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Exactly Solvable Spin-1/2 Systems in Jordan-Wigner Language

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2nd Quantization

- Problems with Many-body wavefunctions:
  1. Can become very tedious (long)
  2. Do not account for particle statistics
  3. Could lead to ambiguity
- In the 2nd quantization, any state could be generating from vacuum $|0\rangle$ with the creation and anhhilation operators, $c_i^\dagger$ and c_i.
- For fermions, the operators satisfy the anticommutation relations:

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

with $c_i |0\rangle = 0$.

$$|100110\rangle \implies c_1^\dagger c_4^\dagger c_5^\dagger |0\rangle \tag{2}$$

Spin Hamiltonian

$$H_{\text{Hubbard}} = -\sum_{\langle i,j \rangle,\sigma} t_{i,j} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. \right) + \sum_{i} U_i n^{\dagger}_{i,\uparrow} n_{i,\downarrow} \tag{3}$$

1. Consider the half-filling case in the limit U/t
2. Applying second-order degenerate perturbation theory
3. $J \propto t^2/U$ terms $\implies$ effective spin-1/2 Hamiltonian

Jordan-Wigner Transformation

Many-body spin-1/2 systems could be difficult to study because spin operators are neither fermionic nor bosonic:

$$\{S_i^+, S_j^-\} = 1; \quad [S_i^+, S_j^-] = 0,\ i \neq j \tag{4}$$

Jordan-Wigner (JW) transformation **maps spin-1/2 systems to non-interacting fermionic systems.**
In the one dimension case:

$$S_i^- = \prod_{j=1}^{i-1} (-S_j^z) c_i; \qquad S_i^+ = c_i^\dagger \prod_{j=1}^{i-1} (-S_j^z) \tag{5}$$

We could denote the string of Pauli matrices by $\hat{K}_i \equiv \prod_{j=1}^{j=i-1} (-S_j^z)$. In general we look for string cancellations.

Transverse Ising Model

The Hamiltonian

$$
\begin{aligned}
H &= -\sum_j \left(\Gamma S_j^x + J S_j^z S_{j+1}^z\right) && (6)\\
&= -\sum_j \left(S_j^x + \bar{\lambda} S_j^z S_{j+1}^z\right) && (7)\\
\bar{\lambda} &\equiv \frac{J}{\Gamma}
\end{aligned}
$$

where Γ present the strength of the magnetic field, J is the strength of the interaction, and $\bar{\lambda}$ is a dimensionless factor.

Rotation and $S^+\, S^-$ operators

$$S^x \to S^z\,,\ S^z \to -S^x$$

Applying the rotation to (6):

$$\tilde{H} = -\sum_j \left(S_j^z + \bar{\lambda} S_j^x S_{j+1}^x\right)$$

using the identities:

$$S_j^x = S_j^+ + S_j^-\,,\ S_j^z = 2S_j^+ S_j^- + 1$$

The Hamiltonian becomes:

$$\tilde{H} = -\sum_j \left(2S_j^+ S_j^- - 1\right) - \bar{\lambda} \sum_j \left(S_j^+ S_{j+1}^+ + S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ + S_j^- S_{j+1}^-\right) \tag{8}$$

Jordan-Wigner Transformation

The Hamiltonian in (8) can be rewritten in fermion operator c and $c^\dagger$ using Jordan Wigner transformation (JW):

$$S_j^+ = c_j^\dagger \, \Pi_k^{j-1} e^{\left(-i\pi S_k^+ S_k^-\right)} = c_j^\dagger \, \Pi_k^{j-1} \left(-S_k^z\right)$$
$$S_j^- = \Pi_k^{j-1} e^{\left(-i\pi S_k^+ S_k^-\right)} c_j = \Pi_k^{j-1} \left(-S_k^z\right) c_j$$

By the employment of JW transformation, the resultant Hamiltonian is

$$\tilde{H} = -\sum_j \left(2c_j^\dagger c_j - 1\right) - \bar{\lambda} \sum_j \left(c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger - c_j c_{j+1}\right) \tag{9}$$

Example for JW transformation

For the term $S_j^+ S_j^-$:

$$\begin{aligned} S_j^+ S_j^- &= \left[c_j^\dagger \Pi_k^{j-1} \left(-S_k^z\right)\right] \left[\Pi_k^{j-1} \left(-S_k^z\right) c_j\right] \\ &= c_j^\dagger \Pi_k^{j-1} \left(-S_k^z\right)^2 c_j \\ &= c_j^\dagger c_j \end{aligned}$$

For the term: $S_j^+ S_{j+1}^+$

$$\begin{aligned} S_j^+ S_{j+1}^+ &= \left[c_j^\dagger \Pi_k^{j-1} \left(-S_k^z\right)\right] \left[c_{j+1}^\dagger \, \Pi_k^j \left(-S_k^z\right)\right] \\ &= \left[c_j^\dagger \Pi_k^{j-1} \left[-(2c_k^\dagger c_k + 1]\right)\right] \left[c_{j+1}^\dagger \, \Pi_k^j \left[-(2c_k^\dagger c_k + 1)\right]\right] \end{aligned}$$

