Brief introduction to Kitaev's honeycomb model

Gábor B. Halász[1,2]

[1]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*
[2]*Quantum Science Center, Oak Ridge, TN 37831, USA*

In this tutorial, we will explore important concepts of topological quantum spin liquids, including fractionalized excitations and topological ground-state degeneracies, by investigating an exactly solvable spin model: the Kitaev model on the honeycomb lattice [1]. These notes provide some background on the Kitaev model. In the tutorial session, we will first briefly cover these notes and then move on to the associated Mathematica worksheet.

KITAEV MODEL ON THE HONEYCOMB LATTICE

The Kitaev model has a spin-1/2 degree of freedom at each site of the honeycomb lattice, with neighboring spins coupled by bond-dependent Ising interactions [1]. Specifically, if the honeycomb bonds are divided into three classes (x, y, z) depending on their orientation [see Fig. 1(a)], the Ising interaction along any α bond $\langle jk \rangle_\alpha$ (with $\alpha = x, y, z$) couples the two neighboring spins at sites j and k by their α components. The Hamiltonian of the Kitaev model thus reads

$$H_{\mathrm{Kitaev}} = -J_x \sum_{\langle jk \rangle_x} \sigma_j^x \sigma_k^x - J_y \sum_{\langle jk \rangle_y} \sigma_j^y \sigma_k^y - J_z \sum_{\langle jk \rangle_z} \sigma_j^z \sigma_k^z, \tag{1}$$

where σ_j^α is the α component of the spin-1/2 degree of freedom at site j. Note that the coupling strengths $J_{x,y,z}$ can in general be different on the three kinds of bonds. For completeness, we will also consider the extended version of the Kitaev model that includes three-spin interactions mimicking a magnetic field and breaking time-reversal symmetry [1]. In this extended model, each pair of neighboring bonds $\langle jk \rangle_\alpha$ and $\langle kl \rangle_\beta$ connecting through a site k has an associated three-spin interaction $\sigma_j^\alpha \sigma_k^\gamma \sigma_l^\beta$, where γ is the complement of α and β within the set $\{x, y, z\}$ such that, for example, $\gamma = z$ for $\alpha = x$ and $\beta = y$. Therefore, the Hamiltonian of the extended Kitaev model is given by

$$H_{\mathrm{extended}} = -J_x \sum_{\langle jk \rangle_x} \sigma_j^x \sigma_k^x - J_y \sum_{\langle jk \rangle_y} \sigma_j^y \sigma_k^y - J_z \sum_{\langle jk \rangle_z} \sigma_j^z \sigma_k^z - K \sum_{\langle jkl \rangle_{xy}} \sigma_j^x \sigma_k^z \sigma_l^y - K \sum_{\langle jkl \rangle_{yz}} \sigma_j^y \sigma_k^x \sigma_l^z - K \sum_{\langle jkl \rangle_{zx}} \sigma_j^z \sigma_k^y \sigma_l^x, \tag{2}$$

where $\langle jkl \rangle_{\alpha\beta}$ is the path of length two consisting of the two neighboring bonds $\langle jk \rangle_\alpha$ and $\langle kl \rangle_\beta$. Note that, for simplicity, we assume a single coupling strength K for all three-spin interactions.

