Exactly Solvable Systems of Strongly Correlated Electrons in Jordan-Wigner Language

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Abstract

We present here techniques for solving certain strongly interacting spin-1/2 systems. Chiefly, we employ the Jordan-Wigner transformation. In particular, we consider the (spin-1/2) 1D transverse Ising model, XY model, and Kitaev honeycomb model. After obtaining the feminized Hamiltonians using the Jodran-Wigner transformation, a diagonalization is carried out using Fourier and Bogoliubov transformations. Furthermore, the spectrum of elementary excitations as well as the ground-state are examined. In addition, some correlation functions of the solved models are recovered. We also introduce the necessary mathematical background, namely Wick's theorem. Lastly, the research problem of strained or sheared Kitaev honeycomb is proposed.

Contents

1 Introduction

Systems of strongly correlated electrons often exhibit remarkable properties as well as wide array of fascinating phenomena, such as: high-temperature superconductivity, quantum hall effects, topologically protected edge currents, as well as a variety of other electric and magnetic phenomena. Currently, while the physics of certain strongly correlated electron systems is well understood, there is no general approach for solving or understanding this class of systems. In addition to the prospects of applications owing to the before-mentioned properties, possible realizations of Majoranas in strongly correlated systems have further bolstered interest in this field due to possible applications in quantum computing. Although, the strong electron correlations are responsible for such rich properties they also make such models difficult to study.

A model that is often considered the prototypical example of a strongly correlated system is given by the Hubbard Hamiltonian below:

$$H = -\sum_{\langle i,j\rangle,\sigma} t_{i,j}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma} + h.c.\right) + \sum_{i} U_i n^{\dagger}_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

where $n_{i,\sigma} = c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the number operator and $c_{i,\sigma}$, c and $c^{\dagger}$ denote fermionic creation and annihilation operators at site i or j for spin σ. Here, $t_{i,j}$ denotes the hoping integral between nearest neighbors $\langle i,j\rangle$. The hopping term corresponds to the kinetic energy, while the U_i term describes the same-site interactions.

2 Formalism

In this section, it is useful to introduce the formalism of spin Hamiltonians and Jodran-Wigner transformation to exactly solve the models considered in this report.

Spin Hamiltonians Spin Hamiltonian are often obtained for half-filled[1] hubbard models in the limit where U/t is large. Applying second-order degenerate perturbation theory to the Hubbard Hamiltonian, an effective spin-1/2 Hamiltonian can be derived, which contains linear and/or bilnear terms (i.e. at most quadratic - in spin operators - terms). Such an effective spin Hamiltonian describes the physics of the low-lying energy states.

However, often many-body spin-1/2 systems are difficult to study because spin operators are neither fermionic nor bosonic. More accurately, this is because spin-rasing and spin-lowering operators satisfy the fermionic anti-commutation relations when on the same site. However, on different sites they fulfil the bosonic commutations relations. That is, they fulfill the relations below

$$\{\sigma^{+}_{i}, \sigma^{-}_{j}\} = 1; \quad [\sigma^{+}_{i}, \sigma^{-}_{j}] = 0,\ i \neq j \tag{2}$$

For spin 1/2 one may use the Pauli spin matrix representation of spin-operators ($\sigma^{x}_{i}, \sigma^{y}_{i}, \sigma^{z}_{i}$ at site i). These fulfill the following relations

$$\sigma^{x}_{i} = \sigma^{+}_{i} + \sigma^{-}_{i}; \quad \sigma^{y}_{i} = -i(\sigma^{+}_{i} - \sigma^{-}_{i}); \quad \sigma^{z}_{i} = 2\sigma^{+}_{i}\sigma^{-}_{i} - 1 \tag{3}$$

$$\sigma^{+}_{i} = (\sigma^{x}_{i} + i\sigma^{y}_{i})/2; \quad \sigma^{-}_{i} = (\sigma^{x}_{i} - i\sigma^{y}_{i})/2 \tag{4}$$

It is important to note that spin-operator algebra here is represented by the Pauli matrices at site i.

[1] The reason for the restriction to half-filling is to have the perturbation Hamiltonian with only interactions terms $J \propto t^2/U$ with no kinetic terms, proportional to t.

