REVIEW OF TIME-DEPENDENT MAJORANA MEAN FIELD THEORY

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Motivation

We are interested in the Kitaev-Heisenberg-Γ spin Hamiltonian which can be used to describe the material $\alpha-RuCl_3$ [1]:

$$\hat{H} = -\sum_{\langle i,j\rangle\alpha}\left[K\hat{S}_i^\alpha\hat{S}_j^\alpha + J\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j + \Gamma\sum_{\bar{\beta}\neq\beta\neq\alpha}\hat{S}_i^\beta\hat{S}_j^{\bar{\beta}}\right]. \tag{1}$$

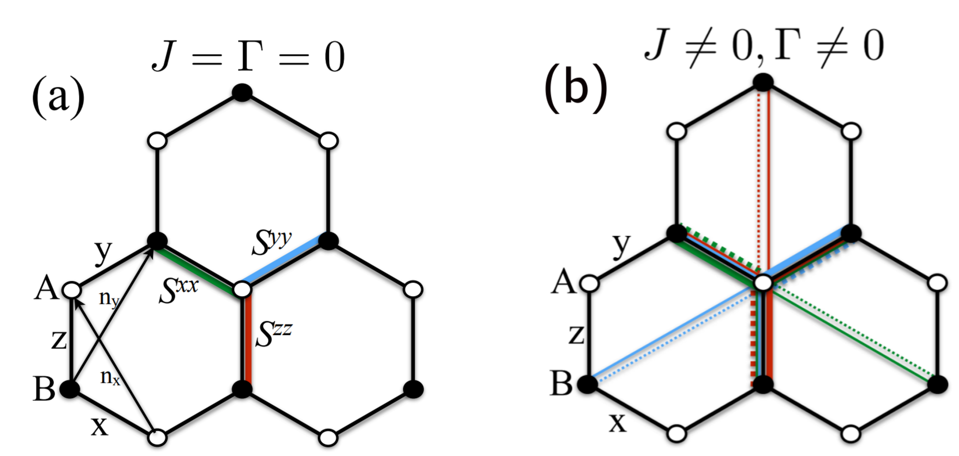


Fig. 1: (a) Kitaev Honeycomb lattice model (b) Kitaev-Heisenberg-Γ model [2]

In this model, it is convenient to rewrite the spins as combinations of Majorana fermions as can be seen from figure (2).

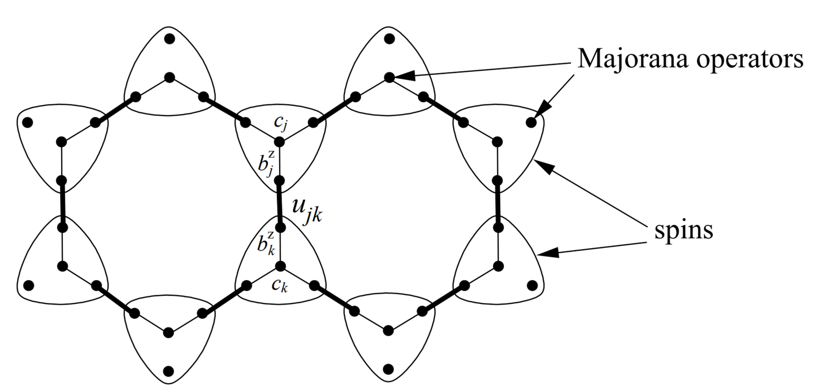


Fig. 2: Spin Hamiltonian on Honeycomb Lattice with Majorana fermions on each site [3]

Theory

We will formulate a way of diagonalizing a general quadratic Hamiltonian of the form:

$$\hat{H} = \frac{1}{4}\sum_{ij}M_{ij}\hat{c}_i\hat{c}_j \tag{2}$$

where $\hat{c}_i$ is a Majorana operator that can be rewritten as fermions and the matrix M can depend on time.