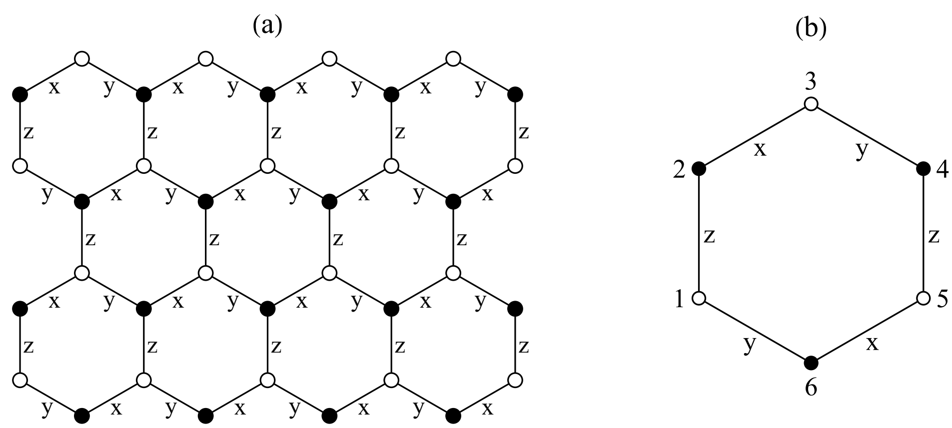

FIG. 1. (a) Honeycomb lattice with three classes of bonds (x, y, z) and two sublattices; sites in sublattices A and B are denoted by white and black dots, respectively. (b) Site numbering convention around a hexagonal plaquette.

MAJORANA FERMIONS AND GAUGE FLUXES

Remarkably, the extended Kitaev model in Eq. (2) has a reasonably simple exact solution [1]. In the first step, one introduces four Majorana fermions (b_j^x, b_j^y, b_j^z, c_j) at each site j of the honeycomb lattice, demands the local fermion-parity constraint

$$D_j \equiv b_j^x b_j^y b_j^z c_j = 1, \tag{3}$$

and writes each spin component σ_j^α as a product of two Majorana fermions:

$$\sigma_j^x = i b_j^x c_j, \qquad \sigma_j^y = i b_j^y c_j, \qquad \sigma_j^z = i b_j^z c_j. \tag{4}$$

These Majorana fermions are their own antiparticles,

$$\left(b_j^\alpha\right)^\dagger = b_j^\alpha, \qquad c_j^\dagger = c_j, \tag{5}$$

and satisfy canonical anticommutation relations:

$$\left\{b_j^\alpha, b_k^\beta\right\} = 2\delta_{jk}\delta_{\alpha\beta}, \qquad \left\{c_j, c_k\right\} = 2\delta_{jk}, \qquad \left\{b_j^\alpha, c_k\right\} = 0. \tag{6}$$

In other words, each Majorana fermion squares to 1, while distinct Majorana fermions anticommute. One can also show that the Majorana fermions provide a faithful representation of the spins as they preserve the canonical spin commutation relations:

$$\left[\sigma_j^x, \sigma_j^y\right] = \left(i b_j^x c_j\right)\left(i b_j^y c_j\right) - \left(i b_j^y c_j\right)\left(i b_j^x c_j\right) = 2 b_j^x b_j^y = \left(2 b_j^x b_j^y\right) D_j = \left(2 b_j^x b_j^y\right)\left(b_j^x b_j^y b_j^z c_j\right) = -2 b_j^z c_j = 2i\sigma_j^z, \tag{7}$$

as well as its cyclic permutations in x, y, z. In terms of the Majorana fermions, the bond-dependent Ising (i.e., Kitaev) interactions and three-spin interactions in Eq. (2) can be written as

$$\begin{aligned}
\sigma_j^x \sigma_k^x &= \left(i b_j^x c_j\right)\left(i b_k^x c_k\right) = -\left(i b_j^x b_k^x\right)\left(i c_j c_k\right), \\
\sigma_j^x \sigma_k^z \sigma_l^y &= \sigma_j^x \sigma_k^z D_k \sigma_l^y = \left(i b_j^x c_j\right)\left(i b_k^z c_k\right)\left(b_k^x b_k^y b_k^z c_k\right)\left(i b_l^y c_l\right) = -\left(i b_j^x c_j\right)\left(i b_k^x b_k^y\right)\left(i b_l^y c_l\right) = -\left(i b_j^x b_k^x\right)\left(i b_l^y b_k^y\right)\left(i c_j c_l\right).
\end{aligned} \tag{8}$$

