

Figure 4: Honeycomb lattice after deformation, showing JW path

Then, it becomes more clear how to define a convenient path for a JW transformation. Using the JW transformation defined in (14) we will thread the brick-wall lattice in a zig-zag fashion, as illustrated in Figure 4. The result after employing the JW transformation is the following Hamiltonian:

$$H = J_x \sum_{x-links} \left(c - c^\dagger\right)_w \left(c^\dagger + c\right)_b - J_y \sum_{y-links} \left(c^\dagger + c\right)_b \left(c - c^\dagger\right)_w - J_z \sum_{z-links} \left(2c^\dagger c - 1\right)_b \left(2c^\dagger c - 1\right)_w \tag{58}$$

Where $w\&b$ denotes the two sub-lattices. Now, we introduce Majorana fermions at each site, which are defined by:

$$A_w \equiv \frac{\left(c - c^\dagger\right)_w}{i}; \quad B_w \equiv \left(c^\dagger + c\right)_w; \quad A_b \equiv \left(c^\dagger + c\right)_b; \quad B_b \equiv \frac{\left(c - c^\dagger\right)_b}{i} \tag{59}$$

The Hamiltonian then takes the form below:

$$H = -iJ_x \sum_{x-links} A_w A_b + iJ_y \sum_{y-links} A_b A_w + J_z \sum_{z-links} B_b B_w A_b A_w \tag{60}$$

We note that the term $B_b B_w A_b A_w$ is not quadratic, but luckily, there is a conserved quantity α_r. Replacing the conserved quantity given below will allow us to separate the Hamiltonian into quadratic sectors:

$$\alpha_r \equiv iB_b B_w \tag{61}$$

$$\therefore H = -iJ_x \sum_{x-links} A_w A_b + iJ_y \sum_{y-links} A_b A_w - iJ_z \sum_{z-links} \alpha_r A_b A_w \tag{62}$$

Where r is the midpoint coordinate of the z-bonds.
Since $B_{b/w}$ is hermitian, and $B_{b/w}^2 = 1$ (17), then $B_{b/w}$ will have eigenvalues of ± 1. Moreover, $B_{b/w}$ operators ***anti-commute*** with $A_{b/w}$ operators, and consequently, $\alpha_r/i = B_{b/w} B_{b/w}$ will ***commute*** with $A_{b/w}$ operators.

$$\{B_i, A_j\} = 0; \qquad [B_i B_j, A_k] = 0; \quad ijk \in \{b, w\} \tag{63}$$

It is now clear why we were able to identify α_r as conserved quantities in our Hamiltonian. We will replace them by their eigenvalue $+1$ which minimizes energy and therefore corresponds to the ground state configuration. Next, we introduce a new spinon excitation fermionic operator which lives on the middle of z-bonds, defined as:

$$d \equiv \frac{A_w + iA_b}{2}; \qquad d^\dagger \equiv \frac{A_w - iA_b}{2} \tag{64}$$

We can observe that

$$[\alpha_r, d_r] = \left[\alpha_r, d_r^\dagger\right] = 0 \tag{65}$$

Finally, the Hamiltonian now reads:

$$H = J_x \sum_r \left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_x}^\dagger + d_{r+\hat{e}_x}\right) + J_y \sum_r \left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_y}^\dagger + d_{r+\hat{e}_y}\right) + J_z \sum_r \left(2d_r^\dagger d_r - 1\right) \tag{66}$$

Where $\hat{e}_x\&\hat{e}_y$ are the basis vectors shown in Figure 4. Now we apply a Fourier transform in 2-D, which is slightly different than (18):

$$d_{\mathbf{r}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} d_{\mathbf{q}}^\dagger e^{i\mathbf{q}\cdot\mathbf{r}}; \quad d_{\mathbf{r}} \quad = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} d_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} \tag{67}$$

And (19) becomes:

$$\sum_{\mathbf{r}} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}} = N\delta_{\mathbf{q}\mathbf{q}'} \tag{68}$$

