جامعة الملك فهد للبترول والمعادن
King Fahd University of Petroleum & Minerals

Intro. to JW Solution to Kitaev Honeycomb Model

A Summary of PHYS497 Progress

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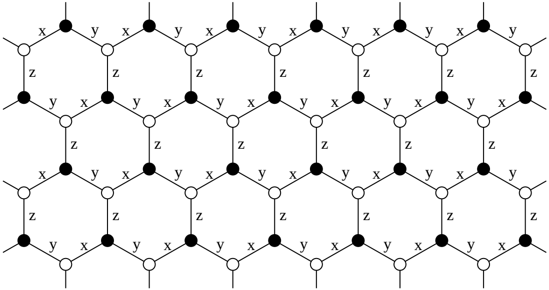
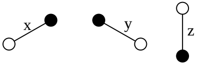
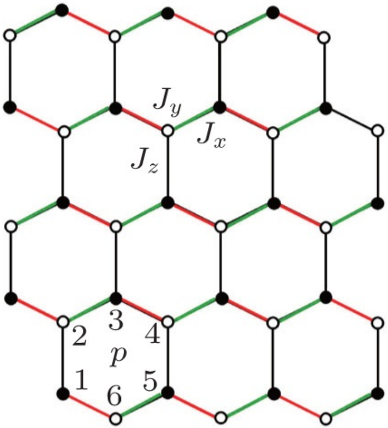
Kitaev's Honeycomb Hamiltonian

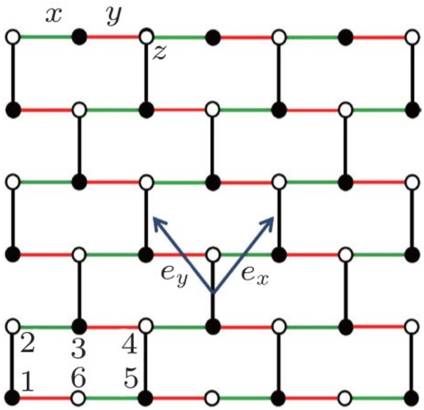
$$H = -J_x \sum_{x-links} \sigma_j^x \sigma_k^x - J_y \sum_{y-links} \sigma_j^y \sigma_k^y - J_z \sum_{z-links} \sigma_j^z \sigma_k^z$$



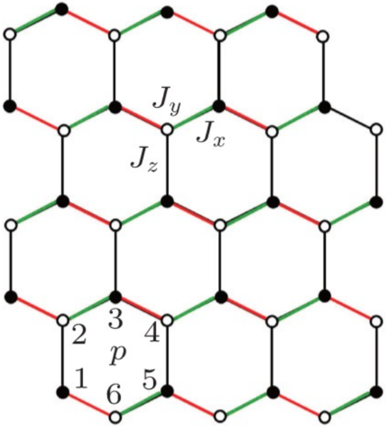


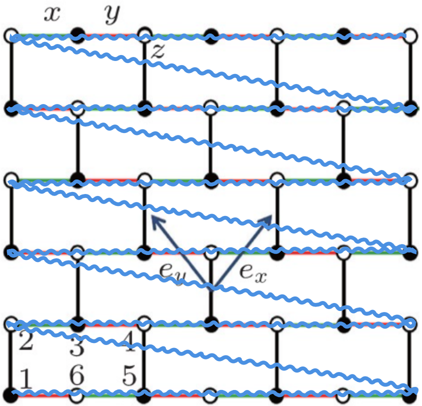
Deforming The Lattice





Threading The Lattice





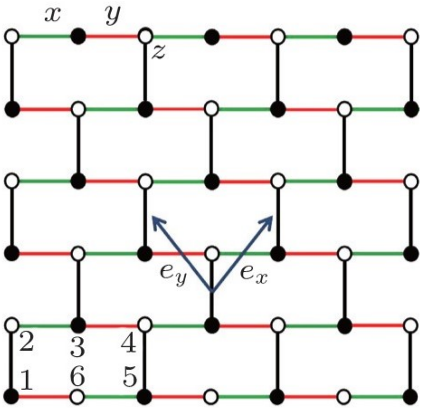
Jordan-Wigner Definition

$$\sigma_{ij}^{+} = 2\left[\prod_{j'<j}\prod_{i'}\sigma_{i'j'}^{z}\right]\underbrace{\left[\prod_{i'<i}\sigma_{i'j}^{z}\right]}_{1D\ String}c_{ij}^{\dagger}$$

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

$$\sigma_{ij}^{x} = \frac{1}{2}\left(\sigma_{ij}^{+} + \sigma_{ij}^{-}\right)$$

$$\sigma_{ij}^{y} = \frac{i}{2}\left(\sigma_{ij}^{-} - \sigma_{ij}^{+}\right)$$



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

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

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

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:

$$\alpha_r \equiv iB_b B_w$$

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.

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

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

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:

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

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

Fourier Transform

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

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

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:

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

Fourier Transform

Here, we have used the short-hand notation.

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

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

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:

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

Diagonalized Hamiltonian

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

The result is this following Hamiltonian in its eigenspace:

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

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

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 $\langle kl \rangle_\beta$

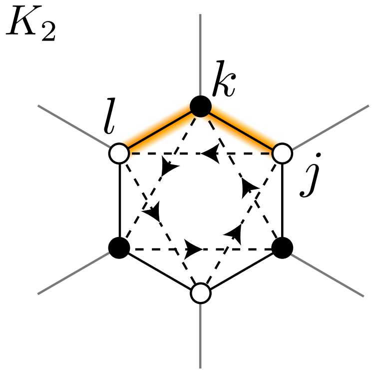


Figure: Representative of the path $\langle jkl \rangle_{yx}$ associated with the K_2 in H

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

Thank you!