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Exact Solution of Kitaev's Honeycomb Model

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1 Kitaev's spin lattice Hamiltonian

The honeycomb lattice with anisotropic nearest neighbor coupling was first proposed by Dr. A. Kitaev in 2006 [1]. It is a paradigmatic example of a quantum spin liquid ground state emerging from a highly frustrated Hamiltonian that can be solved exactly. In Kitaev's honeycomb lattice model, the degrees of freedom

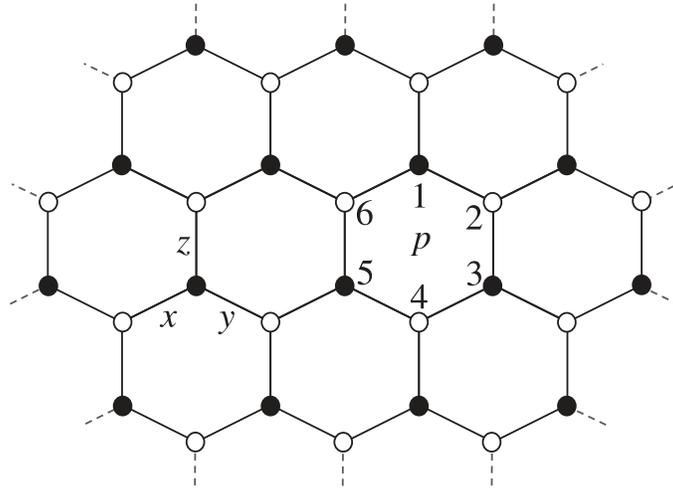


Figure 1: Kitaev's honeycomb lattice. The solid and hollow dots indicate sublattice A and B , with anisotropic coupling in x, y, z directions. A plaquette is labeled p by convention.[2]

live on vertices of honeycomb lattice with nearest neighbor interactions. The interactions between spin degrees of freedom are made anisotropy by directional coupling constants $\{K_x, K_y, K_z\}$. The Hamiltonian reads:

$$H = -K_x \sum_{\langle ij \rangle_x} \sigma_j^x \sigma_k^x - K_y \sum_{\langle ij \rangle_y} \sigma_j^y \sigma_k^y - K_z \sum_{\langle ij \rangle_z} \sigma_j^z \sigma_k^z \quad (1)$$

The schematic model is as shown in Fig.1

2 Majorana fermionisation

We start by mapping one spin-1/2 particle on site i onto two fermionic modes $f_{1,i}$ and $f_{2,i}$, in analogy with two spins.

$$f_{1,i}^\dagger |0\rangle_1 = |1\rangle_1, \quad f_{2,i}^\dagger |0\rangle_2 = |1\rangle_2.$$

The composite modes made by these two modes are:

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

To make the mapping consistent with spin-1/2 particles we need to project out $|01\rangle$ and $|10\rangle$ states and keep only $|00\rangle$ and $|11\rangle$ states that are to be mapped to spin down and spin up:

$$|\uparrow\rangle \equiv |00\rangle \quad \text{and} \quad |\downarrow\rangle \equiv |11\rangle \quad (2)$$

with $f_{1,i} |00\rangle = f_{2,i} |00\rangle = 0$ and $f_{1,i}^\dagger f_{2,i}^\dagger |00\rangle = |11\rangle$. Therefore, to make the map a valid representation we need to restrict the Hilbert space into its subspace \mathcal{L} , whose states satisfy

$$D_i |\psi\rangle = |\psi\rangle \quad (3)$$

where D_i can be viewed as a gauge operator:

$$D_i = (1 - 2f_{1,i}^\dagger f_{1,i})(1 - 2f_{2,i}^\dagger f_{2,i}) \quad (4)$$

It is readily to see that this definition of D_i , when acting on $|11\rangle$ and $|00\rangle$, leaves these states unchanged:

$$D_i |00\rangle = |00\rangle, \quad D_i |11\rangle = |11\rangle$$

$$D_i |10\rangle = -|10\rangle, \quad D_i |01\rangle = -|01\rangle$$

Now, we would like to represent the spin operators in terms of Majorana fermions, i.e. split each of the fermionic modes into 2 Majorana modes. Consider a collection of four Majorana operators c, b^x, b^y, b^z , that act on the 4-dimensional Fock space:

$$\begin{aligned} c_i &= f_{1,i} + f_{1,i}^\dagger \\ b_i^x &= i(f_{1,i}^\dagger - f_{1,i}) \\ b_i^y &= f_{2,i} + f_{2,i}^\dagger \\ b_i^z &= i(f_{2,i}^\dagger - f_{2,i}) \end{aligned} \quad (5)$$

In this Majorana representation we can re-write D_i as:

$$D_i = (1 - 2f_{1,i}^\dagger f_{1,i})(1 - 2f_{2,i}^\dagger f_{2,i}) = c_i b_i^x b_i^y b_i^z \quad (6)$$