Continue JW for $S_j^+ S_{j+1}^+$

Using commutation relation: $\{c_i, c_j^\dagger\} = \delta_{ij}$

$$\begin{aligned}
S_j^+ S_{j+1}^+ &= c_j^\dagger c_{j+1}^\dagger \Pi_k^{j-1} \left[-(2c_k^\dagger c_k + 1]) \right] \left[\Pi_k^j \left[-(2c_k^\dagger c_k + 1) \right] \right] \\
&= c_j^\dagger c_{j+1}^\dagger \Pi_k^{j-1} \left[\left(2c_k^\dagger c_k + 1 \right)^2 \right] \left[-(2c_j^\dagger c_j + 1) \right] \\
&= c_j^\dagger c_{j+1}^\dagger \left[(-2c_j^\dagger c_j - 1) \right] \\
&= -2c_j^\dagger c_{j+1}^\dagger c_j^\dagger c_j - c_j^\dagger c_{j+1}^\dagger \\
&= +2c_j^\dagger (c_j^\dagger c_{j+1}^\dagger) c_j - c_j^\dagger c_{j+1}^\dagger \\
&= -c_j^\dagger c_{j+1}^\dagger
\end{aligned}$$

Fourier Transformation

Applying Fourier transform to the Hamiltonian makes it easier to diagonalize. It has the form:

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_q^N c_q^\dagger \, e^{-iqR_j} \tag{10}$$

$$c_j = \frac{1}{\sqrt{N}} \sum_q^N c_q \, e^{iqR_j} \tag{11}$$

$$q = \frac{m\pi}{N}, \, m \in \{-N, \dots, N\}_{odd}$$

$$R_j \equiv ja = j; \, a = 1$$

Continue Fourier transformation

Hence, Hamiltonian in (9) becomes:

$$\tilde{H} = -\sum_{j}\left[\left(\frac{2}{N}\sum_{q}^{N} c_q^\dagger c_q\, e^{(-iqj+iqj)}\right) - 1\right] - \bar{\lambda}\sum_{j}\frac{1}{N}\sum_{qq'}^{N}\Big[c_q^\dagger c_{q'}^\dagger\, e^{(-iqj-iq'(j+1))}$$
$$+\, c_q^\dagger c_{q'}\, e^{(-iqj+iq'(j+1))} - c_q c_{q'}^\dagger\, e^{(iqj-iq'(j+1))} - c_q c_{q'}\, e^{(+iqj+iq'(j+1))}\Big] \qquad (12)$$

Then using the identity $\sum_{j=1}^{N} e^{ij(q-q')} = N\delta_{q,q'}$, the Hamiltonian becomes:

$$\tilde{H} = N - \sum_{q}\left[2\left(1+\bar{\lambda}\cos q\right) c_q^\dagger c_q + \bar{\lambda}\left(c_q^\dagger c_{-q}^\dagger\, e^{-iq} - c_q c_{-q}\, e^{+iq}\right)\right] \qquad (13)$$

Summation over $q>0$ and $q<0$

This sum can be split into two different sums, one over $q>0$ and the other over $q<0$. Therefore:

$$
\begin{aligned}
\tilde{H} =& N - \sum_{q>0} \left\{ \left[2\left(1+\bar{\lambda}\cos q\right) c_q^\dagger c_q + \bar{\lambda}\left(c_q^\dagger c_{-q}^\dagger \, e^{-iq} - c_q c_{-q} \, e^{+iq} \right) \right] \right. \\
& + \sum_{q<0} \left\{ \left[2\left(1+\bar{\lambda}\cos q\right) c_q^\dagger c_q + \bar{\lambda}\left(c_q^\dagger c_{-q}^\dagger \, e^{-iq} - c_q c_{-q} \, e^{+iq} \right) \right] \right. \\
=& N - \sum_{q>0} \left\{ \left[2\left(1+\bar{\lambda}\cos q\right) c_q^\dagger c_q + \bar{\lambda}\left(c_q^\dagger c_{-q}^\dagger \, e^{-iq} - c_q c_{-q} \, e^{+iq} \right) \right] \right. \\
& \left. + \left[2(1+\bar{\lambda}\cos(-q)) c_{-q}^\dagger c_{-q} + \bar{\lambda}\left(c_{-q}^\dagger c_q^\dagger \, e^{iq} - c_{-q} c_q \, e^{-iq} \right) \right] \right\} \\
=& -2\sum_{q>0} \left[\left(1+\bar{\lambda}\cos q\right) \left(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger\right) - i\bar{\lambda}\sin q \left(c_q^\dagger c_{-q}^\dagger - c_q c_{-q} \right) \right]
\end{aligned}
\tag{14}
$$

Matrix form and Bogoliubov transformation

The previous Hamiltonian can be written in matrix form as follows:

$$\tilde{H} = -2\sum_q \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} \begin{pmatrix} 1+\bar{\lambda}\cos q & -i\bar{\lambda}\sin q \\ i\bar{\lambda}\sin q & -1-\bar{\lambda}\cos q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix}. \tag{15}$$

which can be diagonalized by Bogoliubov transformation. For a 2D matrix:

$$\tilde{H} = \begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} (D) \begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix} \tag{16}$$

$$\begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} \equiv \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} U \tag{17}$$

$$D \equiv \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} \tag{18}$$

$$\begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix} \equiv U^\dagger \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} \tag{19}$$

