Machine learning the Kitaev Honeycomb model

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Based on work with: M. Noormandipoor and Y. Sun.

Outline

1. Introduction
2. The Kitaev Honeycomb model
   - Majorana fermion realization
   - Emerging lattice gauge theory
   - Ising Anyons
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   - Conformal block representation
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Non-Abelian Phases of Matter

- Fractional Quantum Hall Effect with filling fraction $\nu = \frac{5}{2}$ was observed experimentally through measurement of *electric* Hall conductivity by R. Willett, J. P. Eisenstein, H. L. Störmer, D. C. Tsui, A. C. Gossard, and J. H. English [1987].
- Theoretical explanation in terms of a Non-Abelian phase of matter was given by G. Moore and N. Read [1991]. But other explanations in terms of Abelian phases of matter were also proposed and were consistent with experimental results.
- This situation changed with the recent experimental measurement of *thermal* Hall conductivity at $\nu = \frac{5}{2}$ by M. Banerjee, M. Heiblum, V. Umansky, D. E. Feldman, Y. Oreg and A. Stern [2018] .
  $\Rightarrow$ Experimental confirmation of Non-Abelian phases of matter in nature!
- Kitaev Honeycomb model Kitaev [2006] provides a spin lattice realization of a Non-Abelian phase of matter $\Rightarrow$ worth studying further in these exciting times!

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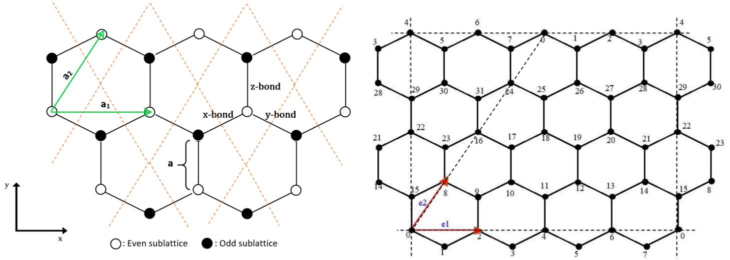
Kitaev Honeycomb model

The Kitaev model is a spin lattice model on a honeycomb lattice:



(a) Honeycomb lattice (b) Periodic boundary conditions

$$\mathbf{a}_1 = \sqrt{3}a\mathbf{e}_x \qquad \& \qquad \mathbf{a}_2 = \frac{\sqrt{3}}{2}a(\mathbf{e}_x, \sqrt{3}\mathbf{e}_y)$$

with Hamiltonian

$$H = -\sum_{\text{x links}} \sigma_i^x \sigma_j^x - \sum_{\text{y links}} \sigma_i^y \sigma_j^y - \sum_{\text{z links}} \sigma_i^z \sigma_j^z - K \sum_{(i,j,k)} \sigma_i^x \sigma_j^y \sigma_k^z$$

Kitaev's solution: realize spin 1/2 particles at each site i by two complex spinless fermionic modes $a_{1,i}$ and $a_{2,i}$

$$|\uparrow\rangle = |00\rangle, \quad |\downarrow\rangle = |11\rangle$$

with $a_1|00\rangle = a_2|00\rangle = 0$ and $|11\rangle = a_1^\dagger a_2^\dagger|00\rangle$. This representation is faithful if one eliminates states with only a single fermionic mode. This can be done by the projector

$$D_i|\Psi\rangle = |\Psi\rangle,$$

where

$$D_i = (1 - 2a_{a,i}^\dagger a_{1,i})(1 - 2a_{2,i}^\dagger a_{2,i}).$$

Defining 'real' and 'imaginary' modes

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

one can realize Pauli matrices by defining

$$\sigma_i^\alpha = ib_i^\alpha c_i \quad \text{for} \quad \alpha = x, y, z$$

Employing this representation the Hamiltonian interactions become

$$\sigma_i^\alpha \sigma_j^\alpha = -i\hat{u}_{ij}c_i c_j \quad \text{and} \quad \sigma_i^x \sigma_j^y \sigma_k^z = -i\hat{u}_{ik}\hat{u}_{jk}D_k c_i c_j,$$

where one defines the link operators

$$\hat{u}_{ij} = ib_i^\alpha b_j^\alpha, \quad \alpha = x, y, z$$

depending on the type of link (ij) as shown in the figure. The $\hat{u}_{ij}$ have the following properties:

$$\hat{u}_{ij} = -\hat{u}_{ji}, \quad \hat{u}_{ij}^2 = 1, \quad \hat{u}_{ij}^\dagger = \hat{u}_{ij}$$