Second Quantization In first quantization, the many-body wavefunction depends on a symmetrized permanent or determinant of all single particle wavefunctions. This can become cumbersome for describing systems with many particles, as the number of degrees of freedom grows rapidly with the number of particles. Moreover, it does not tell us anything about particle statistics. Second quantization provides a framework which enforces particles statistics through creation and annihilation operators. Rather than having a many-body wavefunction, we express a state in terms of creation and annihilation operators acting on a vacuum state $|0\rangle$. For fermions, $c_i^\dagger$ creates a particle at site i while c_i destroys a particle at site i. The operators satisfy the anticommutation relations:

$$\{c_i, c_j^\dagger\} = \delta_{i,j}; \quad \{c_i, c_j\} = 0; \quad \{c_i^\dagger, c_j^\dagger\} = 0 \tag{5}$$

with $c_i |0\rangle = 0$. The Pauli exclusion principle is also enforced ${c^\dagger}^2 = 0$.

Jordan-Wigner Transformation The Jordan-Wigner (JW) transformation maps spin-1/2 systems to non-interacting fermionic systems. It takes the following form in one dimension:

$$\sigma_i^- = \prod_{j=1}^{i-1}(-\sigma_j^z)c_i; \qquad \sigma_i^+ = c_i^\dagger \prod_{j=1}^{i-1}(-\sigma_j^z) \tag{6}$$

The JW transformation includes a string of Pauli matrices, denoted by $\hat{K}_i \equiv \prod_{j=1}^{j=i-1}(-\sigma_j^z)$. An important property in the JW language is the commutation of the string $\hat{K}_i$ with fermionic operators at sites $\geq i$ but anti-commutes with smaller-indexed sites due to (2).

In higher dimensions, such as the case in the 2-dimensional Kitaev honeycomb model, there is a freedom in the choice of path granted it covers all the lattice sites exactly once. Simplifications result when the chosen path leads to cancellations between the strings (of pauli matrices) in the JW transformed Hamiltonian.

3 1D Quantum Chains

Many condensed matter systems can be accurately modelled using 1-dimensional quantum chain models. There has been great success in analytically predicting or explaining experimental results using these models. Many features of quantum phase transitions, which could have potential applications in quantum computation, have been observed in spin chains [1].

In the following we show exact solutions to two simple quantum spin chain models: transverse Ising model [2]; XY model [3]. We will employ a Jordan-Wigner transformation. The chains are transitionally symmetric. Generally, the following transformation are applied the spin Hamiltonian: (1) Jordan-Wigner transformation to fermionize the Hamiltonian, (2) Fourier transformation to exploit the translational symmetry of the Hamiltonian, and lastly (3) Bogoliubov transformation is applied to diagonalize the Hamiltonian. In effect, the Fourier transformation amounts to applying a change of basis from the positional basis with a block tri-diagonal Hamiltonian to the momentum basis where the Hamiltonian could be represented as a block-diagonal Bogoliubov-type Hamiltonian - each block corresponds to a momentum k. The Bogoliubov transformation yields an exact solution in therms of the operators which diagonalize the Hamiltonian in momentum space. These solutions are interpreted as elementary excitation. Therefore, the ground state and elementary excitations are readily obtained after the Bogoluibov diagonalization. Finally, some two-site correlation functions will be examined.

Transverse Ising Model The first model represents an Ising chain of N spin-1/2 particles in a row with only nearest neighbor exchange interaction J in the x-competent of the spin. The chain is subjected to an external magnetic field of strength Γ, which is applied in a transverse direction, say along the z-axis:

$$H = -\sum_i \left(\sigma_i^z + \bar{\lambda}\sigma_i^x\sigma_{i+1}^x\right); \qquad \bar{\lambda} \equiv J/\Gamma \tag{7}$$

At $\Gamma = 0$, J interaction orders the spin along the x direction, as Γ is increased, it destroys the ordered spin system.

XY Model This model is a nearest-neighbor interaction model where there is an anisotropy in the xy-plane:

$$H = \sum_i (1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y. \tag{8}$$

Here, γ is the so-called anisotropy parameter. It can be interpreted in that $\gamma = 0$ represents the isotropic case and $\gamma = \pm 1$ represents Ising case, which is fully anisotropic in x-y plane of spin space. In the anisotropic case ($|\gamma| \neq 1$), note that the spin components no longer commute with the Hamiltonian. Moreover, terms arIsing due to anisotropy oppose the ordering of spins.