Here, U is 2×2 Hermitian matrix that can be constructed using the normalized eigenvector of matrix in the Hamiltonian. Explicitly in this case:

$$U = \frac{1}{\sqrt{2\omega_q(1 + \bar{\lambda}\cos(q) + \omega_q)}} \begin{pmatrix} 1 + \bar{\lambda}\cos(q) + \omega_q & -i\bar{\lambda}\sin(q) \\ i\bar{\lambda}\sin(q) & 1 + \bar{\lambda}\cos(q) + \omega_q \end{pmatrix} \tag{20}$$

where $\omega_q = \sqrt{1 + 2\bar{\lambda}\cos(q) + \bar{\lambda}^2}$ is the eigenvalue of the matrix in $\tilde{H}$ from (15). Eq. (15) becomes:

$$\tilde{H} = 2\sum_q \omega_q \left(\eta_q^\dagger \eta_q - \frac{1}{2}\right) \tag{21}$$

XY Model

The Hamiltonian

$$H = \sum_j \left[(1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y \right] . \tag{22}$$

When $\gamma \to \pm 1$ the model reduces to Ising model.

$$H = \sum_j \left[(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \gamma (S_j^x S_{j+1}^x - S_j^y S_{j+1}^y) \right] \tag{23}$$

Using identities:

$$S_j^x = S_j^+ + S_j^- \ , \ S_j^y = i(S_j^- - S_j^+) \tag{24}$$

H becomes:

$$H = 2 \sum_j \left[(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) + \gamma (S_j^+ S_{j+1}^+ + S_j^- S_{j+1}^-) \right] \tag{25}$$

The Hamiltonian

applying JW transform:

$$S_j^+ = c_j^\dagger \, \Pi_k^{j-1} e^{\left(-i\pi S_k^+ S_k^-\right)} = c_j^\dagger \, \Pi_k^{j-1} \left(-S_k^z\right)$$
$$S_j^- = \Pi_k^{j-1} e^{\left(-i\pi S_k^+ S_k^-\right)} c_j = \Pi_k^{j-1} \left(-S_k^z\right) c_j$$

$$H = 2 \sum_j \left[(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger) + \gamma (c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) \right] \quad (26)$$

Fourier Transformation

By applying a Fourier transform:

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_q^N c_q^\dagger \, e^{-iqR_j} \tag{27}$$

$$c_j = \frac{1}{\sqrt{N}} \sum_q^N c_q \, e^{iqR_j} \tag{28}$$

$$q = \frac{m\pi}{N}, \, m \in \{-N, \dots, N\}_{odd}$$

$$R_j \equiv ja = j; \, a = 1$$

$$H = 2 \sum_q \left[(2\cos(q) c_q^\dagger c_q + \gamma(e^{-iq} c_q^\dagger c_{-q}^\dagger - c_q c_{-q} e^{iq}) \right] \tag{29}$$

Summation over $q > 0$ and $q < 0$, and matrix form
Breaking the sum into $q > 0$ and $q < 0$ results in:

$$H = 4\sum_{q>0}\left[\cos(q)(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) - i\gamma\sin(q)(c_q^\dagger c_{-q}^\dagger - c_{-q}c_q)\right], \tag{30}$$

which can be written in matrix form:

$$H = 4\sum_q \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} \begin{pmatrix} \cos q & -i\gamma\sin q \\ i\gamma\sin q & -\cos q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} \tag{31}$$

Bogoliubov transformation and diagonalization

$$\tilde{H} = \begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} (D) \begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix}$$

$$\begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} \equiv \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} U$$

$$D \equiv \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix} \qquad \equiv U^\dagger \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix}$$

$$U = \frac{1}{\sqrt{2\omega_q[\cos(q) + \omega_q]}} \begin{pmatrix} \cos(q) + \omega_q & i\gamma \sin(q) \\ i\gamma \sin(q) & \cos(q) + \omega_q \end{pmatrix} \tag{32}$$

Bogoliubov transformation and diagonalization

Therefore we find the diagonalized Hamiltonian:

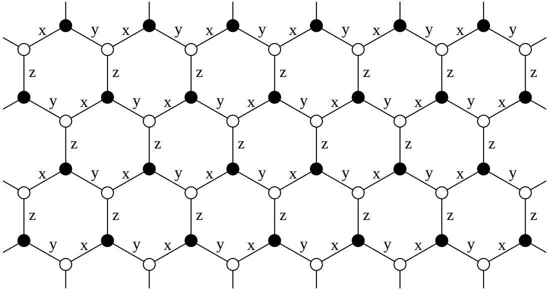
$$\omega_q = \sqrt{\cos^2(q) + \gamma^2 \sin^2(q)} \tag{33}$$

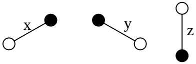
$$H = 4 \sum_q \omega_q \left(\eta_q^\dagger \eta_q - \frac{1}{2} \right) \tag{34}$$