The Hamiltonian can then be rewritten as

$$H = \frac{i}{4}\sum_{i,j}\hat{A}_{ij}c_i c_j, \quad \hat{A}_{ij} = 2\hat{u}_{ij} + 2K\sum_k \hat{u}_{ik}\hat{u}_{jk}$$

Emerging lattice gauge theory

First note that

$$[H, D_i] = 0,$$

$\longrightarrow$ diagonalising Hamiltonian is compatible with restricting to physical subspace $D_i = +1$ for all i:

$$H|\Psi\rangle = E|\Psi\rangle \quad \text{and} \quad D_i|\Psi\rangle = |\Psi\rangle$$

Consider now the plaquette operators

$$\hat{w}_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z = \prod_{i,j \in p} \hat{u}_{ij}$$

These operators have eigenvalues ± 1 and commute with the Hamiltonian and with the D_i operators:

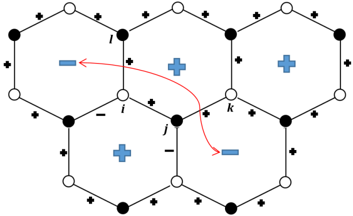
$$[\hat{w}_p, H] = 0 \quad \text{and} \quad [\hat{w}_p, D_i] = 0$$

We see that u_{ij} constitute local $\mathbb{Z}_2$ gauge degrees of freedom as

$$\{\hat{u}_{ij}, D_i\} = 0$$

Vortex sectors

Changing eigenvalues of plaquette operators creates *vortices*. These are always created in pairs as shown below:



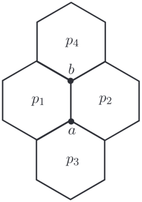
Vortices can be created by applying the operators (and combinations):

$$\hat{O}_1 = \exp\left(-i\frac{\pi}{2}\hat{\sigma}_a^z\right)$$

creates vortex-pair in plaquettes 1 and 2

$$\hat{O}_2 = \exp\left(-i\frac{\pi}{2}\hat{\sigma}_a^x\right)\exp\left(-i\frac{\pi}{2}\hat{\sigma}_b^y\right)$$

creates vortex-pair in plaquettes 3 and 4



Groundstate energy

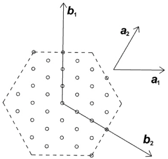
The *groundstate* is the lowest energy eigenstate of the Hamiltonian
$\longrightarrow$ resides in the no-vortex sector
Its energy can be obtained by diagonalizing the Hamiltonian in momentum space:

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}}(\gamma_{\mathbf{k}}^{\dagger}\gamma_{\mathbf{k}} - \frac{1}{2}), \quad E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$$

where $\gamma_{\mathbf{k}}^{\dagger}$ and $\gamma_{\mathbf{k}}$ are fermionic (Majorana) creation and annihilation operators,

$$\epsilon_{\mathbf{k}} = 2[-\cos(k_1) - \cos(k_2)],$$
$$\Delta_{\mathbf{k}} = 2[\sin(k_1) + \sin(k_2)],$$

and $\mathbf{k}$ resides in the first Brillouin zone of the lattice:



Ising Anyons

We see that the groundstate has energy

$$E_{\mathrm{gr}} = -\frac{1}{2}\sum_{\mathbf{k}} E_{\mathbf{k}}$$

Moreover, note that acting with $\gamma_{\mathbf{k}}^{\dagger}$ creates *quasiparticle* excitations
$\longrightarrow$ these have higher energy
It turns out that vortices carry Majorana modes and when one fuses two vortices, the resulting Hilbert space is two-dimensional: 0 quasiparticles/1 quasiparticle
$\longrightarrow$ reminiscent of Ising anyons!
Kitaev showed that the following correspondence to the Ising model holds:

Honeycomb lattice		Ising model
Groundstate	$\leftrightarrow$	$\mathbf{1}$, vacuum
Vortex	$\leftrightarrow$	σ, non-Abelian anyon
Quasiparticle excitation	$\leftrightarrow$	ψ, fermion

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RBM representation

The previous method presented only gives the energy eigenvalues
To obtain the wavefunctionsone has to diagonalize the Hamiltonian in spin basis
$\longrightarrow$ 2^N-dimensional vector space (where N is the number of sites)
$\longrightarrow$ grows exponentially with spin number