- ***Bogoliubov Transformation***

The linear homogeneous transformation used to diagonalize Hamiltonian (2) is:

$$\hat{\boldsymbol{\beta}} = \mathcal{T}\hat{\boldsymbol{\alpha}} \tag{3}$$

where $\hat{\boldsymbol{\alpha}}^T = \left(\hat{a}_1...\hat{a}_N\hat{a}_1^\dagger...\hat{a}_N^\dagger\right)$, $\hat{\boldsymbol{\beta}}^T = \left(\hat{b}_1...\hat{b}_N\hat{b}_1^\dagger...\hat{b}_N^\dagger\right)$, and $\mathcal{T} = \begin{pmatrix} X & Y \\ Y^* & X^*\end{pmatrix}$ when $\hat{b}_j^\dagger = (\hat{b}_i)^\dagger$ [4]. Additionally under the same condition, there exists an operator, $\hat{S}$, acting in the Fock space [4] such that:

$$\hat{b}_i = \hat{S}\hat{a}_i\hat{S}^\dagger,\quad \hat{b}_i^\dagger = \hat{S}\hat{a}_i^\dagger\hat{S}^\dagger\ . \tag{4}$$

Using equations (2-4) and $\hat{a}_i\left|v\right\rangle_a = 0$, we find the vacuum state [1] of the Bogoliubov-transformed quasi-particles to be written in the following form:

$$\left|v\right\rangle_b = \sqrt{\det X}\ e^{\frac{1}{2}\left(\sum_{ij}F_{ij}\hat{a}_i^\dagger\hat{a}_j^\dagger\right)}\left|v\right\rangle_a \tag{5}$$

where $F = -(X)^{-1}Y$.

- ***TDMFT***

We will start by re-scaling the Majorana fermions $\hat{c}_i \mapsto \sqrt{2}\hat{c}_i$ given in equation (2) so M can be diagonalized using a unitary matrix [1]:

$$\hat{H}(t) = \frac{1}{2}\sum_{ij}\hat{\tilde{c}}_i M_{ij}^{(t;\theta_{ij})}\hat{\tilde{c}}_j\ .$$

At time $t=0$, we can diagonalize the Hamiltonian using $\hat{\tilde{\boldsymbol{c}}} = U_0\hat{\tilde{\boldsymbol{a}}}$ as done in equation (3). The evolution of the vacuum state is performed as $\left|v\right\rangle_t = \hat{U}(t)\left|v\right\rangle$ where the evolution operator for the time-dependent Hamiltonian has the following form:

$$\hat{U}(t,t_0) = \exp\left\{-i\int_{t_0}^{t}dt'\hat{H}(t')\right\}\ .$$

Here the evolution operator can be approximated as a product of N step-evolution operators such that $\Delta t = \frac{t}{N} \implies t_n = n\Delta t$:

$$\hat{U}(t,t_0) \approx \prod_n e^{-i\hat{H}(t_n)\Delta t} \tag{6}$$

which can be visualized as shown in figure 3:

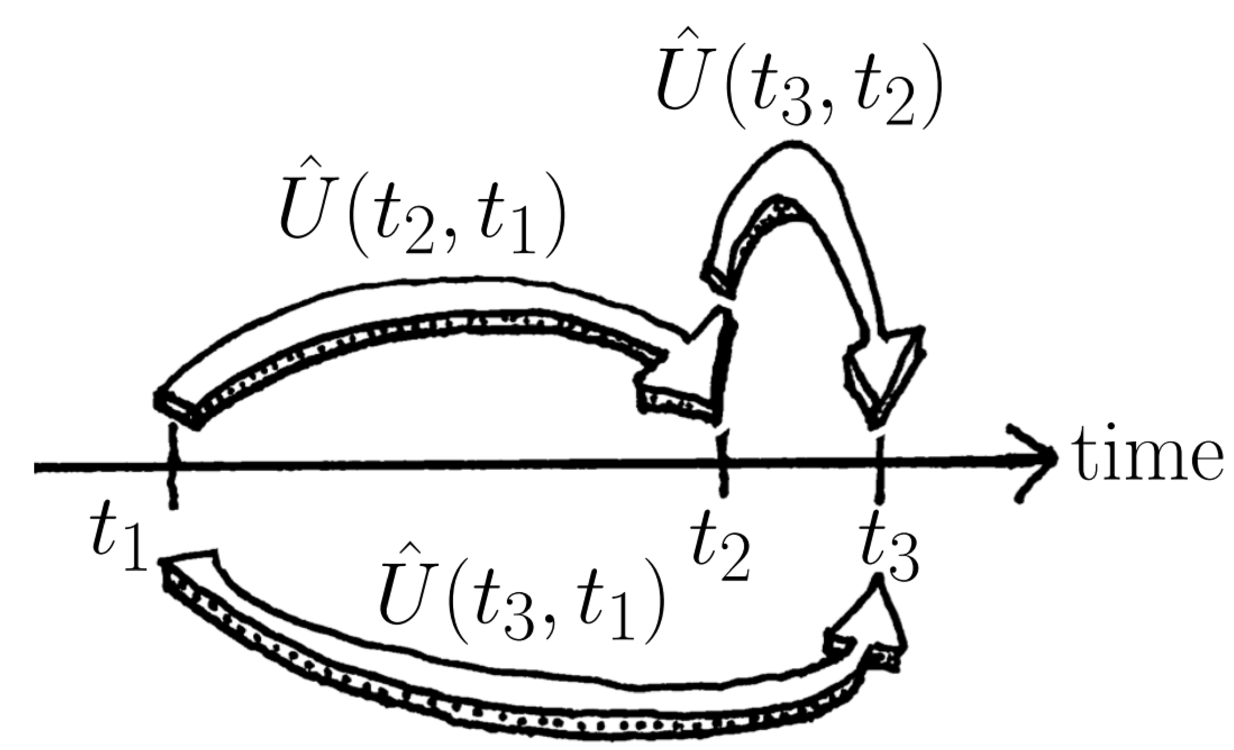


Fig. 3: Graphical Representation of the Composition Law of $\hat{U}(t_3,t_1)$ [5]

We define time-dependent operators $\hat{a}_i^{(t)}$ to always track the time-evolved state $\left|v\right\rangle_t$ such that $\hat{a}_i^{(t)}\left|v\right\rangle_t = 0$. Hence, the time-dependence of the elements of $\hat{\boldsymbol{a}}^{(t)}$ is written as:

$$\hat{\boldsymbol{a}}_i^{(t)} = \hat{U}(t,0)\ \hat{\boldsymbol{a}}_i\ (\hat{U}(t,0))^\dagger \ \Rightarrow\ \hat{\boldsymbol{a}}_i^{(t+\Delta t)} = e^{-i\hat{H}(t)\Delta t}\ \hat{\boldsymbol{a}}_i^{(t)}\ e^{i\hat{H}(t)\Delta t}\ .$$

From this result and equation (5) we find:

$$\left|v\right\rangle_{t+\Delta t} = \sqrt{\det X}\ e^{\frac{1}{2}\left(\sum_{ij}F_{ij}\hat{a}_i^\dagger\hat{a}_j^\dagger\right)}\left|v\right\rangle_t$$

and

$$\hat{\boldsymbol{a}}^{(t+\Delta t)} = \begin{pmatrix} X & Y \\ Y^* & X^*\end{pmatrix}\hat{\boldsymbol{a}}^{(t)}\ .$$

Applications

- ***Kitaev-Heisenberg-Γ Model***

Substituting the Majorana fermions, $\hat{S}_i^\alpha = \frac{1}{2}\hat{c}_i\hat{b}_i^\alpha$, for each spin as shown in figure 2, the Hamiltonian given in equation (1) takes the form:

$$\hat{H} = \sum_{\langle i,j\rangle\alpha}\left[\frac{K}{4}(i\hat{c}_i\hat{c}_j)(i\hat{b}_i^\alpha\hat{b}_j^\alpha) + \frac{J}{4}\sum_\beta(i\hat{c}_i\hat{c}_j)(i\hat{b}_i^\beta\hat{b}_j^\beta) + \frac{\Gamma}{4}\sum_{\bar{\beta}\neq\beta\neq\alpha}(i\hat{c}_i\hat{c}_j)(i\hat{b}_i^\beta\hat{b}_j^{\bar{\beta}})\right]. \tag{7}$$