Kitaev Honeycomb Model

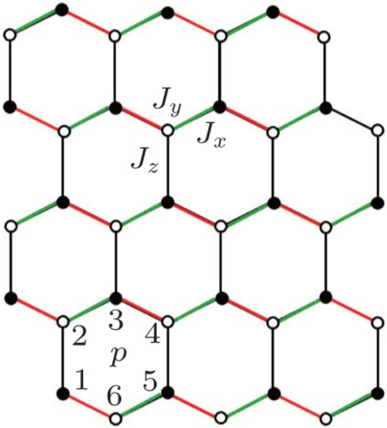
Kitaev's Honeycomb Hamiltonian

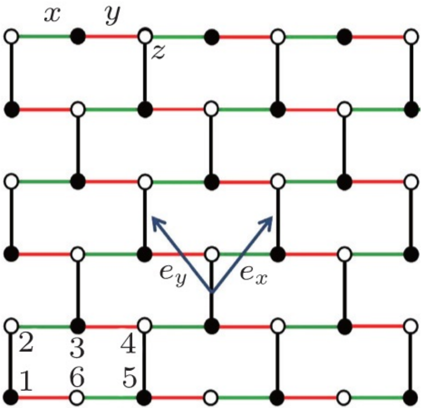
$$H = -J_x \sum_{x-links} \sigma_j^x \sigma_k^x - J_y \sum_{y-links} \sigma_j^y \sigma_k^y - J_z \sum_{z-links} \sigma_j^z \sigma_k^z$$



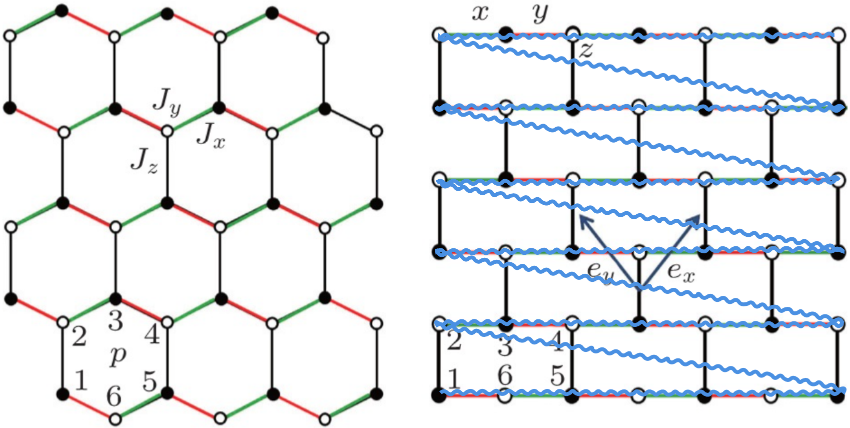


Deforming The Lattice





Threading The Lattice



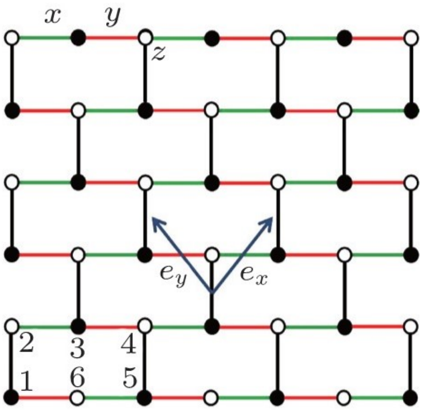
Jordan-Wigner Definition

$$\sigma^+_{ij} = 2\left[\prod_{j'<j}\prod_{i'}\sigma^z_{i'j'}\right]\underbrace{\left[\prod_{i'<i}\sigma^z_{i'j}\right]}_{1D\ String} c^\dagger_{ij}$$

$$\sigma^z_{ij} = 2c^\dagger_{ij}c_{ij} - 1$$

$$\sigma^x_{ij} = \frac{1}{2}\left(\sigma^+_{ij} + \sigma^-_{ij}\right)$$

$$\sigma^y_{ij} = \frac{i}{2}\left(\sigma^-_{ij} - \sigma^+_{ij}\right)$$



Example

We will now transform one part of the Hamiltonian as an example: Using:

$$\sigma^x_{ij} = \frac{1}{2}\left(\sigma^+_{ij} + \sigma^-_{ij}\right)$$

$$\sigma^x_{i,j}\sigma^x_{i+1,j} \implies \frac{1}{4}\left(\sigma^+_{i,j}\sigma^+_{i+1,j} + \sigma^+_{i,j}\sigma^-_{i+1,j} + \sigma^-_{i,j}\sigma^+_{i+1,j} + \sigma^-_{i,j}\sigma^-_{i+1,j}\right)$$

Employing JW transformation:

$$\implies c^\dagger_{i,j}c^\dagger_{i+1,j} + c^\dagger_{i,j}c_{i+1,j} - c_{i,j}c^\dagger_{i+1,j} - c_{i,j}c_{i+1,j}$$

$$\implies \left(c^\dagger_{i,j} - c_{i,j}\right)\left(c^\dagger_{i+1,j} + c_{i+1,j}\right)$$

After JW

$$\left(c^{\dagger}_{i,j} - c_{i,j}\right)\left(c^{\dagger}_{i+1,j} + c_{i+1,j}\right) \implies \left(c - c^{\dagger}\right)_w \left(c^{\dagger} + c\right)_b$$

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

Quartic terms $\implies c^{\dagger}_b c_b c^{\dagger}_w c_w$

Majorana Fermions

Majorana fermions obey these relations:

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

Defining new Majorana operators at each site:

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

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

The Hamiltonian reads:

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

Conserved Quantities

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

The term $B_b B_w A_b A_w$ is not quadratic, but luckily, there is a conserved quantity α_r:

$$\alpha_r \equiv i B_b B_w$$

Since $B_{b/w}$ is hermitian, and $B_{b/w}^2 = 1$, 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.