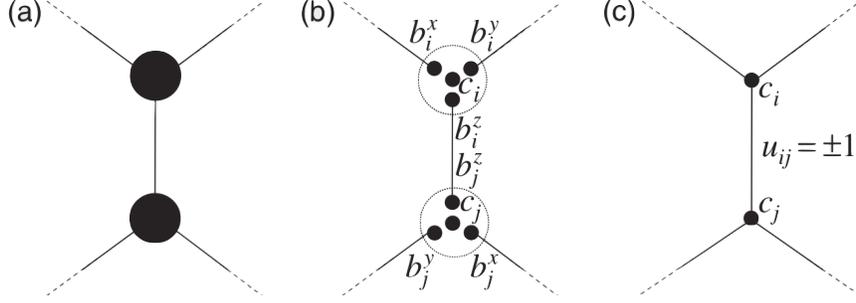


Figure 2: (a) 2 spins on vertices are represented by (b) 4 majoranas c , b^x , b^y , b^z . Since \hat{u}_{jk} commute with Hamiltonian which has eigenvalue ± 1 , we can further simplify the representation to (c) [2]

Then we re-write the spin operators in terms of the same Majorana modes:

$$\begin{aligned}\tilde{\sigma}^x &= ib^x c \\ \tilde{\sigma}^y &= ib^y c \\ \tilde{\sigma}^z &= ib^z c\end{aligned}\tag{7}$$

Each majorana operator is $\sqrt{2}$ -dimensional. Hence, the mapped Hilbert space $\tilde{\mathcal{L}}$ is $(\sqrt{2}^4)^N = 4^N$, in contrast with the original physical Hilbert space \mathcal{L} , that is 2^N dimensional. Then, each spin operator σ_i is expressed in terms of four

majorana operator. One can check that the newly defined Majorana operators obey pauli algebra. (A Mapped version of spin). In this way, the Hamiltonian is mapped to:

$$\tilde{H} = - \sum_{\langle jk \rangle_\alpha} K_\alpha \tilde{\sigma}_j^\alpha \tilde{\sigma}_k^\alpha = - \sum_{\langle jk \rangle_\alpha} K_\alpha b_j^\alpha b_k^\alpha c_j c_k = i \sum_{\langle jk \rangle_\alpha} \left(K_\alpha (ib_j^\alpha b_k^\alpha) \right) c_j c_k \tag{8}$$

Define the following two new operators:

$$\begin{aligned}\hat{u}_{jk} &\equiv ib_j^\alpha b_k^\alpha \\ \hat{A}_{jk} &\equiv K_\alpha \hat{u}_{jk}\end{aligned}\tag{9}$$

Thus the Hamiltonian can be written compactly as:

$$\tilde{H} = i \sum_{\langle jk \rangle_\alpha} \hat{A}_{jk} c_j c_k \tag{10}$$

The convenience of this representation comes from several nice properties of link operator \hat{u}_{jk} :

(i) \hat{u}_{jk} , thus \hat{A}_{jk} , is anti-symmetric under index exchange.

$$\hat{u}_{jk} = -\hat{u}_{kj}, \quad \hat{A}_{jk} = -\hat{A}_{kj}.$$

This property follows directly from the anti-commutation relation of Majorana fermions.

(ii) \hat{u}_{jk} is Hermitian:

$$\hat{u}_{jk}^\dagger = \hat{u}_{jk}.$$

This property follows directly from the anti-commutation relation of Majorana fermions, and that Majoranas are their own anti-particles.

(iii) The eigenvalue of \hat{u}_{jk} is ± 1

It is obvious since b^α is defined to be a Majorana operator which satisfies anti-commutation $\{b_j^\alpha, b_k^\alpha\} = 2\delta_{jk}$, hence:

$$\hat{u}_{jk}^2 = -b_j^\alpha b_k^\alpha b_j^\alpha b_k^\alpha = b_k^\alpha b_j^\alpha b_j^\alpha b_k^\alpha = 1.$$

Therefore \hat{u}_{jk} must have eigenvalues ± 1 .

(iv) operators defined on different links commute, i.e. $[\hat{u}_{jk}, \hat{u}_{lm}] = 0$.

If links do not share a common site:

$$\begin{aligned} [\hat{u}_{jk}, \hat{u}_{lm}] &= \hat{u}_{jk}\hat{u}_{lm} - \hat{u}_{lm}\hat{u}_{jk} = -b_j^\alpha b_k^\alpha b_l^\beta b_m^\beta + b_l^\beta b_m^\beta b_j^\alpha b_k^\alpha \\ &= -b_j^\alpha b_k^\alpha b_l^\beta b_m^\beta + b_j^\alpha b_k^\alpha b_l^\beta b_m^\beta = 0 \end{aligned}$$

where we have applied the anti-commutation relation 4 times on $b_l^\beta b_m^\beta b_j^\alpha b_k^\alpha$ to re-arrange them into the same index order as the other term. It's similar to show that the answer is the same even if they share a same site, for the upper index α and β must be different in that case.

(v) \hat{u}_{jk} is a constant of motion, i.e. $[\hat{u}_{jk}, H] = 0$.