3.1 Jordan-Wigner Transformation

When all quadratic (in spin operators) terms are between nearest-neighbors, then JW strings cancel neatly:

$$\sigma_i^+\sigma_{i+1}^+ = c_i^\dagger c_{i+1}^\dagger; \quad \sigma_i^+\sigma_{i+1}^- = c_i^\dagger c_{i+1}; \quad \sigma_i^-\sigma_{i+1}^+ = -c_i c_{i+1}^\dagger; \quad \sigma_i^-\sigma_{i+1}^- = -c_i c_{i+1} \tag{9}$$

Next, applying the JW transformation (6) to the spin Hamiltonians (7, 8) we find:

Transverse Ising Model

$$H = N - \sum_i [2\sigma_i^+\sigma_i^- - \bar{\lambda}(\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-)] \quad \xrightarrow{\text{JW}} \quad H = N - \sum_i [2c_i^\dagger c_i + \bar{\lambda}(c_i^\dagger c_{i+1}^\dagger + c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger - c_i c_{i+1})] \tag{10}$$

XY Model

$$H = 2\sum_i \left[(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) + \gamma(\sigma_i^+\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-)\right] \quad \xrightarrow{\text{JW}} \quad H = 2\sum_i \left[(c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger) + \gamma(c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1})\right] \tag{11}$$

3.2 Fourier Transformation

Next, we transform to momentum space to obtain a block-diagonal Hamiltonian.

$$c_i = \frac{1}{\sqrt{N}}\sum_q^N c_q e^{-iqR_i}; \qquad c_i^\dagger = \frac{1}{\sqrt{N}}\sum_q^N c_q^\dagger e^{iqR_i} \tag{12}$$

Again, the Fourier transformed Hamiltonians are nicely simplified owing to the quadratic terms being on the same site or between nearest neighbors, expressed in units of lattice spacing ($R_j = aj = j$):

$$\sum_i c_i^\dagger c_i = \sum_q c_q^\dagger c_q; \qquad \sum_i c_i^\dagger c_{i+1} = \sum_q e^{-iq}\, c_q^\dagger c_q; \qquad \sum_i c_i c_{i+1} = \sum_q e^{iq}\, c_q c_{-q} \tag{13}$$

We find that the Hamiltonians reduce to

$$H = N - \sum_i [2c_i^\dagger c_i + \bar{\lambda}(c_i^\dagger c_{i+1}^\dagger + c_i^\dagger c_{i+1} + h.c.)] \quad \xrightarrow{\text{Fourier}} \quad H = N - \sum_q \left[2(1+\bar{\lambda}\cos q)c_q^\dagger c_q + \bar{\lambda}(e^{-iq}c_q^\dagger c_{-q}^\dagger - e^{iq}c_q c_{-q})\right]$$

(Trnv. Ising)

$$H = 2\sum_i \left[(c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger) + \gamma(c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1})\right] \quad \xrightarrow{\text{Fourier}} \quad H = \sum_q \left[4\cos q\, c_q^\dagger c_q + 2\gamma(e^{-iq}\, c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q})\right]$$

(XY Model)

3.3 Bogoliubov Diagonalization

To diagonalize the Hamiltonian, a Bogoliubov transformation is carried out where the fermionic operators diagonalizing the Hamiltonian are a linear combination of the old fermionic operators. For fermionic Bogoluibov-type Hamiltonians, this is done using a unitary transformation, $U^\dagger U = 1$:

$$\vec{c}^\dagger H\vec{c} = (\vec{c^\dagger}U^\dagger)(UHU^\dagger)(U\vec{c}) = \vec{\eta}^\dagger D\vec{\eta}; \qquad \vec{c} \equiv \left(c_q,\ c_{-q}^\dagger\right)^T \tag{14}$$

Note that below, the Bogoliubov Hamiltonian is expressed over positive modes for convenience.

Transverse Ising Model

$$H = -2\sum_{q>0}\left[(1+\bar{\lambda}\cos q)(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + i\bar{\lambda}\sin q\,(c_q^\dagger c_{-q}^\dagger - c_{-q}c_q)\right]; \qquad H_q = \begin{pmatrix} 1+\bar{\lambda}\cos q & -i\bar{\lambda}\sin q \\ i\bar{\lambda}\sin q & -(1+\bar{\lambda}\cos q)\end{pmatrix} \tag{15}$$

$$\xrightarrow{\text{Bogoliubov}} \quad H = 2\sum_q \omega_q \eta_q^\dagger \eta_q + E_0; \qquad E_0 = -\sum_q \omega_q \tag{16}$$

$$\eta_q = \underbrace{\left(\sqrt{\frac{1+\bar{\lambda}\cos q+\omega_q}{2\omega_q}}\right)}_{u_q} c_q + \underbrace{\left(\frac{i\bar{\lambda}\sin q}{\sqrt{2\omega_q(1+\bar{\lambda}\cos q+\omega_q)}}\right)}_{iv_q} c_{-q}^\dagger; \qquad \omega_q = \sqrt{1+2\bar{\lambda}\cos q+\bar{\lambda}^2} \tag{17}$$