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

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

Conserved Quantities

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

Since $B_{b/w}$ is hermitian, and $B_{b/w}^2 = 1$, 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.

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

Spinon Operators

We will replace α_r quantities 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:

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

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

Fourier Transform

Now we apply a Fourier transform in 2-D, which is slightly different:

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

The identity becomes:

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

Summing over positive modes, the Hamiltonian will read:

$$\begin{aligned} H &= \sum_{q>0} \left[\epsilon_q (d_q^\dagger d_q - d_{-q} d_{-q}^\dagger) + i\Delta_q (d_q^\dagger d_{-q}^\dagger - d_{-q} d_q)\right] \\ &= \sum_{q>0} \begin{bmatrix} d_q^\dagger & d_{-q} \end{bmatrix} \begin{bmatrix} \epsilon_q & i\Delta_q \\ -i\Delta_q & -\epsilon_q \end{bmatrix} \begin{bmatrix} d_q \\ d_{-q}^\dagger \end{bmatrix} \end{aligned}$$

Bogoliubov Diagonalization

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

Here, we have used the short-hand notation.

$$\sum_q \implies \sum_{q_x} \sum_{q_y}; \quad \sum_{q>0} \implies \sum_{q_x>0} \sum_{q_y>0}$$

Bogoliubov Diagonalization

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

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

Then eigenvalues are given as:

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

The unitary matrix U is:

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

Fourier Transform

$$H = \sum_q \underbrace{\begin{bmatrix} d_q^\dagger & d_{-q} \end{bmatrix} U^\dagger}_{\begin{bmatrix} \eta_q^\dagger & \eta_{-q} \end{bmatrix}} \underbrace{UhU^\dagger}_{D} \underbrace{U \begin{bmatrix} d_q \\ d_{-q}^\dagger \end{bmatrix}}_{\begin{bmatrix} \eta_q & \eta_{-q}^\dagger \end{bmatrix}^T}$$

The result is this following Hamiltonian in its eigenspace:

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + E_0$$

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

Ground-State Energy and Elementary Excitations

Kitaev Model

The ground state ($E_q = 0$) imposes $\alpha_q = \beta_q = 0$:

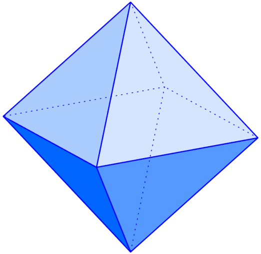
$$\omega_q = \sqrt{\alpha_q^2 + \beta_q^2}; \quad \alpha_q = 2J_z - 2J_x \cos q_x - 2J_y \cos q_y; \quad \beta_q = 2J_x \sin q_x + 2J_y \sin q_y \tag{35}$$

$$q_x = \pm \arccos\left(\frac{J_x^2 + J_z^2 - J_y^2}{2J_x J_z}\right); \qquad q_y = \pm \arccos\left(\frac{J_y^2 + J_z^2 - J_x^2}{2J_y J_z}\right) \tag{36}$$

Kitaev Model

Consequently, this implies the **conditions for gapless excitations in the ground state**:

$$
\begin{aligned}
|J_x| &\leq |J_y| + |J_z| \\
|J_y| &\leq |J_z| + |J_x| \\
|J_z| &\leq |J_x| + |J_y|
\end{aligned}
\tag{37}
$$



Ground States

Transverse

$$E_0 = -\sum_q \sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2} \tag{38}$$

XY Model

$$E_0 = -\sum_q \sqrt{1 - (1-\gamma^2)\sin^2 q} \tag{39}$$

Ground States

We evaluate the the thermodynamic limit, $N \to \infty$:

Transverse

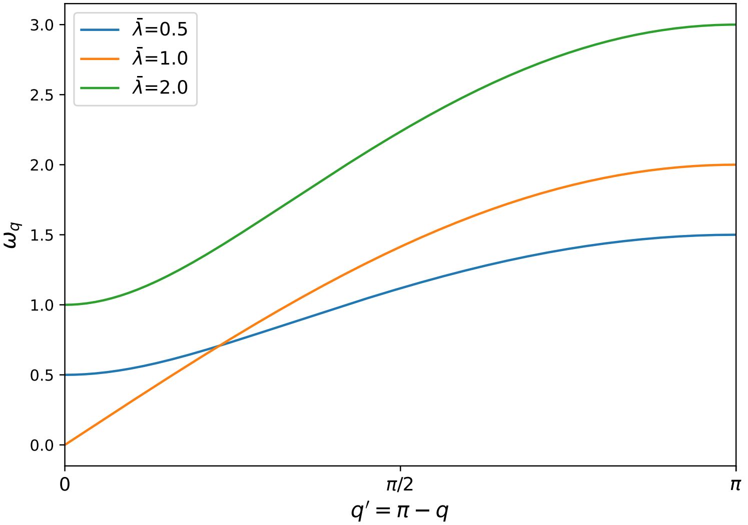
$$E_0/N = -\frac{1}{\pi}\int_0^{\pi} \sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2}\, dq = -\frac{2}{\pi}(1+\bar{\lambda})\,\mathbf{E}\left(\sqrt{4\bar{\lambda}/(1+\bar{\lambda})^2}\right) \tag{40}$$