Follows (iv) and the Majorana representation of Hamiltonian

As is shown in (v) that \hat{u}_{jk} commutes with Hamiltonian, defining its eigenvalues good quantum numbers. Also, due to (ii), (iii) and (iv), we can specify the eigenvalues, $u_{jk} = \pm 1$, of all link operators \hat{u}_{jk} simultaneously. We therefore are tempted to decompose the system's extended Hilbert space $\tilde{\mathcal{L}}$ into sectors $\tilde{\mathcal{L}}_{\{u_{jk}\}}$ that are defined by the configurations of u_{jk} on all links:

$$\tilde{\mathcal{L}} = \bigoplus_{\{u_{jk}\}} \tilde{\mathcal{L}}_{\{u_{jk}\}} \quad (11)$$

If we choose to work in the subspaces of $\tilde{\mathcal{L}}_{\{u_{jk}\}}$, i.e. represent the extended Hamiltonian \tilde{H} under the basis defined by these link operators, we can shake off the *hat* on $\{\hat{u}_{jk}\}$ and represent the Hamiltonian by their eigenvalues $\{u_{jk}\}$:

$$\tilde{H} = i \sum_{\langle jk \rangle_\alpha} A_{jk} c_j c_k \quad (12)$$

Note here in this representation $A_{jk} = K_\alpha u_{jk}$ are just numbers indexed by links - a simple anti-symmetric matrix.

3 The exact solution

It seems we are done by Eq.(12). Since u_{jk} are good quantum numbers, we are tempted to label states by $\{u_{jk}\}$. Just apply Fourier transformation on $\tilde{H} = i \sum_{\langle jk \rangle_\alpha} A_{jk} c_j c_k$, then it can be represented in non-interacting Majoranas in k space, thus can be diagonalized directly, in the same way we did for graphene. However, we have not apply the gauge operator! That means there will be unphysical states in the solution which have to be gauged out.

We have simplified the Hamiltonian in the last section by working under the subspace $\tilde{\mathcal{L}}_{\{u_{jk}\}}$. Yet along with this extended representation we also introduced redundencies that contains unphysical states. In fact what we now have is a emergent lattice gauge theory with the gauge operator D_i defined in section 2. It is crucial to keep in mind that up till now we have been working in the extended Hilbert space $\tilde{\mathcal{L}}$ that contains unphysical states (We have not fixed the gauge!). To eliminate the unphysical states we must enforce the gauge operator $D_i = 1$ in order to maintain in the subspace \mathcal{L} , that is:

$$D_i = c_i b_i^x b_i^y b_i^z \equiv 1 \quad (13)$$

In other words, the states that satisfy $D_i |\psi_p\rangle = |\psi_p\rangle$ for all i are the physical states of the system ($|\psi_p\rangle$ is abbrev. of $|\psi_{physical}\rangle$), whereas those which satisfy $D_i |\psi_u\rangle = -|\psi_u\rangle$ for any i in the lattice are redundant unphysical states. ($|\psi_u\rangle$ is abbrev. of $|\psi_{unphysical}\rangle$). One can check under this restriction we retain the pauli algebra.

Another way to put condition (13) upon the extended Hilbert space is to define a projection operator. We need to do is to define a projection operator to project out the unphysical states, i.e. find an operator $P_{\tilde{\mathcal{L}} \rightarrow \mathcal{L}}$ that satisfies $P_{\tilde{\mathcal{L}} \rightarrow \mathcal{L}} |\psi_p\rangle = |\psi_p\rangle$ and $P_{\tilde{\mathcal{L}} \rightarrow \mathcal{L}} |\psi_u\rangle = 0$. It is readily to see such an projection operator can be simply defined as follows:

$$P_{\tilde{\mathcal{L}} \rightarrow \mathcal{L}} = \prod_i \left(\frac{1 + D_i}{2} \right) \quad (14)$$

Constraints defined by Eq.(13) and Eq.(14) are equivalent. The question is how do we implement the constraint to the extended Hilbert space. Dr. A. Kitaev came up with a solution by construction. Consider a plaquette operator :

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z \quad (15)$$

This plaquette operator has several nice proverties:

(i) W_p has eigenvalues $w_p = \pm 1$

Follows from Pauli algebra:

$$\sigma_i^{a2} = 1, \quad [\sigma_i^a, \sigma_j^b] = 2i\delta_{ij}\epsilon^{abc}\delta_j^c$$

Hence $W_p^2 = 1$, $w_p = \pm 1$

(ii) W_p on different plaquettes commute with each other: $[W_p, W_{p'}] = 0$. This follow directly from Pauli algebra.

(iii) W_p commutes with Hamiltonian: $[W_p, H] = 0$

WLOG, we look at the bond (1,2) that coincides with a particular W_p .

$$\begin{aligned} [W_p, H] &= [W_p, \sigma_1^c \sigma_2^c] = [\sigma_1^a \sigma_2^b, \sigma_1^c \sigma_2^c] = [\sigma_1^a, \sigma_1^c] \sigma_2^c \sigma_2^b + \sigma_1^a \sigma_1^c [\sigma_2^b, \sigma_2^c] \\ &= 2i(-\sigma_1^b \sigma_2^c \sigma_2^b + \sigma_1^a \sigma_1^c \sigma_2^a) = -2(\sigma_1^b \sigma_2^a - \sigma_1^a \sigma_2^b) = 0 \end{aligned}$$

where {a,b,c} are in cyclic order.

To be consistent with the Majorana representation, we are tempted to rewrite W_p in terms of Majorana previously defined. Fantastically, we can apply the constraint along with rewriting W_p in Majoranas! That is:

$$\tilde{W}_p = \prod_{\langle jk \rangle \in \partial p} \hat{u}_{jk} \quad (j \in A \text{ sublattice}, k \in B \text{ sublattice}) \quad (16)$$

where ∂p is the boundary of a plaquette p .