Our Ansatz: Use a *Restricted Boltzmann Machine* (RBM) to reduce the number of free parameters to polynomial in spin number
$\longrightarrow$ express wavefunction as

$$|\Phi\rangle = \sum_{\mathbf{s}} \Phi_\Omega(\mathbf{s})|\mathbf{s}\rangle$$

where $\mathbf{s} = (s_1, s_2, \ldots, s_N)$ and the s_i are projections of the spins on the z axis. For example,

$$|\mathbf{s}\rangle = |\uparrow\uparrow \cdots \downarrow \cdots \uparrow\rangle,$$

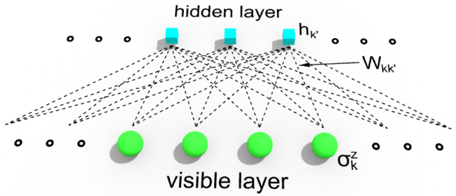
and

$$\Phi_\Omega(\mathbf{s}) = \sum_{\{h_k\}} e^{\sum_k a_k \sigma_k^z + \sum_{k'} b_{k'} h_{k'} + \sum_{kk'} W_{kk'} h_k \sigma_{k'}^z}.$$

In the above representation, $\{h_k\} = \{-1, 1\}^M$ is the set of possible configurations of hidden layer nodes and

$$\Omega = (a_k, b_{k'}, W_{kk'})$$

is the set of weights and biases of the RBM. Pictorially, we have



The weights and biases of the RBM have to be trained in such a way that the final state represents the desired quantum state of the model.

parameters is polynomial in system size $\longrightarrow$ computationally feasible

Summing over the values of $\{h_k\}$, we get

$$\Phi_\Omega(\mathbf{s}) = e^{\sum_k a_k \sigma^z_k} \times \prod_{k'} \cosh\left(\sum_k W_{kk'}\sigma^z_k + b_{k'}\right)$$

Training

In order to find the groundstate, the RBM is trained by minimizing

$$E_\Omega = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

via *stochastic gradient descent* . After each training step we *project* onto translation invariant states in order to restrict RBM to physical parameter space:

$$|\Phi'\rangle = \sum_{m,n} \hat{T}_{m\mathbf{a}_1 + n\mathbf{a}_2} |\Phi\rangle \ ,$$

where $\hat{T}_{m\mathbf{a}_1 + n\mathbf{a}_2}$ are operators translating m steps along the $\mathbf{a}_1$ direction and n steps along the $\mathbf{a}_2$ direction. $\hat{T}_{m\mathbf{a}_1 + n\mathbf{a}_2}$ can be realized as a permutation matrix acting on quantum states or a permutation of RBM parameters.

Results

We use several different methods to compute the groundstate energy and compare them:

a) Analytic formula (i: periodic bdc, ii: anti-periodic bdc)
b) Original method of Kitaev (using Majorana fermion representation of spins)
c) Direct diagonalization of Hamiltonian for small system sizes
d) RBM results using the **NetKet** package
e) RBM results using our own package written using **PyTorch**

lattice size	2×2	2×3	2×4	3×3	3×4	4×4	5×5	6×6	7×7	3×3 with $K=0.2$
a.i	-6.4721	-9.8003	-12.5851	-14.2915	-18.9869	-25.1282	-39.3892	-56.7529	-77.1249	
a.ii	-6	-9.2915	-12.4721	-14.2915	-19.0918	-25.4164	-39.3892	-56.2668	-77.1249	
b	-6	-9.2915	-12.4721	-14.2915	-19.0918	-25.4164	-39.3892	-56.2668	-77.1249	
c	-6.9282	-9.8003	-12.9443	-14.2915	-19.0918	-	-	-	-	-17.5260
d	-6.9282	-9.8003	-12.573	-13.7374	-18.0466	-24.0783	-37.305	-52.920	-71.793	
e	-6.9282	-9.8003	-12.9293	-14.2787						-17.393

Excited states can be created from the groundstate by applying string operators

$$\hat{S} = \prod_{\alpha-links} \exp\left(-i\frac{\pi}{2}\hat{\sigma}^{\alpha}_{\circ}\right) .$$

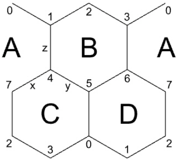
These have representations at the level of the RBM:

$$\hat{S}^z_l : (W_{lk'}, a_l) \mapsto \left(W_{lk'}, a_l - i\frac{\pi}{2}\right)$$

$$\hat{S}^x_l : (W_{lk'}, a_l) \mapsto (-W_{lk'}, -a_l)$$

$$\hat{S}^y_l : (W_{lk'}, a_l) \mapsto \left(-W_{lk'}, -a_l - i\frac{\pi}{2}\right) .$$