Noting that each bond $\langle jk \rangle_\alpha$ connects two sites j and k in opposite sublattices A and B of the honeycomb lattice [see Fig. 1(a)], one can then define appropriate bond variables in a sublattice-consistent way,

$$u_{jk} = u_{kj} = \begin{cases} i b_j^\alpha b_k^\alpha & (j \in A, k \in B), \\ i b_k^\alpha b_j^\alpha & (j \in B, k \in A), \end{cases} \tag{9}$$

and express the Hamiltonian of the extended Kitaev model [i.e., Eq. (2)] in terms of these bond variables as

$$\begin{aligned}
H_{\text{extended}} = {} & J_x \sum_{\langle jk \rangle_x} i u_{jk} c_j c_k + J_y \sum_{\langle jk \rangle_y} i u_{jk} c_j c_k + J_z \sum_{\langle jk \rangle_z} i u_{jk} c_j c_k \\
& + K \sum_{\langle jkl \rangle_{xy}} i u_{jk} u_{kl} c_j c_l + K \sum_{\langle jkl \rangle_{yz}} i u_{jk} u_{kl} c_j c_l + K \sum_{\langle jkl \rangle_{zx}} i u_{jk} u_{kl} c_j c_l.
\end{aligned} \tag{10}$$

Here, it is implicitly assumed that $j \in A$ and $k \in B$ in the first three terms. Importantly, the bond variables u_{jk} commute with each other as well as the Hamiltonian in Eq. (10), which implies that they are compatible quantum numbers for the eigenstates of Eq. (10). Also, since u_{jk} are both hermitian and unitary, their only allowed eigenvalues are $u_{jk} = \pm 1$. At the same time, the bond variables are not compatible with the local fermion-parity constraints in Eq. (3) because any D_j and u_{jk} sharing a common site j anticommute with each other. Therefore, one can interpret the bond variables $u_{jk} = \pm 1$ as static $\mathbb{Z}_2$ gauge fields and the local fermion parities D_j as the corresponding $\mathbb{Z}_2$ gauge transformations. Since they are manifestly gauge dependent, the gauge fields themselves are not measurable quantities but merely provide a redundant description of measurable quantities (cf. vector potential in electromagnetism). In contrast, the products of the gauge fields around the hexagonal plaquettes p of the lattice, also known as gauge fluxes, are gauge invariant and hence measurable (cf. magnetic flux in electromagnetism). Indeed, following the site numbering convention in Fig. 1(b), the gauge flux at plaquette p can be explicitly written in terms of the physical spins as

$$\begin{aligned}
W_p &= u_{12} u_{23} u_{34} u_{45} u_{56} u_{61} = \left(i b_1^z b_2^z\right)\left(i b_3^x b_2^x\right)\left(i b_3^y b_4^y\right)\left(i b_5^z b_4^z\right)\left(i b_5^x b_6^x\right)\left(i b_1^y b_6^y\right) \\
&= \left(i b_1^y b_1^z\right)\left(i b_2^z b_2^x\right)\left(i b_3^x b_3^y\right)\left(i b_4^y b_4^z\right)\left(i b_5^z b_5^x\right)\left(i b_6^x b_6^y\right) = \sigma_1^x D_1 \sigma_2^y D_2 \sigma_3^z D_3 \sigma_4^x D_4 \sigma_5^y D_5 \sigma_6^z D_6 = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z.
\end{aligned} \tag{11}$$

Therefore, the $\mathbb{Z}_2$ gauge fields u_{jk} provide a redundant description of the $\mathbb{Z}_2$ gauge fluxes W_p. Specifically, if the lattice has m unit cells, thus supporting $3m$ gauge fields with 2^{3m} different configurations $u_{jk} = \pm 1$, there are only 2^m physically distinct gauge configurations that correspond to the different eigenvalues $W_p = \pm 1$ of the m gauge fluxes. Each flux sector $W_p = \pm 1$ can then be represented with one of 2^{2m} physically equivalent gauge configurations $u_{jk} = \pm 1$ that are related to each other by the 2^{2m} gauge transformations generated by the $2m$ local fermion parities D_j.