To show this, we substitute each spin operator in terms of its Majorana map defined in Eq.(7):

$$\tilde{W}_p = \tilde{\sigma}_1^x \tilde{\sigma}_2^y \tilde{\sigma}_3^z \tilde{\sigma}_4^x \tilde{\sigma}_5^y \tilde{\sigma}_6^z = (ib_1^x c_1)(ib_2^y c_2)(ib_3^z c_3)(ib_4^x c_4)(ib_5^y c_5)(ib_6^z c_6) \quad (17)$$

Now we are well-prepared to apply the constraint defined in Eq.(13)! We wish to enforce $b_i^x b_i^y b_i^z c_i \equiv 1$, in other words, to enforce

$$b_i^x b_i^y b_i^z \equiv c_i \quad (18)$$

This is done by applying an c_i operator on both sides and noting that c_i is a Majorana operator which gives $c_i^2 = 1$. Therefore we can rewrite \tilde{W}_p as follows:

$$\begin{aligned} \tilde{W}_p &= (ib_1^x c_1)(ib_2^y c_2)(ib_3^z c_3)(ib_4^x c_4)(ib_5^y c_5)(ib_6^z c_6) \\ &= i(b_1^x b_1^x b_1^y b_1^z)(ib_2^y b_2^x b_2^y b_2^z)(ib_3^z b_3^x b_3^y b_3^z)(ib_4^x b_4^x b_4^y b_4^z)(ib_5^y b_5^x b_5^y b_5^z)(ib_6^z b_6^x b_6^y b_6^z) \\ &= i(b_1^y b_1^z)(ib_2^x b_2^z)(ib_3^x b_3^y)(ib_4^y b_4^z)(ib_5^x b_5^z)(ib_6^x b_6^y) \\ &= (ib_2^z b_1^z)(ib_2^x b_3^x)(ib_4^y b_3^y)(ib_4^z b_5^z)(ib_6^x b_5^x)(ib_6^z b_1^z) \\ &= \hat{u}_{21} \hat{u}_{23} \hat{u}_{43} \hat{u}_{45} \hat{u}_{65} \hat{u}_{61} \\ &= \prod_{\langle jk \rangle \in \partial p} \hat{u}_{jk} \quad \text{for } j \in A \text{ \& } k \in B \end{aligned} \quad (19)$$

\tilde{W}_p has several nice properties:

(i) $[\tilde{W}_p, \hat{u}_{ij}] = 0$

So we can specify eigenvalues simultaneously.

(ii) \tilde{W}_p commute with Hamiltonian: $[\tilde{W}_p, H] = 0$.

This follows directly from that different link operators commute, and is consistent with the spin representation.

(iii) W_p commute with gauge operator: $[\tilde{W}_p, D_i] = 0$

Therefore we can label the ground states in terms of eigenvalues of \tilde{W}_p on all plaquettes! All eigenstates of plaquette operators \tilde{W}_p belongs to the physical Hilbert space \mathcal{L} since it is defined along with the constraint in Eq.(18). In other words:

$$|\psi_{\{w_p\}}\rangle = \mathcal{P}_{\tilde{\mathcal{L}} \rightarrow \mathcal{L}} |\psi_{\{u_{ij}\}}\rangle \quad (20)$$

It is important to point out that this projection only project a state in $\tilde{\mathcal{L}}$ into \mathcal{L} , yet does not effect eigenvalues E . Since the eigenvalue of a physical state $|\psi_p(E)\rangle$ is determined only by $\{w_p\}$. So to look at dispersion relation, we don't have to play this projection.

So we have a procedure for finding the full solution, i.e. the eigenstates and eigen values of H :

1. Fix a set of $\{w_p\}$ for all plaquettes, which defines a physical eigenstate.
2. For such a state defined by (1), there are many u_{jk} which give the same $\{w_p\}$ configuration. Find one valid configuration of $\{u_{jk}\}$.
3. Diagonalize the quadratic Hamiltonian and find eigen energy E .
4. Project into \mathcal{L} and get the corresponding eigenstate $|\psi_p(E)\rangle$.
5. Repeat 1 - 4. To find ground state, look at minimum E .

It is worth pointing out that the model is actually an emergent Z_2 gauge theory. Each D_i operator flips the sign of all 3 links that are connected to site i , on which D_i acts. The physical states can retrieved by a series of gauge transformation defined by D_i , which eventually should reach a state that satisfies $D_i |\psi\rangle = |\psi\rangle$. The action of this gauge operator keeps the states in the same vortex configuration, while symmetrize the state in link sector u_{ij} by constructing an equal weight superposition of all $\{u_{ij}\}$ configuration. See Fig.3.