Decoupling the Hamiltonian using the mean-fields $\langle i\hat{c}_i\hat{c}_j\rangle$ and $\left\langle i\hat{b}_i^\alpha\hat{b}_j^\beta\right\rangle$, we can get the approximate Hamiltonian:

$$\hat{H}_{MF} = \hat{H}_c + \hat{H}_b + C \tag{8}$$

where

$$\hat{H}_c = \sum_{\langle i,j\rangle\alpha}\left\{\frac{(K+J)}{4}\left\langle i\hat{b}_i^\alpha\hat{b}_j^\alpha\right\rangle + \frac{J}{4}\sum_{\beta\neq\alpha}\left\langle i\hat{b}_i^\beta\hat{b}_j^\beta\right\rangle + \frac{\Gamma}{4}\sum_{\bar{\beta}\neq\beta\neq\alpha}\left\langle i\hat{b}_i^\beta\hat{b}_j^{\bar{\beta}}\right\rangle\right\}i\hat{c}_i\hat{c}_j\ ,$$

$$\hat{H}_b = \sum_{\langle i,j\rangle\alpha}\langle i\hat{c}_i\hat{c}_j\rangle\left\{\frac{(K+J)}{4}(i\hat{b}_i^\alpha\hat{b}_j^\alpha) + \frac{J}{4}\sum_{\beta\neq\alpha}(i\hat{b}_i^\beta\hat{b}_j^\beta) + \frac{\Gamma}{4}\sum_{\bar{\beta}\neq\beta\neq\alpha}(i\hat{b}_i^\beta\hat{b}_j^{\bar{\beta}})\right\}\ ,$$
$$C = -\left\langle\hat{H}_c\right\rangle\ .$$

- ***Spin Correlator***

We now use the machinery developed earlier to find the analytical expression for the dynamical spin correlator in the ground state:

$$S_{ij}^{zz}(t) = \left\langle\hat{S}_i^z(t)\hat{S}_j^z\right\rangle = \left\langle\hat{U}(t)^\dagger\ \hat{S}_i^z\ \hat{U}(t)\ \hat{S}_j^z\right\rangle_0\ . \tag{9}$$

Letting E_{MF} be the ground state energy from the mean-field decoupled Hamiltonian and using the Majorana substitution and equation (8), we find

$$S_{ij}^{zz}(t) = \frac{1}{4}e^{(iE_{MF}\Delta t - i\psi_C(t))}\left\langle\hat{c}_i\ e^{-i\hat{H}_c(\mathcal{M}_t^c)}\ \hat{c}_j\ \hat{b}_i^z\ e^{-i\hat{H}_b(\mathcal{M}_t^b)}\ \hat{b}_j^z\right\rangle_0\ .$$