The Hamiltonian of the extended Kitaev model in Eq. (10) can be interpreted as a quadratic problem of Majorana fermions coupled to static $\mathbb{Z}_2$ gauge fields. Indeed, the first three (last three) terms are first-neighbor (second-neighbor) hopping terms for the Majorana fermions c_j that are modulated by the $\mathbb{Z}_2$ gauge fields u_{jk}. Therefore, the elementary excitations of the model are Majorana fermions and $\mathbb{Z}_2$ gauge fluxes. Note that, if the lattice has m unit cells, the $2m$ Majorana fermions c_j in Eq. (10) are equivalent to m complex fermions (see next section) and the original $2m$ spin degrees of freedom in Eq. (2) are thus correctly recovered in terms of m complex fermions and m gauge fluxes.

QUADRATIC MAJORANA PROBLEMS

In each flux sector $W_p = \pm 1$ represented with an appropriate gauge configuration $u_{jk} = \pm 1$, the Hamiltonian of the extended Kitaev model in Eq. (10) reduces to a quadratic Majorana problem, $H = \sum_{j,k} iM_{jk} c_j c_k$, where M is a $2m \times 2m$ real matrix (and m is the number of unit cells). To solve such a problem, it is first useful to rewrite it in a manifestly antisymmetric form as

$$H = \frac{1}{2} \sum_{j,k} iM_{jk} \left(c_j c_k - c_k c_j \right) = \sum_{j,k} S_{jk} c_j c_k, \qquad S_{jk} \equiv \frac{i}{2} \left(M_{jk} - M_{kj} \right). \tag{12}$$

Since S is a $2m \times 2m$ antisymmetric purely imaginary (hence, hermitian) matrix, its $2m$ eigenvalues are real and come in pairs $\pm\lambda$, while the corresponding eigenvectors $v_{\pm\lambda}$ are complex conjugates of each other. It is then natural to express each Majorana fermion c_j in terms of complex-fermion eigenmodes ψ_λ as

$$c_j = \sqrt{2} \sum_{\lambda} \left(v_\lambda \right)_j \psi_\lambda = \sqrt{2} \sum_{\lambda > 0} \left[\left(v_\lambda \right)_j \psi_\lambda + \left(v_{-\lambda} \right)_j \psi_{-\lambda} \right] = \sqrt{2} \sum_{\lambda > 0} \left[\left(v_\lambda \right)_j \psi_\lambda + \left(v_\lambda \right)_j^* \psi_{-\lambda} \right], \tag{13}$$

where the prefactor $\sqrt{2}$ is required to correctly preserve the canonical anticommutation relations. Since the Majorana fermion c_j is hermitian [see Eq. (5)], the fermion eigenmodes must satisfy $\psi_{-\lambda} = \psi_\lambda^\dagger$. Hence, there are only m physically independent complex fermions $\psi_{\lambda > 0}$, while the remaining m complex fermions $\psi_{\lambda < 0}$ are their antiparticles. Finally, by substituting Eq. (13) into Eq. (12), and using $\sum_j (v_\lambda)_j^* (v_\mu)_j = \delta_{\lambda\mu}$, the Hamiltonian of the extended Kitaev model becomes

$$H = \sum_{\lambda > 0} 2\lambda \left[\psi_\lambda^\dagger \psi_\lambda - \psi_\lambda \psi_\lambda^\dagger \right] = \sum_{\lambda > 0} 4\lambda \left[\psi_\lambda^\dagger \psi_\lambda - \frac{1}{2} \right]. \tag{14}$$

In other words, each fermion excitation $\psi_{\lambda > 0}$ with real-space wave function $(v_\lambda)_j$ has an excitation energy $\varepsilon_\lambda = 4\lambda$, while the ground-state energy of the Hamiltonian in Eq. (12) takes the form

$$E_{\mathrm{GS}} = - \sum_{\lambda > 0} 2\lambda = -\frac{1}{2} \sum_{\lambda > 0} \varepsilon_\lambda. \tag{15}$$

Importantly, the Hamiltonian in Eq. (12) and, hence, its ground-state energy in Eq. (15) depend on the flux sector of the extended Kitaev model. Any increases in E_{GS} as a result of creating gauge fluxes can be interpreted as flux excitation energies.