4 Ground state energy

According to H. Lieb[3], the ground state of this system has to be vortex-free (v.f.), i.e. $w_p = +1$ for all plaquettes. This Greatly simplify the problem at hand. Our goal now is to find the energy dispersion which isn't effect by

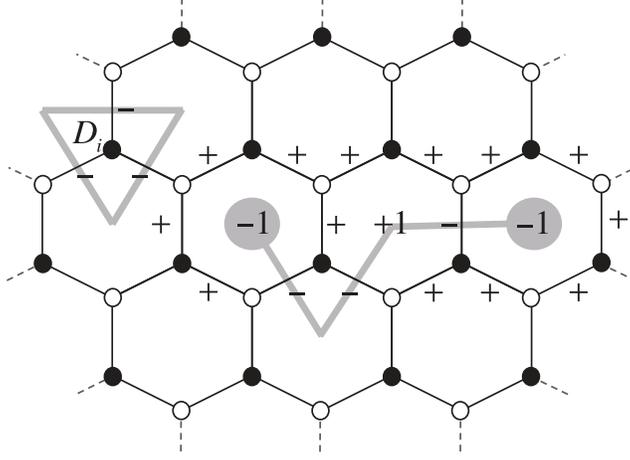


Figure 3: In the Z_2 gauge field, each D_i operator flips the sign of all 3 u_{ij} links that are connected to site. We can denote $u_{ij} = -1$ by a string perpendicular to the link. In this string-net picture, the string must end at vortex $w_p = -1$, unless it forms a closed loop as shown in the upper left corner. [2]

the gauge, we can trivially satisfy $w_p = +1$ by setting all link variables to be $u_{jk} = +1$. Now we begin diagonalize the Majorana Hamiltonian:

$$\tilde{H}_{v.f.} = i \sum_{\langle jk \rangle_\alpha} K_\alpha c_j c_k \quad (21)$$

where u_{jk} are set to be +1 for all links. Note by fixing the link configuration the Majorana Hamiltonian becomes translationally symmetric!

The system has a discrete translational symmetry under $\vec{r}' = \vec{r} + n_1 \vec{a}_1 + n_2 \vec{a}_2$ for integer n_i , in the honeycomb lattice the basis vectors \vec{a}_i are:

$$\begin{aligned} \vec{a}_1 &= \frac{a}{2}(\sqrt{3}, 3) \\ \vec{a}_2 &= \frac{a}{2}(-\sqrt{3}, 3) \end{aligned} \quad (22)$$

where a is the lattice constant. We can rewrite the Hamiltonian as:

$$\tilde{H}_{v.f.} = i \sum_{j \in A} \sum_{\delta} K_\alpha c_j c_{j+\delta} \quad (23)$$

where δ indicates 3 nearest neighbors of site j :

$$\begin{aligned} \delta_x &= \frac{a}{2}(\sqrt{3}, 1) \\ \delta_y &= \frac{a}{2}(-\sqrt{3}, 1) \\ \delta_z &= a(0, -1) \end{aligned} \quad (24)$$

Go to momentum space by Fourier transform:

$$\begin{aligned} c_j &= \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_j} a_{\vec{k}}; & a_{\vec{k}} &= \frac{1}{\sqrt{N}} \sum_{j \in A} e^{-i\vec{k}\cdot\vec{r}_j} c_j \\ c_k &= \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_k} b_{\vec{k}}; & b_{\vec{k}} &= \frac{1}{\sqrt{N}} \sum_{k \in B} e^{-i\vec{k}\cdot\vec{r}_k} c_k \end{aligned} \quad (25)$$

with the orthogonality:

$$\sum_{j \in A} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_j} = N \delta_{\vec{k}\vec{k}'} \quad (26)$$

Plug these into the vortex-free Hamiltonian:

$$\begin{aligned} \tilde{H}_{v.f.} &= \frac{i}{N} \sum_{j \in A} \sum_{\vec{k}, \vec{k}'} \sum_{\delta} K_{\delta} e^{i\vec{k}\cdot\vec{r}_j} a_{\vec{k}} e^{-i\vec{k}'\cdot(\vec{r}_j+\delta)} b_{-\vec{k}'} \\ &= \sum_{\vec{k}, \vec{k}'} \sum_{\delta} \left(\sum_{j \in A} \frac{1}{N} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_j} \right) K_{\delta} i e^{-i\vec{k}'\cdot\delta} a_{\vec{k}} b_{-\vec{k}'} \\ &= \sum_{\vec{k}} \left(\sum_{\delta} K_{\delta} e^{-i\vec{k}\cdot\delta} \right) i a_{\vec{k}} b_{-\vec{k}} \\ &\equiv \sum_{\vec{k}} i f^*(\vec{k}) a_{\vec{k}} b_{-\vec{k}} \end{aligned} \quad (27)$$

where we have defined $f(\vec{k}) = \sum_{\delta} K_{\delta} e^{i\vec{k}\cdot\delta}$. Due to the symmetry in momentum space, we can re-arrange the above equation as:

$$\begin{aligned} \tilde{H}_{v.f.} &= \sum_{\vec{k}} i f^*(\vec{k}) a_{\vec{k}} b_{-\vec{k}} = \frac{1}{2} \sum_{\vec{k}} i f(\vec{k}) a_{-\vec{k}} b_{\vec{k}} - i f^*(\vec{k}) b_{-\vec{k}} a_{\vec{k}} \\ &= \sum_{\vec{k}} \Psi_{\vec{k}}^{\dagger} \hat{h}_{\vec{k}} \Psi_{\vec{k}} \end{aligned} \quad (28)$$

where we have defined:

$$\Psi_{\vec{k}} = \begin{bmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{bmatrix}, \quad \hat{h}_{\vec{k}} = \frac{1}{2} \begin{bmatrix} 0 & i f(\vec{k}) \\ -i f^*(\vec{k}) & 0 \end{bmatrix} \quad (29)$$