$\longrightarrow$ can create vortices and measure plaquette operator eigenvalues + energy:



(c) 2×2 lattice

Spin Flip Operator (acting successively)	W_A	W_B	W_C	W_D	Energy
Groundstate	0.9489	0.9517	0.9525	0.9553	-6.078
$\hat{S}^x_5$	0.9489	-0.9517	0.9525	-0.9553	-4.011
$\hat{S}^y_7$	-0.9489	-0.9517	0.9525	0.9553	-1.804
$\hat{S}^z_3$	0.9489	0.9517	0.9525	0.9553	0.061

(d) Vortex sectors

Conformal block representation

Using the correspondence between (2+1)d topological field theories and 2d CFTs, wavefunctions are identified with conformal blocks:
$\longrightarrow$ for $SU(p)_k$ WZW models we have

$$\Psi_0(z_1,\dots,z_N) = \prod_{i<j}^{N}(z_i - z_j)^{n+k/p}\langle\mathcal{O}_R(z_1)\dots\mathcal{O}_R(z_N)\rangle e^{-\sum_i |z_i|^2/4l_B^2}$$

In order to guarantee a single groundstate on the 2-sphere, the conformal block $\langle\mathcal{O}_R(z_1)\dots\mathcal{O}_R(z_N)\rangle$ is computed in the representation $R = \mathrm{Sym}_k$, satisfying

$$\underbrace{\mathrm{Sym}_k \times \mathrm{Sym}_k \times \dots \times \mathrm{Sym}_k}_{p} = \mathbf{1}$$

The Kitaev model is in the same universality class as the $SU(2)_2$ WZW model, i.e. $p = k = 2 \longrightarrow$ *Pfaffian state*:

$$\Psi_0^{\mathrm{Pf}}(\{z_i\}) = \mathrm{Pf}\left(\frac{|ij\rangle_1}{z_i - z_j}\right)\prod_{i<j}(z_i - z_j)^{n+1} e^{-\frac{1}{4l_B^2}\sum_j |z_j|^2}$$

We have identified $\mathcal{O}_R$ with the spin 1 field ψ of the Ising CFT
The state $|ij\rangle_1$ is a spin singlet state formed from two spin 1 states

$$|ij\rangle_1 = |1_i\rangle|-1_j\rangle + |-1_i\rangle|1_j\rangle - 2|0_i\rangle|0_j\rangle$$

Spin 1 states can be viewed as partons composed of fermionic creation (annihilation) operators giving *color* states

$$|a\rangle = c_a^\dagger|0\rangle, \quad a = 1, 2, 3,$$

with the identification

$$|\pm\rangle = -(\pm|1\rangle + i|2\rangle)/\sqrt{2} \quad \text{and} \quad |m = 0\rangle = |3\rangle$$

$\longrightarrow$ can obtain our spin $\frac{1}{2}$ states as projections of these!
$\longrightarrow$ we insert for each lattice site of the Honeycomb an Ising spin 1 field ψ and project down to a spin $\frac{1}{2}$ state
$\longrightarrow$ since $|ij\rangle_1$ is spin 1 singlet, the corresponding spin $\frac{1}{2}$ projection should be invariant under permutations of σ^x, σ^y and σ^z
$\longrightarrow$ generated by $\hat{U}_{C_6}$ operator

We are interested in groundstate wave-functions on the *torus*
$\longrightarrow$ the two-point correlation function of two ψ-fields is

$$\langle \psi(z_i)\psi(z_j)\rangle \sim \frac{\vartheta[\alpha](z_i - z_j)}{\vartheta_1(z_i - z_j)}$$

which implies that our Pfaffian state is given by

$$\Psi^{\mathrm{Pf}}_{0,\alpha}(z_1, \ldots, z_N) = e^{-\sum_i |z_i|^2/4l_B^2} F^{\alpha}_{\mathrm{cm}}(\sum_i z_i)\mathrm{Pf}\left(\frac{\vartheta[\alpha](z_i - z_j)}{\vartheta_1(z_i - z_j)}|ij\rangle_1\right)\prod_{i<j}\vartheta_1(z_i - z_j)$$

There are three states with even spin structure $\alpha = (0,0)$, $(1/2,0)$, and $(0,1/2)$
$\longrightarrow$ groundstate is triple-degenerate!
Moreover, the wave-function is translation invariant under