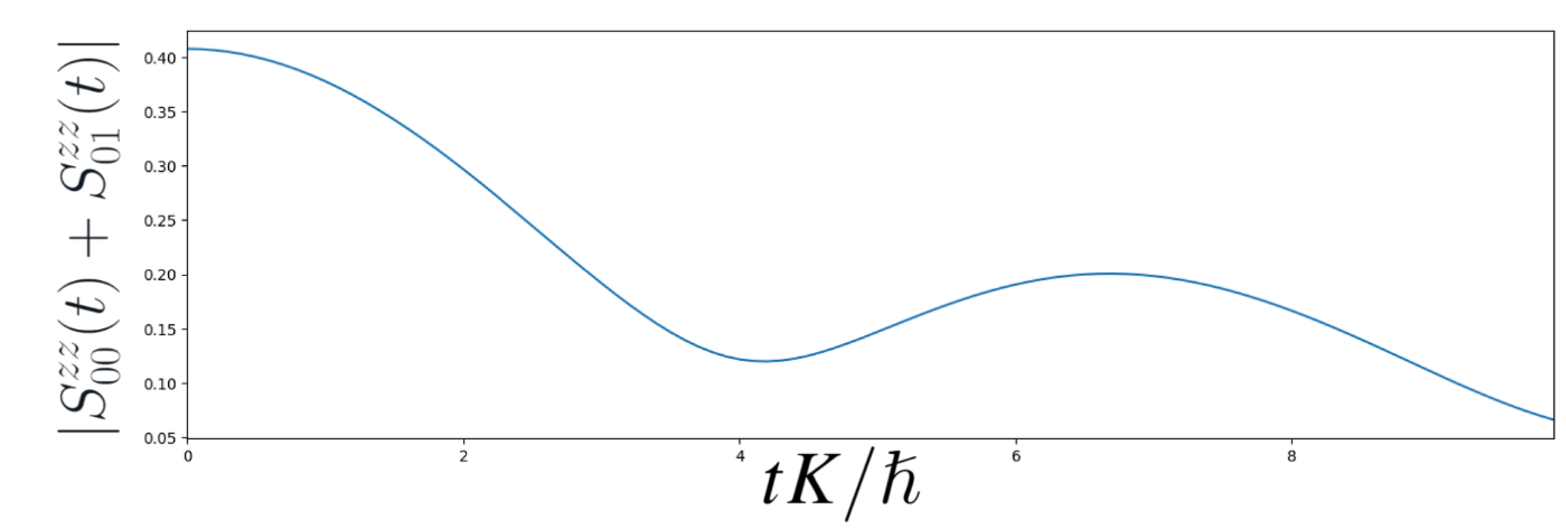
For the mean-field Hamiltonian, the ground state is a tensor product of c-type and b-type vacuum states, $\left|v\right\rangle = \left|v\right\rangle_c\otimes\left|v\right\rangle_b$:

$$S_{ij}^{zz}(t) = \frac{1}{4}e^{(iE_{MF}\Delta t - i\psi_C(t))}\underbrace{\left\langle\hat{c}_i\ e^{-i\hat{H}_c(\mathcal{M}_t^c)}\ \hat{c}_j\right\rangle_c}_{J_{ij}}\left\langle\hat{b}_i^z\ e^{-i\hat{H}_b(\mathcal{M}_t^b)}\ \hat{b}_j^z\right\rangle_b \tag{10}$$

with

$$J_{ij} = 2\sqrt{\det X}\sum_{kl}U_{0,ik}X_{kl}^{-1}U_{0,lj}^\dagger\ .$$

Considering a small perturbation $\frac{J}{K} = -0.04$ and $\frac{\Gamma}{K} = 0$, we plot the combination of dynamical spin correlators, $|S_{00}^{zz}(t) + S_{01}^{zz}(t)|$, for a cylinder of size $N_x = 16$ and $N_y = 4$ with open boundary condition along x and periodic boundary condition along y. Site 0 is connected with site 1 by a z bond and is far away from the open boundary.



This approach is also applicable to driven system [6].

References

[1] Tessa Cookmeyer and Joel E. Moore. "Dynamics of fractionalized mean-field theories: Consequences for Kitaev materials". In: *Phys. Rev. B* 107 (22 June 2023), p. 224428.

[2] Johannes Knolle, Subhro Bhattacharjee, and Roderich Moessner. "Dynamics of a quantum spin liquid beyond integrability: The Kitaev-Heisenberg-Γ model in an augmented parton mean-field theory". In: *Phys. Rev. B* 97 (13 Apr. 2018), p. 134432.

[3] Alexei Kitaev. "Anyons in an exactly solved model and beyond". In: *Annals of Physics* 321.1 (2006). January Special Issue, pp. 2–111. ISSN: 0003-4916.

[4] Jean-Paul. Blaizot and Georges. Ripka. *Quantum theory of finite systems / Jean-Paul Blaizot and Georges Ripka.* eng. Cambridge, Mass: MIT Press, 1986. ISBN: 0262022141.

[5] Tom Lancaster and Stephen J. Blundell. *Quantum Field Theory for the Gifted Amateur.* Oxford University Press, 2014. ISBN: 978-0-19-969933-9.

[6] Hui-Ke Jin, Johannes Knolle, and Michael Knap. "Fractionalized Prethermalization in a Driven Quantum Spin Liquid". In: *Phys. Rev. Lett.* 130 (22 June 2023), p. 226701.