Now the Hamiltonian is block diagonal in terms of $\hat{h}_{\vec{k}}$, we can extract the eigen value by diagonalizing the block $\hat{h}_{\vec{k}}$, which is simply:

$$\epsilon(\vec{k}) = \pm \frac{1}{2} |f(\vec{k})| \quad (30)$$

Note that the equation we derived above is not periodic in reciprocal space: $\hat{h}_{\vec{k}} \neq \hat{h}_{\vec{k}+\vec{G}}$, we apply a simple gauge transformation to recover the periodicity. Note that in the honeycomb lattice:

$$\vec{\delta}_2 - \vec{\delta}_1 = -\vec{a}_1, \quad \vec{\delta}_2 - \vec{\delta}_1 = -\vec{a}_1 \quad (31)$$

Apply a gauge transformation $f(\vec{k}) \rightarrow \tilde{f}(\vec{k})$ and $b(a)_{\vec{k}} \rightarrow \tilde{b}(\tilde{a})_{\vec{k}}$ by:

$$\tilde{b}_{\vec{k}} = ie^{i\vec{k}\cdot\vec{\delta}_1} b_{\vec{k}}, \quad \tilde{a}_{\vec{k}} = a_{\vec{k}}, \quad \tilde{f}(\vec{k}) = ie^{-i\vec{k}\cdot\vec{\delta}_1} f(\vec{k}) \quad (32)$$

where, by applying Eq.(31), we have:

$$\begin{aligned} \tilde{f}(\vec{k}) &= i \left(K_z + K_y e^{i\vec{k}\cdot(\vec{\delta}_2 - \vec{\delta}_1)} + K_x e^{i\vec{k}\cdot(\vec{\delta}_3 - \vec{\delta}_1)} \right) \\ &= i (K_z + K_y e^{-i\vec{k}\cdot\vec{a}_2} + K_x e^{-i\vec{k}\cdot\vec{a}_1}) \end{aligned} \quad (33)$$

It's readily to see Eq.(33) is indeed periodic in reciprocal lattice.

The system is in its gapless phase when there exists solutions for $\epsilon(\vec{k}) = 0$ for particular triplets of $\{K_\alpha\}$, and is gapped otherwise. In fact, One can show that the gapless phase must satisfy the triangle inequalities:

$$|K_x| \leq |K_y| + |K_z|, \quad |K_y| \leq |K_x| + |K_z|, \quad |K_z| \leq |K_x| + |K_y| \quad (34)$$

The full phase diagram is summarized in the triangular plot as follows:

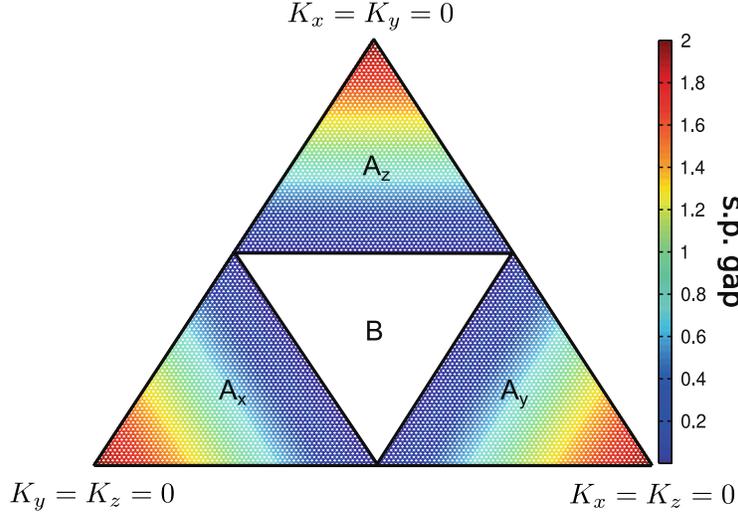


Figure 4: The phase diagram of Kitaev's Hamiltonian with $K_x + K_y + K_z = 1$. The central triangle B is gapless in which the center denotes $K_x = K_y = K_z$. The other 3 outer triangles are gapped phases with gap width indicated in the colorbar. [4]

In particular, the geometry of dispersion at the center of triangle B where $K_x = K_y = K_z$ is exactly identical to graphene (though it is dispersion of majorana).