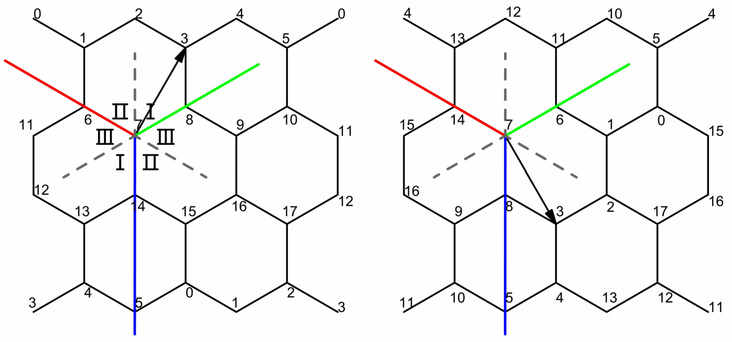
$$z_i \mapsto z_i + m\mathbf{a}_1 + n\mathbf{a}_2 \quad \forall\ i.$$

$\longrightarrow$ physical reason for projection onto translation invariant states in the RBM!

Recall the Kitaev Hamiltonian

$$H = -\sum_{\text{x links}} \sigma_i^x \sigma_j^x - \sum_{\text{y links}} \sigma_i^y \sigma_j^y - \sum_{\text{z links}} \sigma_i^z \sigma_j^z - K \sum_{(i,j,k)} \sigma_i^x \sigma_j^y \sigma_k^z$$

$\longrightarrow$ invariant under simultaneous permutation of x-, y-, and z-links as well as a permutation of the Pauli matrices. While we identified the second operation as the action of the $\hat{U}_{C_6}$-operator, the first one is the $\hat{C}_6$-operator.
For a 3×3 lattice the action is given by:



Thus we see that $\hat{C}_6$-operator permutes sites clockwise by 120 degrees. As an action on the difference of site-coordinates, it has the following representation:

$$\hat{C}_6(z_i - z_j) = e^{2\pi i/3}(z_i - z_j) = (\tau - 1)(z_i - z_j)$$

where $\tau = e^{i\pi/3}$ is the complex structure of the 3×3 lattice with periodic boundary conditions.
But this is nothing else than a modular transformation:

$$\begin{aligned} & \vartheta[\alpha](\tau, (\tau-1)(z_i - z_j) = \vartheta \begin{bmatrix} \epsilon \\ \epsilon' \end{bmatrix} (\tau, (\tau-1)(z_i - z_j)) \\ = \quad & \kappa\left([\alpha], \gamma\right)^{-1} (\tau - 1)^{-\frac{1}{2}} e^{-i\pi \frac{(z_i - z_j)^2}{\tau - 1}} \vartheta \begin{bmatrix} -\epsilon - \epsilon' - 1/2 \\ \epsilon \end{bmatrix} \left(-\frac{1}{\tau - 1}, z_i - z_j \right) \\ = \quad & \kappa\left([\alpha], \gamma\right)^{-1} (\tau - 1)^{-\frac{1}{2}} e^{-i\pi \frac{(z_i - z_j)^2}{\tau - 1}} \vartheta \begin{bmatrix} -\epsilon - \epsilon' - 1/2 \\ \epsilon \end{bmatrix} (\tau, z_i - z_j). \end{aligned}$$

giving

$$\hat{C}_6 \frac{\vartheta[\alpha](\tau, z_i - z_j)}{\vartheta_1(\tau, z_i - z_j)} = \kappa([\alpha], \gamma)^{-1} \kappa\left(\begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}, \gamma \right) \frac{\vartheta[\beta](\tau, z_i - z_j)}{\vartheta_1(\tau, z_i - z_j)}$$

$$\alpha = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \to \beta = \begin{bmatrix} 1/2 \\ 0 \end{bmatrix}, \quad \alpha = \begin{bmatrix} 1/2 \\ 0 \end{bmatrix} \to \beta = \begin{bmatrix} 0 \\ 1/2 \end{bmatrix}, \quad \alpha = \begin{bmatrix} 0 \\ 1/2 \end{bmatrix} \to \beta = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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Summary and Outlook

- The Kitaev Honeycomb model is a spin lattice model admitting topological order.
- It has a topological sector where it supports Ising anyons with non-Abelian braiding statistics.
- We construct the eigen-wavefunctions of the Hamiltonian using a Restricted Boltzmann machine,
- find the lowest energy eigenstate using stochastic gradient descent,
- built excited states using vortex pairs,
- identify the groundstates with certain conformal blocksof the Ising model on the torus involving ψ-fields.
- Our Ansatz has the right symmetries of the Hamiltonian which can be shown using modularity.
- In future: plan to extend our map to conformal blocks to excited states using σ-fields

Thank you!