XY Model

$$H = 2\sum_{q>0}\left[\cos q\,(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + \gamma i\sin q\,(c_{-q}c_q - c_q^\dagger c_{-q}^\dagger)\right]; \qquad H_q = \begin{pmatrix} \cos q & -i\gamma\sin q \\ i\gamma\sin q & -\cos q\end{pmatrix} \tag{18}$$

$$\xrightarrow{\text{Bogoliubov}} \quad H = 2\sum_q \omega_q \eta_q^\dagger \eta_q + E_0; \qquad E_0 = -\sum_q \omega_q \tag{19}$$

$$\eta_q = \underbrace{\left(\sqrt{\frac{\cos q+\omega_q}{2\omega_q}}\right)}_{u_q} c_q + \underbrace{\left(\frac{i\gamma\sin q}{\sqrt{2\omega_q(\cos q+\omega_q)}}\right)}_{iv_q} c_{-q}^\dagger; \qquad \omega_q = \sqrt{1-(1-\gamma^2)\sin^2 q} \tag{20}$$

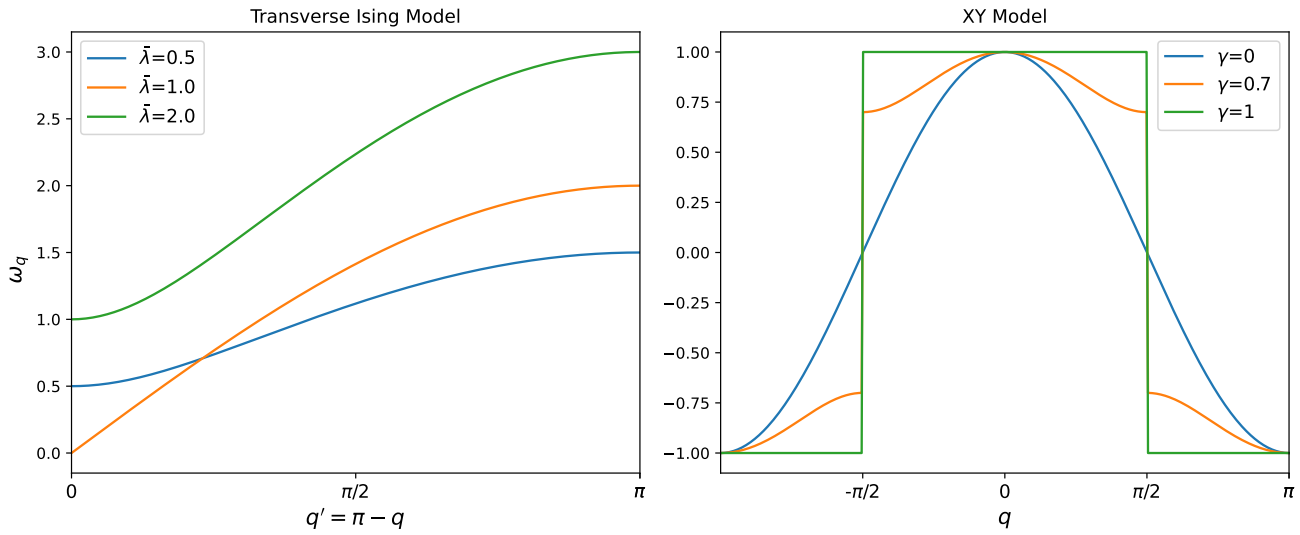

Figure 1: Elementary excitation energy for different parameter values

3.4 Ground State

For the ground state, the ground state energy can be evaluated the thermodynamic limit, $E_0/N = -\int_{-\pi}^{\pi} \frac{dq}{2\pi}\omega_q$:

$$E_0/N = -\frac{1}{\pi}\int_0^{\pi} \sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2}\, dq = -\frac{2}{\pi}(1+\bar{\lambda})\,\mathbf{E}\left(\sqrt{4\bar{\lambda}/(1+\bar{\lambda})^2}\right) \qquad \text{(Trnv. Ising Model)}$$

$$E_0/N = -\frac{1}{\pi}\int_0^{\pi/2} \sqrt{1 - (1-\gamma^2)\sin^2 q}\, dq = -\mathbf{E}\left(\sqrt{1-\gamma^2}\right)/\pi \qquad \text{(XY Model)}$$

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

3.5 Elementary Excitations

Transverse Ising Model The lowest excitation occurs at $q' = 0,\ 3.5$. With exception to the critical value of $\bar{\lambda} = 1$, the system is always gapped. The critical value for which the systems is gapless (no energy cost to excitations) to a highly disordered state.