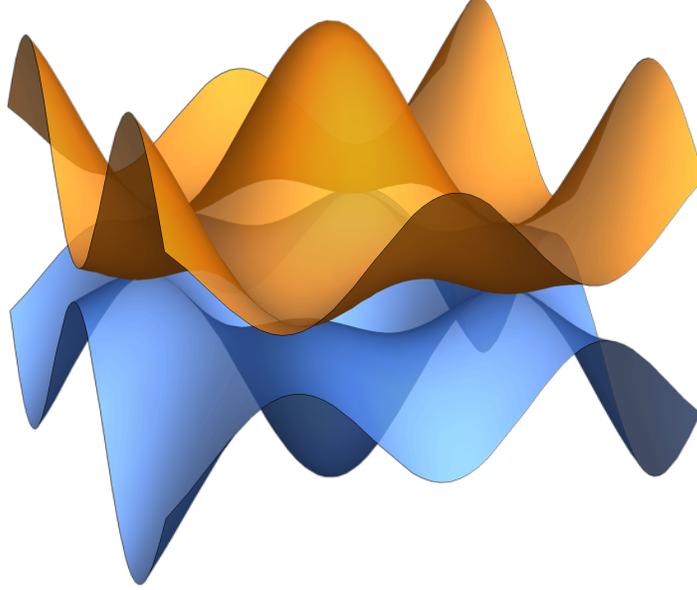


Figure 5: Energy dispersion at $K_x = K_y = K_z$ is identical to graphene

5 Toric code limit

5.1 From Honeycomb to Toric code Hamiltonian

Amazingly, the Kitaev's honeycomb is an effective Toric code Hamiltonian at high anisotropic regime, where one of the K_α go to ∞ . According to Kitaev's derivation [1], at 4th order perturbation of Kitaev Honeycomb model:

$$H_{eff}^{(4)} = cons - \frac{K_x^2 K_y^2}{16K_z^3} \sum_p Q_p \quad (35)$$

where p runs over the square lattice plaquettes of the dimer lattice.

$$Q_p = \sigma_{p_1}^y \sigma_{p_2}^z \sigma_{p_3}^y \sigma_{p_4}^z \quad (36)$$

On the new square lattice (TC lattice), the plaquettes in old lattice become plaquettes and stars. So the effective Hamiltonian becomes:

$$H_{eff} = -J_{eff} \left(\sum_s \tilde{Q}_s + \sum_p \tilde{Q}_p \right) \quad (37)$$

Note here \tilde{Q}_s , \tilde{Q}_p are still in the same form of the original Q_p defined in Eq.7, since by now, we only changed the representation of the lattice vectors rather than spins. These two operators has a mixing of σ^y and σ^x , but we can apply

an unitary transformation to eliminate this mixing. We can define a unitary transformation that rotates the above Hamiltonian into the TC model. To do that, let us first look at the degrees of freedom in real space:

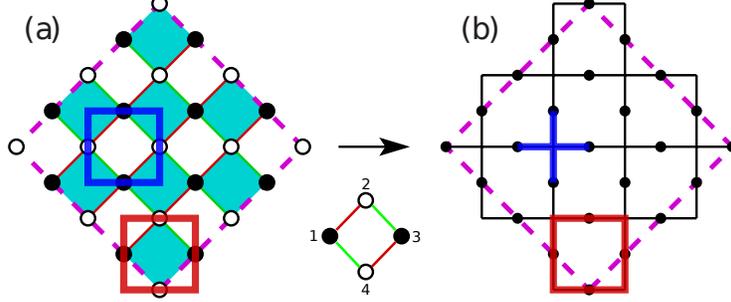


Figure 6: An illustration of mapping to the new square lattice embedded on a torus, with the purple dashed lines defining the pairs of equivalent sides. The blue square in (a) is mapped into the blue star in (b), while the red square in (a) remains a red square in (b). The label convention is as showed in the small square at the middle.

We can rotate the hilbert space so that $\tilde{Q}_p = \sigma_{p_1}^y \sigma_{p_2}^z \sigma_{p_3}^y \sigma_{p_4}^z$ becomes $\tilde{Q}'_p = \sigma_{p_1}^z \sigma_{p_2}^z \sigma_{p_3}^z \sigma_{p_4}^z$ on red plaquette, and $\tilde{Q}_s = \sigma_{p_1}^y \sigma_{p_2}^z \sigma_{p_3}^y \sigma_{p_4}^z$ becomes $\tilde{Q}'_p = \sigma_{p_1}^x \sigma_{p_2}^x \sigma_{p_3}^x \sigma_{p_4}^x$. This can be achieved if we do the following rotation respectively of \bullet and \circ sites.

$$\begin{aligned} \sigma_{\bullet}^x &\rightarrow \sigma_{\bullet}^y, & \sigma_{\bullet}^y &\rightarrow \sigma_{\bullet}^z, & \sigma_{\bullet}^z &\rightarrow \sigma_{\bullet}^x \\ \sigma_{\circ}^x &\rightarrow -\sigma_{\circ}^y, & \sigma_{\circ}^y &\rightarrow \sigma_{\circ}^x, & \sigma_{\circ}^z &\rightarrow \sigma_{\circ}^z \end{aligned} \quad (38)$$

We thus recover the Toric code Hamiltonian:

$$H_{TC} = -J_1 \sum_c A_v - J_2 \sum_p B_p \quad (39)$$

where

$$A_v = \prod_v \sigma_v^x, \quad B_p = \prod_p \sigma_p^z \quad (40)$$

5.2 Topological Entanglement Entropy of Toric code

Let's partition the system in to 2 parts: $\{A_{in}, A_{out}\}$, where $A_{in/out}$ is inside/outside of A 's boundary. The wavefunction are respectively $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$. Further let's suppose the boundary that separates two areas consists of L links, which is labeled by $h \equiv \{h_1, h_2, h_3, \dots, h_L\}$. Note that $h_m = 0$ or 1 .

Given a particular h , the wavefunctions is then described by $|\psi_{in,h}\rangle$ and $|\psi_{out,h}\rangle$, since h can be viewed as a boundary condition of both in and out states, the wavefunction must be h -dependent.