XY Model

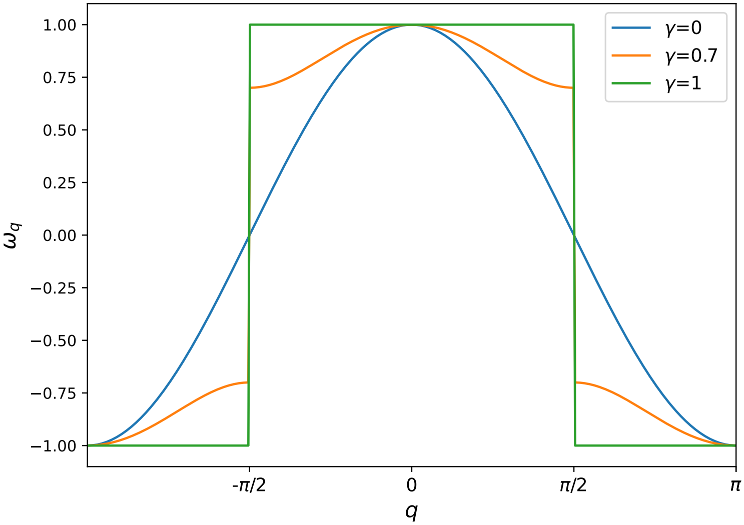
$$E_0/N = -\frac{1}{\pi}\int_0^{\pi/2} \sqrt{1 - (1-\gamma^2)\sin^2 q}\, dq = -\mathbf{E}\left(\sqrt{1-\gamma^2}\right)/\pi \tag{41}$$

where $\mathbf{E}(k)$ is the complete elliptic integral of the second kind.

Excitations: Transverse Ising Model



Excitations: XY Model



Correlation Functions for Transverse and XY Models

Correlation Functions

$$C_{ij}^{x} = \langle 0|S_i^x S_j^x|0\rangle \; ; \qquad C_{ij}^{y} = \langle 0|S_i^y S_j^y|0\rangle$$ (Both)

$$C_{ij}^{z} = \langle 0|S_i^z S_j^z|0\rangle$$ (XY)

$$C_{ij}^{z} = \langle 0|S_i^z S_j^z|0\rangle - \langle 0|S_i^z|0\rangle^2$$ (Tnsv.)

Majorana Fermions

Majorana Fermions

$$A_i \equiv c_i^\dagger + c_i; \qquad B_i \equiv c_i^\dagger - c_i \tag{42}$$

$$\{B_i, A_j\} = 0; \quad \{A_i, A_j\} = 2\delta_{ij}; \quad \{B_i, B_j\} = -2\delta_{ij} \tag{43}$$

Therefore:

$$S_i^x S_j^x = A_i \hat{K}_i \hat{K}_j A_j; \quad S_i^y S_j^y = B_i \hat{K}_i \hat{K}_j B_j \tag{44}$$

$$S_i^z = B_i A_i; \quad \hat{K}_i \hat{K}_j = \prod_{i \le k < j} A_k B_k \tag{45}$$

where $\hat{K}_i \equiv \prod_{k=1}^{i-1}(-S_k^z)$.

Majorana Fermions

Rewriting the correlation functions in terms of Majorana operators:

$$
\begin{aligned}
C_{ij}^{x} &= \langle 0|S_i^x S_j^x|0\rangle && (46)\\
&= \langle 0|(S_i^+ + S_i^-)(S_j^+ + S_j^-)|0\rangle && (47)\\
&= \langle 0|(c_i^\dagger + c_i)\hat{K}_i\hat{K}_j(c_j^\dagger + c_j)|0\rangle && (48)\\
&= \langle 0|A_i\Pi_{i\leq k<j}A_kB_kAj|0\rangle && (49)\\
C_{ij}^{x} &= \langle \Pi_{i\leq k<j}B_kA_{k+1}\rangle && (50)
\end{aligned}
$$

Majorana Fermions

Rewriting the correlation functions in terms of Majorana operators:

$$C_{ij}^{x} = \langle \Pi_{i\leq k<j} B_k A_{k+1} \rangle \quad (51)$$

$$C_{ij}^{y} = \langle \Pi_{i\leq k<j} B_{k+1} A_k \rangle \quad (52)$$

$$C_{ij}^{z} = \langle B_i A_i B_j A_j \rangle - \langle B_i A_i \rangle^2 \quad \text{(Trnv. Ising)}$$

$$C_{ij}^{z} = \langle B_i A_i B_j A_j \rangle \quad \text{(XY Model)}$$

Wick's Theorem

Wick's Theorem

For a string of fermionic operators:

$$
\begin{aligned}
\hat{A}\hat{B}\hat{C}\hat{D}\ldots = {} & :\hat{A}\hat{B}\hat{C}\hat{D}\ldots: \\
& + \sum_{\text{singles}} \operatorname{sgn}(\sigma) :\hat{A}^{\bullet}\hat{B}^{\bullet}\hat{C}\hat{D}\ldots: \\
& + \sum_{\text{doubles}} \operatorname{sgn}(\sigma) :\hat{A}^{\bullet}\hat{B}^{\bullet\bullet}\hat{C}^{\bullet\bullet}\hat{D}^{\bullet}\ldots: \\
& + \ldots + \sum_{\text{full contractions}} \hat{A}^{\bullet}\hat{B}^{\bullet}\hat{C}^{\bullet\bullet}\hat{D}^{\bullet\bullet}\ldots
\end{aligned}
$$

where $\hat{A}^{\bullet}\hat{B}^{\bullet} \equiv \hat{A}\hat{B} - :\hat{A}\hat{B}:$ and σ is the parity of the permutation.