MOMENTUM-SPACE SOLUTION

It can be rigorously proven [2] that the ground-state energy in Eq. (15) is minimized in the absence of any non-trivial gauge fluxes, i.e., in the flux sector where $W_p = +1$ for all plaquettes p. In this ground-state flux sector, the Hamiltonian in Eq. (12) is translation invariant and thus allows for a simple solution in momentum space. Specifically, if one searches for the eigenvectors of the appropriate matrix S in the general form of

$$\left(v_{\mathbf{q}} \right)_j = \begin{cases} v_{\mathbf{q},A} \, e^{i\mathbf{q}\cdot\mathbf{R}_j} & (j \in A), \\ v_{\mathbf{q},B} \, e^{i\mathbf{q}\cdot\mathbf{R}_j} & (j \in B), \end{cases} \tag{16}$$

where $\mathbf{q}$ is the momentum and $\mathbf{R}_j$ is the position of site j, the eigenvalue problem reduces to

$$\begin{bmatrix} K\left\{\sin\left(\mathbf{q}\cdot\mathbf{r}_{y,x}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{z,y}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{x,z}\right)\right\} & \frac{i}{2}\left\{J_x e^{i\mathbf{q}\cdot\mathbf{r}_x}+J_y e^{i\mathbf{q}\cdot\mathbf{r}_y}+J_z e^{i\mathbf{q}\cdot\mathbf{r}_z}\right\} \\ -\frac{i}{2}\left\{J_x e^{-i\mathbf{q}\cdot\mathbf{r}_x}+J_y e^{-i\mathbf{q}\cdot\mathbf{r}_y}+J_z e^{-i\mathbf{q}\cdot\mathbf{r}_z}\right\} & K\left\{\sin\left(\mathbf{q}\cdot\mathbf{r}_{x,y}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{y,z}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{z,x}\right)\right\} \end{bmatrix} \begin{bmatrix} v_{\mathbf{q},A} \\ v_{\mathbf{q},B} \end{bmatrix} = \lambda_{\mathbf{q}} \begin{bmatrix} v_{\mathbf{q},A} \\ v_{\mathbf{q},B} \end{bmatrix}, \tag{17}$$

where $\mathbf{r}_\alpha$ is a first-neighbor bond vector from any $j\in A$ site to the $j\in B$ site connected to it by an α bond, while $\mathbf{r}_{\alpha,\beta}\equiv\mathbf{r}_\alpha-\mathbf{r}_\beta$ is a second-neighbor bond vector. The excitation energy of the corresponding complex-fermion eigenmode is then given by

$$\varepsilon_{\mathbf{q}} = 4\left|\lambda_{\mathbf{q}}\right| = 2\sqrt{\left|J_x e^{i\mathbf{q}\cdot\mathbf{r}_x}+J_y e^{i\mathbf{q}\cdot\mathbf{r}_y}+J_z e^{i\mathbf{q}\cdot\mathbf{r}_z}\right|^2+4K^2\left\{\sin\left(\mathbf{q}\cdot\mathbf{r}_{y,x}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{z,y}\right)+\sin\left(\mathbf{q}\cdot\mathbf{r}_{x,z}\right)\right\}^2}. \tag{18}$$

Note that the two eigenvalues $\pm\lambda_{\mathbf{q}}$ from Eq. (17) correspond to the complex fermion and its antiparticle, respectively.

[1] A. Y. Kitaev, Ann. Phys. **321**, 2 (2006).
[2] E. H. Lieb, Phys. Rev. Lett. **73**, 2158 (1994).