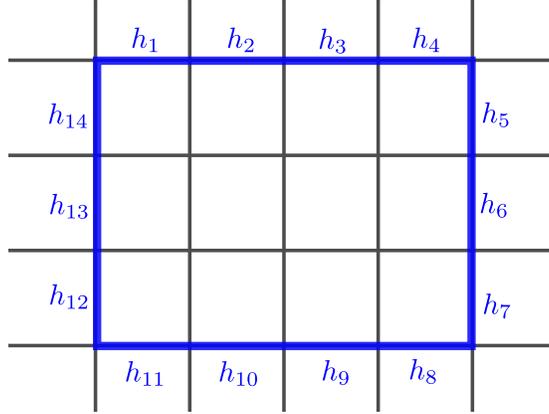


Figure 7: An illustration of partition of TC lattice. The full Hilbert space can be factorized as in and out lattice. the full wavefunction is $\{h\}$ -dependent.

The full wave function $|\Psi\rangle$ is then:

$$|\Psi_{TC}\rangle = \sum_h \sum_{in,out} C_{in,out} |\psi_{in,h}\rangle \otimes |\psi_{out,h}\rangle \quad (41)$$

We can apply a Schmidt decomposition (See Appendix) to the inner summation:

$$\sum_{in,out} C_{in,out} |\psi_{in,h}\rangle |\psi_{out,h}\rangle = \sum_{\phi} D_{\phi} |\phi_{in,h}\rangle |\phi_{out,h}\rangle \quad (42)$$

where D_{ϕ} is an abbrev. of the diagonal matrix $D_{\phi,\phi'}\delta_{\phi,\phi'}$. We now arrive at a new basis at which the full wavefunction is diagonal in terms of in/out states. Note that the diagonal matrix D_{ϕ} is in fact an Identity matrix (up to constant). This is because all orbitals must be equal weight. To see this, recall that the Star operator doesn't change the ground state:

$$A_v |\Psi\rangle = |\Psi\rangle \quad (43)$$

i.e.

$$A_v \sum_{\phi} D_{\phi} |\phi\rangle = \sum_{\phi} D_{\phi} |\phi\rangle$$

This is true if and only if all D_{ϕ} are equal of each orbit. Hence the full wavefunction becomes:

$$|\Psi_{TC}\rangle = \sum_h \sum_{\phi} |\phi_{in,h}\rangle |\phi_{out,h}\rangle \quad (44)$$

Since the full wavefunction $|\Psi_{TC}\rangle$ is diagonal in both ϕ and h , and the summation is over all possible configurations. According to the uniqueness of the diagonal basis, we can manually set $\phi \equiv \delta_{h,\phi}$, and $|\phi_{in/out,h}\rangle \equiv |\psi_{in/out,h}\rangle$ without changing the physical state. That is:

$$|\Psi_{TC}\rangle = \sum_h \sum_\phi \delta_{h,\phi} |\psi_{in,h}\rangle |\psi_{out,h}\rangle = \sum_h |\psi_{in,h}\rangle |\psi_{out,h}\rangle \quad (45)$$

This is great, because it's diagonal, and there're no redundant notation anymore. since the summation over h is constrained by $\sum_i^L h_i = \text{even number}$, Eq.5 can be rewrite as:

$$|\Psi_{TC}\rangle = \sum_{\{\sum h=2n\}} |\psi_{in,h}\rangle |\psi_{out,h}\rangle \quad (46)$$

where n is a positive integer.

Now by counting the number of elements in $\{\sum_i h_i = \text{even number}\}$, we are able to tell the number of states. since $h = 0, 1$, the number of elements is simply $\frac{1}{2} \times 2^L = 2^{L-1}$. Then the entropy is:

$$S \propto \log 2^{L-1} = L \log 2 - \log 2 \quad (47)$$

The first term is obviously from the area law, the second being the topological entanglement entropy.

$$\gamma = -\log 2 \quad (48)$$

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Appendix

1 The Schmitdt Decomposition

Suppose Ψ is a matrix state produced by the inside and the outside, with dimensions $D_A \times D_B$.

$$|\Psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle.$$

This can be factorized as

$$|\Psi\rangle = UDV^\dagger.$$

Suppose $D_B < D_A$, and ψ_{ij} are entries of matrix Ψ after the factorization by SVD, ψ_{ij} can be written as:

$$\psi_{ij} = \sum_{\alpha}^{D_B} U_{i\alpha} \lambda_{\alpha} (V^\dagger)_{\alpha j} = \sum_{\alpha}^{D_B} U_{i\alpha} \lambda_{\alpha} V_{\alpha j}^*.$$

Now plug this ψ_{ij} into $|\Psi\rangle$ in the original basis expression:

$$|\Psi\rangle = \sum_i^{D_A} \sum_j^{D_B} \sum_{\alpha}^{D_B} U_{i\alpha} \lambda_{\alpha} V_{\alpha j}^* |i\rangle |j\rangle.$$

This again can be factorized:

$$|\Psi\rangle = \sum_{\alpha}^{D_B} \left(\sum_i^{D_A} U_{i\alpha} |i\rangle \right) \lambda_{\alpha} \left(\sum_j^{D_B} V_{\alpha j}^* |j\rangle \right) = \sum_{\alpha}^{D_B} \lambda_{\alpha} |\alpha\rangle_A |\alpha\rangle_B.$$