Wick's Theorem

Wick's Theorem for VEVs

$$\langle 0|ABCDEF\ldots|0\rangle = \sum_{\sigma} \mathrm{sgn}(\sigma) \prod_{\text{all pairs}} \text{contraction pair} \tag{53}$$

Then, by Wick's theorem we could express correlation functions VEV with full contractions of four elementary contractions: $\langle A_i A_j \rangle$, $\langle B_i B_j \rangle$, $\langle A_i B_j \rangle$, and $\langle B_i A_j \rangle$.

$$C^x_{ij} = \langle \Pi_{i \le k < j} B_k A_{k+1} \rangle \tag{54}$$

$$C^y_{ij} = \langle \Pi_{i \le k < j} B_{k+1} A_k \rangle \tag{55}$$

$$C^z_{ij} = \langle B_i A_i B_j A_j \rangle - \langle B_i A_i \rangle^2 \tag{Trnv. Ising}$$

$$C^z_{ij} = \langle B_i A_i B_j A_j \rangle \tag{XY Model}$$

Wick's Theorem

- By commutation relations: $\langle B_i A_j \rangle = - \langle B_j A_i \rangle$
- Meanwhile we find $\langle A_i A_j \rangle = - \langle B_i B_j \rangle = \delta_{i,j}$.
- However, neither $\langle A_i A_i \rangle$ or $\langle B_i B_i \rangle$ occur in the correlation functions.
- Therefore, we could express the correlation functions entirely in $\langle B_i A_j \rangle$.

Evaluating $\langle B_i A_j \rangle$ in the Bogoliubov operators:

$$\boxed{\langle B_i A_j \rangle = \delta_{ij} - \frac{2}{N} \sum_q \left(u_q v_q \sin q(R_j - R_i) - u_q^2 \cos q(R_j - R_i) \right)} \tag{56}$$

Correlation Functions

Thus, with $G_r \equiv \langle B_i A_{i+r} \rangle$:

$$C_r^x = \begin{vmatrix} G_1 & G_2 & \dots & G_r \\ G_0 & G_1 & \dots & G_{r-1} \\ \dots & \dots & \dots & \dots \\ G_{2-r} & G_2 & \dots & G_1 \end{vmatrix}; \qquad C_r^y = \begin{vmatrix} G_{-1} & G_0 & \dots & G_{r-2} \\ G_{-2} & G_{-1} & \dots & G_{r-1} \\ \dots & \dots & \dots & \dots \\ G_{-r} & G_{1-r} & \dots & G_{-1} \end{vmatrix} \tag{57}$$

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

In the thermodynamic limit ($N \to \infty$):

$$\boxed{G_r = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \left(\frac{\alpha_q}{\omega_q} \cos qr - \frac{\beta_q}{\omega_q} \sin qr \right)} \tag{58}$$

where α_q and β_q are matrix elements of the Hamiltonian.

Correlation Functions

Transverse

$$G_r(\bar{\lambda}) = \frac{1}{\pi}\int_0^{\pi} \frac{\cos qr \ + \ \bar{\lambda}\cos[q(r+1)]}{\sqrt{1+\bar{\lambda}^2+2\bar{\lambda}\cos q}}\, dq \tag{59}$$

$$G_r(1) = \frac{2}{\pi}\frac{(-1)^r}{2r+1}; \qquad G_r(0) = \delta_{0,r}; \qquad \lim_{\bar{\lambda}\to\infty} G_r(\bar{\lambda}) = \delta_{-1,r} \tag{60}$$

XY Model

$$G_r(\gamma) = \frac{1}{\pi}\int_0^{\pi} \frac{(1-\gamma)\cos[q(r+1)] + (1+\gamma)\cos[q(r-1)]}{\sqrt{1-(1-\gamma^2)\sin^2 q}}\, dq \tag{61}$$

$$G_r(\pm 1) = -\delta_{-1,r}; \qquad G_r(0) = (-1)^{(r+1)/2}(2/\pi r) \qquad (r \text{ odd})$$

while $G_r = 0$ for r even.

Long-Range Order

From here, either a numerical approach or theorems for evaluating the determinant could be used.

XY Model

- No long-range order for the isotropic case.
- There is non-vanishing long-range order for some values of anisotropy parameter γ.

Transverse

- The model shows a finite long-range order in the ground state when the transverse field is less than a critical value $\bar{\lambda} < 1$.

Research Proposals

Extended Kitaev Honeycomb Model

An extended Kitaev honeycomb model can be written as:

$$H = H_1 + H_2$$

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

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).