Using (67) and (68), and summing over positive modes, the Hamiltonian will read:

$$H = \sum_{q>0} \left[\epsilon_q (d_q^\dagger d_q - d_{-q} d_{-q}^\dagger) + i\Delta_q (d_q^\dagger d_{-q}^\dagger - d_{-q} d_q)\right] \tag{69}$$

$$= \sum_{q>0} \begin{bmatrix} d_q^\dagger & d_{-q} \end{bmatrix} \begin{bmatrix} \epsilon_q & i\Delta_q \\ -i\Delta_q & -\epsilon_q \end{bmatrix} \begin{bmatrix} d_q \\ d_{-q}^\dagger \end{bmatrix} \tag{70}$$

$$\epsilon_q = 2J_z - 2J_x \cos q_x - 2J_y \cos q_y; \quad \Delta_q = 2J_x \sin q_x + 2J_y \sin q_y; \quad q_i \equiv \mathbf{q} \cdot \hat{e_i}; \quad i \in \{x, y\} \tag{71}$$
$$\tag{72}$$

Here, we have used the short-hand notation.

$$\sum_q \Longrightarrow \sum_{q_x} \sum_{q_y}; \quad \sum_{q>0} \Longrightarrow \sum_{q_x>0} \sum_{q_y>0} \tag{73}$$

Which now has a similar form to (23), thus, we can diagonalize it using (24). The result is this following Hamiltonian in its eigenspace:

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + E_0 \tag{74}$$

$$E_0 = -\frac{1}{2} \sum_q \omega_q; \quad \omega_q = \sqrt{\epsilon_q^2 + \Delta_q^2} \tag{75}$$

4 Research Questions

Kitaev's honeycomb model only encompasses nearest neighbor interactions. However, what physical properties can one study by including the next nearest neighbor (NNN) interactions? For example, an extended Kitaev honeycomb model can be written as:

$$H = H_1 + H_2 \tag{76}$$

$$H_2 = -iK_2 \sum_{(\alpha\beta\gamma)} \sum_{\langle jkl \rangle_{\alpha\beta}} \epsilon_{(\alpha\beta\gamma)} \left(\sigma_j^\alpha \sigma_k^\alpha\right) \left(\sigma_k^\beta \sigma_l^\beta\right) = K_2 \sum_{(\alpha\beta\gamma)} \sum_{\langle jkl \rangle_{\alpha\beta}} \sigma_j^\alpha \sigma_k^\gamma \sigma_l^\beta \tag{77}$$

Here, H_1 is the original Kitaev honeycomb model, H_2 includes the NNN interactions, K_2 is the NNN Kitaev coupling, $\epsilon_{(\alpha\beta\gamma)}$ is Levi-Civita symbol, and $(\alpha\beta\gamma)$ is a general permutation of (xyz). We define $\langle jkl \rangle_{\alpha\beta}$ to be the path consisting of the two bonds $\langle jk \rangle_\alpha$ and $\langle kl \rangle_\beta$. Illustrated in Figure 5:

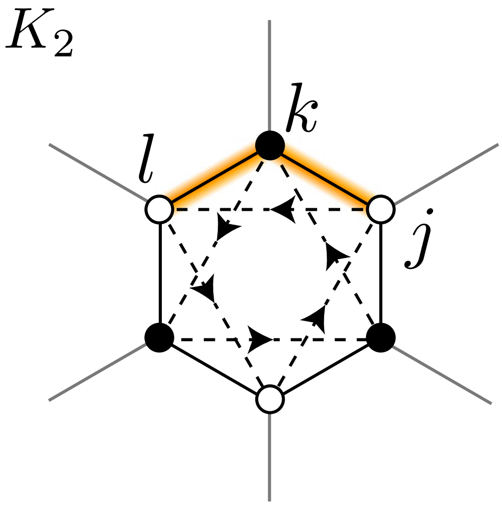

Figure 5: Representative of the path $\langle jkl \rangle_{yx}$ associated with the K_2 in (77)

- How does this impact thermal conductivity?
- Can we find Kitaev spin liquid candidate materials?
- How does the magnetic field dependence on thermal conductivity change by including these interactions?
- Will the model still be exactly solvable?

This research proposes a method to study a generalize Kitaev honeycomb model by extending it to encompass such interactions, and check how this affect the physical properties of the model.

5 Methodology

An extended Kitaev honeycomb model can be written as:

$$H = H_1 + H_2 + H_3 \tag{78}$$

Here, H_3 includes the next next nearest neighbor interactions.
The way to approach such a Hamiltonian, is to first study it up to H_2, checking the solvability of the model. Then attempt to include H_3.

The research scheme is to first write the Hamiltonian in fermionic language using (11). Then to introduce Majorana fermions to check what conserved quantities are present in the system. Then, to use such quantities to attempt performing a Fourier transform defined in (67). Finally, if the results have similar form to Bogoliubov Hamiltonians, we employ (26).

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