XY Model The XY model is only gapless in the isotropic case $\gamma = 0$. Otherwise, it is gapped with the energy gap proportional to the anisotropy factor γ, with the maximum energy gap at $\gamma = \pm 1$.

Correction to Pfeuty [2] (Fig. 1) and Chakrabarti [1] (Fig. 2.2)

$\bar{\lambda} = 2$ is incorrectly denoted by $\bar{\lambda} = 1.5$ (figure 3.5 here).

$$\omega(q' = 0, \bar{\lambda} = 3/2) = \sqrt{1 + 2\,(3/2)\cos(\pi) + (3/2)^2} = \sqrt{1 - 3 + 9/4} = 1/2 \neq 1$$
$$\omega(q' = 0, \bar{\lambda} = 2) = \sqrt{1 + 2\,(2)\cos(\pi) + 2^2} = \sqrt{1 - 4 + 4} = 1 \qquad (q' = \pi - q = 0 \to q = \pi)$$

3.6 Correlation Functions

We end this section by illustrating a scheme that allows us to reduce the correlation functions to simpler expressions. Here, we utilize Majorana fermion operators and Wick's theorem. The spin-spin correlation functions given below are useful for examining the short- and long-range ordering of the system.

$$C_{ij}^x = \langle 0|\sigma_i^x\sigma_j^x|0\rangle\,; \quad C_{ij}^y = \langle 0|\sigma_i^y\sigma_j^y|0\rangle\,; \quad C_{ij}^z = \langle 0|\sigma_i^z\sigma_j^z|0\rangle - {m^z}^2 \qquad \text{(Trnv. Ising)}$$
$$C_{ij}^x = \langle 0|\sigma_i^x\sigma_j^x|0\rangle\,; \quad C_{ij}^y = \langle 0|\sigma_i^y\sigma_j^y|0\rangle\,; \quad C_{ij}^z = \langle 0|\sigma_i^z\sigma_j^z|0\rangle \qquad \text{(XY Model)}$$

where $m^z = \langle 0|\sigma_i^z|0\rangle$.

Majorana Fermions Let us start by defining the Majorana operators we will use:

$$A_i \equiv c_i^\dagger + c_i \qquad B_i \equiv c_i^\dagger - c_i$$

which satisfy the following commutation relations:

$$\{B_i, A_j\} = 0; \quad \{A_i, A_j\} = 2\delta_{ij}; \quad \{B_i, B_j\} = -2\delta_{ij} \tag{21}$$

The following expressions can then be shown to be true using the JW transformation:

$$\sigma_i^z = B_iA_i; \quad \hat{K}_i\hat{K}_j = \prod_{i\le k<j} A_kB_k \tag{22}$$

The correlation functions can then be rewritten in terms of Majorana operators using the preceding relations (22):

$$C_{ij}^x = \langle \Pi_{i\le k<j} B_kA_{k+1}\rangle\,; \quad C_{ij}^y = \langle \Pi_{i\le k<j} B_{k+1}A_k\rangle \tag{23}$$
$$C_{ij}^z = \langle 0|\sigma_i^z\sigma_j^z|0\rangle - {m^z}^2 = \langle B_iA_iB_jA_j\rangle - \langle B_iA_i\rangle^2 \qquad \text{(Trnv. Ising)}$$
$$C_{ij}^z = \langle B_iA_iB_jA_j\rangle \qquad \text{(XY Model)}$$

Wick's Theorem To further simplify our expressions we need to make use of Wick's theorem. It is often used to reduce the computation of expectation values to pairs of contractions[2] ($\hat{A}^\bullet\hat{B}^\bullet \equiv \hat{A}\hat{B} - :\hat{A}\hat{B}:$). In the case of Vacuum Expectation Values:

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

where $A, B, C,$ .etc are fermionic operators.

In our case, applying Wick's theorem to the VEVs of the Majorna strings in (23) yields full contraction terms that are products of the following elementary contractions: $\langle A_iA_j\rangle$, $\langle B_iB_j\rangle$, $\langle A_iB_j\rangle$, and $\langle B_iA_j\rangle$.

$$\langle A_iA_j\rangle = \delta_{ij}; \quad \langle B_iB_j\rangle = -\delta_{ij}; \quad \langle A_iB_j\rangle = -\langle B_iA_j\rangle \tag{24}$$

[2] A more general introduction of Wick's theorem is found in the Appendix

Since neither $\langle A_i A_i \rangle$ nor $\langle B_i B_i \rangle$ occur in C^x, C^y, C^z, full contractions can be written in terms a single contraction, $\langle B_i A_j \rangle$. To compute the VEV of $B_i A_j$, we apply the Fourier and Bogoliubov transformations Eqs. (12,16,19): The contraction function can then be written as

$$\langle B_i A_j \rangle = \delta_{ij} - \frac{2}{N} \sum_q \left(u_q v_q \sin qr - u_q^2 \cos qr \right). \tag{25}$$

We note that the other contractions $\langle A_i A_j \rangle$ and $\langle B_i B_j \rangle$ given above were obtained in a similar fashion.