Extended Kitaev Honeycomb Model

We define $\langle jkl \rangle_{\alpha\beta}$ to be the path consisting of the two bonds $\langle jk \rangle_\alpha$ and $\langle kl \rangle_\beta$

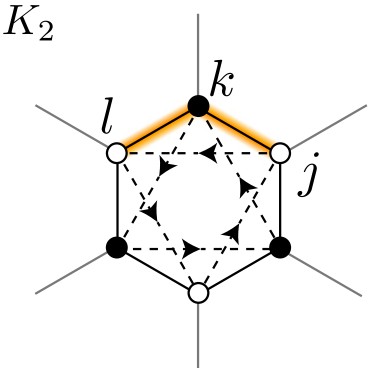


Figure: Representative of the path $\langle jkl \rangle_{yx}$ associated with the K_2 in H

Research Questions

- Will the model still be exactly solvable?
- 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?

The scheme is the following:

1. Write the Hamiltonian in fermionic language
2. Introduce Majorana fermions
3. Perform a 2D Fourier transform
4. Bogoliubov diagonalization

3D Kitaev Model

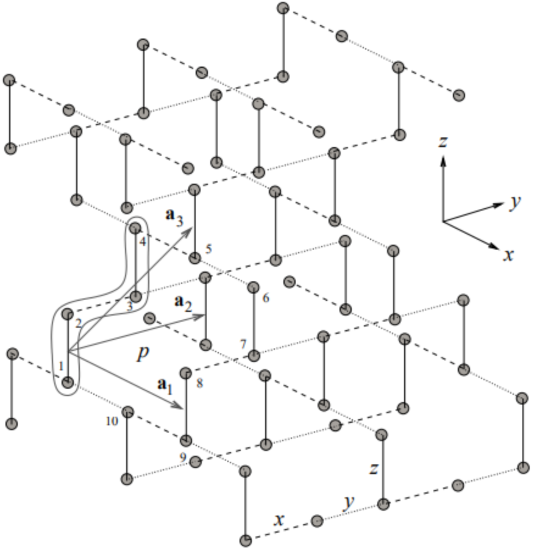
This model is expected to have applications in topological quantum computing. It has a gapped phase and a gapless one, same as for Kitaev honeycomb. Furthermore, the model has been proven to be exactly solvable. The Hamiltonian has the form:

$$H = -\left(J_x \sum_{<i,j>_x} \sigma_i^x \sigma_j^x + J_y \sum_{<i,j>_y} \sigma_i^y \sigma_j^y + J_z \sum_{<i,j>_z} \sigma_i^z \sigma_j^z \right) \tag{62}$$

The lattice can be constructed by deleting, from cubic lattice, sites , ijk in Cartesian coordinates , that satisfy the following relations:

1. k=0 mod 4 and i=0 mod 2.
2. k=1 mod 4 and j =0 mod 2.
3. k=2 mod 4 and i=1 mod 2.
4. k=3 mod 4 and j=1 mod 2.

3D Kitaev Lattice



Suggested way to solving the Hamiltonian

Given that a convenient path for JW transformation is found, I propose that this Model can be solved exactly using the following steps:

1. Expressing the Hamiltonian in σ^+, σ^-
2. Jordan Wigner transformation.
3. Introducing Majorana fermions.
4. Identify the conserved quantity/quantities.
5. Defining spinons.
6. Fourier transformation.
7. Breaking the sum over $\mathbf{q} > 0$
8. Matrix form.
9. diagonalization.

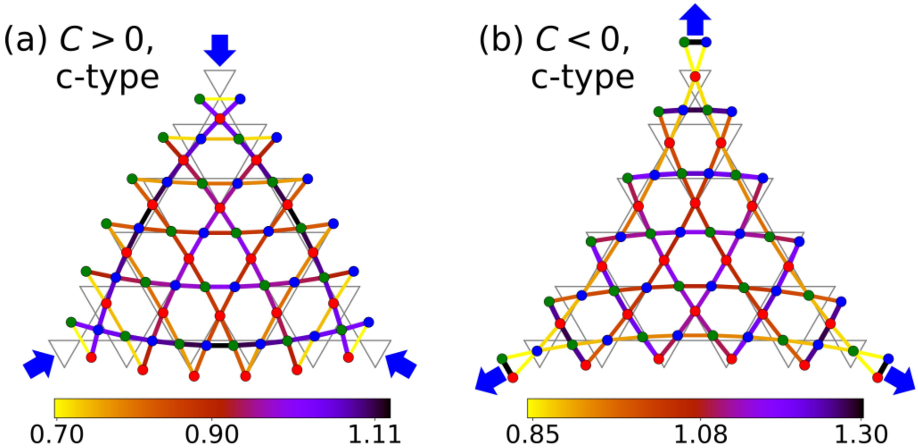
Distorted Kitaev Honeycomb Model

Background

- Applying strain to a condensed matter system could manipulate its excitation spectrum or cause phase transition.
- Deforming the lattice vectors could induce a pseudo magnetic field.

Objectives

1. Formulate expressions for different lattice distortions that can be studied.
2. Attempt to exactly solve the model in JW language.
3. Find the ground state for the distorted lattice.
4. Is the quantity α_r still conserved (commutes with the Hamiltonian)?
5. Examine wether or not the strain gives rise to novel phases.
6. Examine characteristics of the excitation spectrum



Distorted Kagome Heisenberg Antiferromagnet (Nayga & Vojta, 2022)

Thank you!

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