Noting that this contraction only depends on qr where $r \equiv R_j - R_i$ (i.e. $B_i A_j = A_{i+1} B_{j+1}$), the correlation functions can be expressed as a determinant, with $G_r \equiv \langle B_i A_{i+r} \rangle$:

$$C_r^x = \begin{vmatrix} G_1 & G_2 & \dots & G_r \\ G_0 & G_1 & \dots & G_{r-1} \\ \dots & \dots & \dots & \dots \\ G_{2-r} & G_2 & \dots & G_1 \end{vmatrix} \qquad C_r^y = \begin{vmatrix} G_{-1} & G_0 & \dots & G_{r-2} \\ G_{-2} & G_{-1} & \dots & G_{r-1} \\ \dots & \dots & \dots & \dots \\ G_{-r} & G_{1-r} & \dots & G_{-1} \end{vmatrix} \tag{26}$$

$$C_r^z = -G_r G_{-r} \quad \text{(Trnv. Ising)} \qquad C_r^z = G_0^2 - G_r G_{-r} \quad \text{(XY Model)} \tag{27}$$

In the thermodynamic limit:

$$G_r = \delta_{0,r} - 2 \int_{-\pi}^{\pi} \frac{dq}{2\pi} \left(u_q v_q \sin qr - u_q^2 \cos qr \right)$$

Transverse Ising Chain For the case of a transverse field Ising chain we find

$$G_r = \frac{1}{\pi} \int_0^{\pi} \frac{\cos qr \ + \ \bar{\lambda} \cos[q(r+1)]}{\sqrt{1 + \bar{\lambda}^2 + 2\bar{\lambda} \cos q}} \, dq = I_r + \bar{\lambda} I_{r+1}; \qquad I_r = \frac{1}{\pi} \int_0^{\pi} \frac{\cos qr}{\omega_q} \, dq \tag{28}$$

Here, we may consider the three limiting cases of parameter $\tilde{\lambda}$ given below:

$$G_r(\bar{\lambda} = 1) = \frac{2}{\pi} \frac{(-1)^r}{2r+1} \tag{29}$$

$$G_r(\bar{\lambda} = 0) = \frac{1}{\pi} \int_0^{\pi} \cos qr \, dq = \delta_{0,r} \tag{30}$$

$$G_r(\bar{\lambda} \to \infty) = \frac{1}{\pi} \int_0^{\pi} \cos q(r+1) \, dq = \delta_{-1,r} \tag{31}$$

(30) implies through (26) no ordering at any range because the determinants have all zero elements. In contrasts to highly ordered case (31) for the latter where there is a non-zero valued diagonal.

XY Model For the XY model our expression for the Greens function G_r takes the form

$$G_r = \frac{1}{\pi} \int_0^{\pi} \frac{(1-\gamma)\cos[q(r+1)] + (1+\gamma)\cos[q(r-1)]}{\sqrt{1 - (1-\gamma^2)\sin^2 q}} \, dq = \begin{cases} (1-\gamma) I_{r+1} + (1+\gamma) I_{r-1}, \ r \text{ odd} \\ 0, \ r \text{ even} \end{cases}$$

with $I_r = \frac{2}{\pi} \int_0^{\pi/2} \cos(qr)/\omega_q \, dq$.

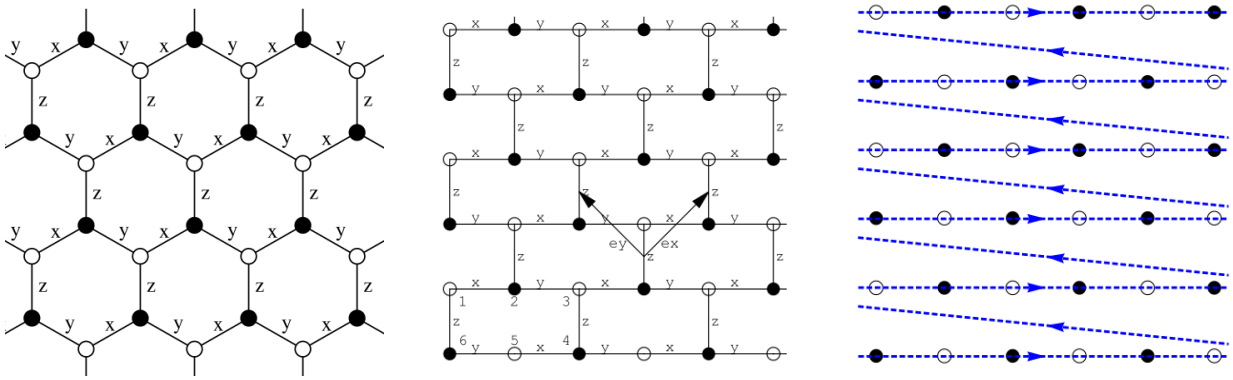

Figure 2: Links on Kitaev honeycomb [4, 5]

We consider two limiting cases below

$$G_r(\gamma = |1|) = -\frac{1}{\pi}\frac{\sin \pi r}{r+1} \equiv \delta_{r,-1} \tag{32}$$

$$G_r(\gamma = 0) = \frac{2(-1)^{1/2(r+1)}}{\pi r} \tag{33}$$

4 Kitaev Honeycomb Model

The Kitaev honeycomb model has been a subject of interest both due to exhibiting Topological Quantum Order (TQO) as well as anyons relevant to potential applications in quantum computing.

$$H = -\left(J_x \sum_{x\text{-bonds}} \sigma^x_R \sigma^x_{R'} + J_y \sum_{y\text{-bonds}} \sigma^y_R \sigma^y_{R'} + J_z \sum_{z\text{-bonds}} \sigma^z_R \sigma^z_{R'} \right) \tag{34}$$

The Kitaev model is a spin-1/2 system on a hexagonal lattice with three types of nearest neighbor interactions along each link direction. The Kitaev model is defined on a bipartite lattice composed of two triangular sublattices as seen in Fig.4. We have denoteed the black sublattice by b and we use the index w for the white sublattice.

A Jordan-Wigner transformation along a path which lead to string cancellation could be obtained by following a path which spans the lattice sites row-wise. A suggestive representation is to deform the lattice into a brick-wall lattice[5] as shown in Fig.4. One may then express spin operators in terms of fermions by the expression, which is given below:

$$\sigma^+_{ij} = 2\left[\prod_{j'<j}\prod_{i'} \sigma^z_{i'j'}\right]\left[\prod_{i'<i} \sigma^z_{i'j}\right] c^\dagger_{ij} \tag{35}$$

We may then fermionize (34) to obtain:

$$H = -\left(J_x \sum_{x\text{-bonds}} \left(c^\dagger - c\right)_w \left(c^\dagger + c\right)_b + J_y \sum_{y\text{-bonds}} \left(c^\dagger + c\right)_b \left(c^\dagger - c\right)_w + J_z \sum_{z\text{-bonds}} \left(2c^\dagger c - 1\right)_b \left(2c^\dagger c - 1\right)_w \right) \tag{36}$$

Introducing Majorana fermions as below:

$$A_w = i\left(c^\dagger - c\right)_w; \quad B_w = \left(c^\dagger + c\right)_w; \quad A_b = \left(c^\dagger + c\right)_b; \quad B_b = i\left(c^\dagger - c\right)_b, \tag{37}$$

we may then rewrite the Hamiltonian in terms of Majorana fermions.

$$H = -J_x \sum_{x\text{-bonds}} iA_wA_b + J_y \sum_{y\text{-bonds}} iA_bA_w + iJ_z \sum_{z\text{-bonds}} \underbrace{(iB_bB_w)}_{\lambda_r} A_bA_w \tag{38}$$

The quantity λ_r, where r point to te midpoint between black and white sites, is a conserved quantity since it commutes with the Hamiltonian (and each $A_{b/w}A_{w/b}$ term).

While the Hamiltonian cannot be directly diagonalized in the Majorana operators, it is possible to diagonalize it by introducing the following fermions (called spinons):

$$d_r = (A_w + iA_b)/2; \quad d_r^\dagger = (A_w - iA_b)/2, \tag{39}$$

where again, r is the midpoint along the z-axis between two adjacent black and white sites. In terms of spinons we may express the Hamiltonian as:

$$H = \sum_r \left[J_x\left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_x}^\dagger - d_{r+\hat{e}_x}\right) + J_y\left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_y}^\dagger - d_{r+\hat{e}_y}\right) + J_z\lambda_r\left(2d_r^\dagger d_r - 1\right)\right] \tag{40}$$

where the unit vectors $\hat{e}_x$ and $\hat{e}_y$ point to the centers of the x- and y-links as shown in Fig.4.

Next, a discrete Fourier transformation in 2D can be defined as:

$$d_R = \frac{1}{\sqrt{N}}\sum_q e^{-i(\mathbf{q}\cdot\mathbf{R})}d_q; \quad d_R^\dagger = \frac{1}{\sqrt{N}}\sum_q e^{i(\mathbf{q}\cdot\mathbf{R})}d_q^\dagger \tag{41}$$

Furthermore, for sufficiently large systems, the ground state can be found in the sector, where all $\lambda_r = 1$ [4, 5]. Therefore, the exact solution for the ground state is obtainable in a similar fashion to the 1D quantum chains using the Fourier transform followed by a Bogoluibov transformation. We find the results given below:

$$\xrightarrow{\text{Fourier}} \quad H_{gs} = \sum_q \left[\alpha_q d_q^\dagger d_q + i\beta_q\left(d_q^\dagger d_{-q}^\dagger - d_{-q}d_q\right)/2\right] \tag{42}$$

$$\xrightarrow{\text{Bogoluibov}} \omega_q = \sqrt{\alpha_q^2 + \beta_q^2}; \quad \alpha_q = 2J_z - 2J_x\cos q_x - 2J_y\cos q_y; \quad \beta_q = 2J_x\sin q_x + 2J_y\sin q_y \tag{43}$$

The gapless excitations at $E_q = 0$ in the ground state would impose the condition $\alpha_q = \beta_q = 0$. These condition can be solved in terms of the model parameters J_x, J_y, and J_z:

$$\begin{aligned} q_x &= \pm\arccos\left(\frac{J_x^2 + J_z^2 - J_y^2}{2J_xJ_z}\right) \\ q_y &= \pm\arccos\left(\frac{J_y^2 + J_z^2 - J_x^2}{2J_yJ_z}\right) \end{aligned} \quad \rightarrow \quad \begin{aligned} |J_x| &\le |J_y| + |J_z| \\ |J_y| &\le |J_z| + |J_x| \\ |J_z| &\le |J_x| + |J_y| \end{aligned} \tag{44}$$

The latter inequalities represent the conditions for gapless excitations in the ground state.

5 Research Proposal

Title: "Distorted Kitaev Honeycomb Model"

Background: Applying strain to a condensed matter system could manipulate its excitation spectrum through gauge fields or cause the system to transition between different phases. Deforming the lattice vectors could induce a pseudo magnetic field. This has been studied on graphene [6]. However, this has only been recently considered for spin Hamiltonians [7], which examined a kagome Heisenberg antiferromagnet.

Objectives:

- Formulate expressions for different lattice distortions that can be studied analytically.
- Attempt to exactly solve the model in JW language.
- Find the ground state for the distorted lattice.
- Is the quantity λ_r still conserved (commutes with the Hamiltonian)?
- Examine wether or not the strain gives rise to novel phases.
- Examine characteristics of the excitation spectrum
- Study the effect of the distortion on the order and disorder of the system (correlation functions).

References

[1] B. K. Chakrabarti, A. Dutta, and P. Sen, *Quantum Ising phases and transitions in transverse Ising models*, vol. 41. Springer Science & Business Media, 2008.

[2] P. Pfeuty, "The one-dimensional ising model with a transverse field," *ANNALS of Physics*, vol. 57, no. 1, pp. 79–90, 1970.

[3] E. Lieb, T. Schultz, and D. Mattis, "Two soluble models of an antiferromagnetic chain," *Annals of Physics*, vol. 16, no. 3, pp. 407–466, 1961.

[4] A. Kitaev, "Anyons in an exactly solved model and beyond," *Annals of Physics*, vol. 321, no. 1, pp. 2–111, 2006.

[5] H.-D. Chen and Z. Nussinov, "Exact results of the kitaev model on a hexagonal lattice: spin states, string and brane correlators, and anyonic excitations," *Journal of Physics A: Mathematical and Theoretical*, vol. 41, p. 075001, feb 2008.

[6] M. R. Masir, D. Moldovan, and F. Peeters, "Pseudo magnetic field in strained graphene: Revisited," *Solid State Communications*, vol. 175-176, pp. 76–82, dec 2013.

[7] M. M. Nayga and M. Vojta, "Strain tuning of highly frustrated magnets: Order and disorder in the distorted kagome heisenberg antiferromagnet," *Physical Review B*, vol. 105, mar 2022.