



The Kitaev Honeycomb lattice

and some numerical observations

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Overview

- o Theory
 - The model
 - Vortices and Fermions
 - Spectral Properties phase diagram
- o Numerical
 - Sparse representations
- o Results
 - Toral hexagonal lattice structures
 - Spectral Phase diagrams
- o Future work
 - ICHEC
 - Larger Lattice systems

The Model

 Hexagonal lattice system with spin exchange parameter dependent on direction



Anyons in an exactly solvable model and beyond, A. Kitaev, cond-mat/0506438

The Model

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$$H = -J_{xx} \sum_{xx-links} \sigma_{j}^{x} \sigma_{k}^{x} - J_{yy} \sum_{yy-links} \sigma_{j}^{y} \sigma_{k}^{y} - J_{zz} \sum_{zz-links} \sigma_{j}^{z} \sigma_{k}^{z}$$

o Plaquette operators

$$W_p = \sigma_1^z \sigma_2^y \sigma_3^x \sigma_4^z \sigma_5^y \sigma_6^x$$

with eigenvalues [-1,1].

 In the quasi-particle description to be described later we will call the -1 state a vortex and the +1 state vortex free. The vortices display anyonic statistics.



Anyons in an exactly solvable model and beyond, A. Kitaev, cond-mat/0506438

Vortices

 Commutes with Hamiltonian and therefore can be simultaneously diagonalised

 $[W_p,H]=0$

 Any Energy eigenstate has expectation value

 $w_{p} = \left\langle E_{n} \left| W_{p} \right| E_{n} \right\rangle = \pm 1$

 This allows us to split the Hilbert space into sectors labelled by a fixed configuration of plaquette eigenvalues.

$$L = \bigoplus_{w_{1,\ldots,w_{m}}} L_{w_{1,\ldots,w_{m}}}$$



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Vortex free sector



The Fermionic picture

- It is possible to map this spin ½ model to a free majorana fermionic picture. (Jordan-Wigner Transformation)
- Represent each spin with 2 fermionic modes $a_1 \& a_2$ so that the no-fermion state represents a spin up and 2-fermion state represents a spin down.



 Majorana fermions are defined as the 'real' and 'imaginary' parts of the fermionic creation and annihilation operators in the following way

$$c_{2k-1} \equiv a_k + a_k^+ \qquad \qquad c_{2k} \equiv \frac{a_k - a_k^+}{i}$$

• They are Hermitian and satisfy the relations

$$c_i = c_i^+ \qquad \{c_{i,j}c_{j,j}\} = 2\delta_{ij}$$

The Fermionic picture

• There are 4 Majorana operators corresponding to each spin

$$c_{1} = a_{1} + a_{1}^{+} = b^{x} \qquad c_{3} = a_{2} + a_{2}^{+} = b^{z}$$
$$c_{2} = \frac{a_{1} - a_{1}^{+}}{i} = b^{y} \qquad c_{4} = \frac{a_{2} - a_{2}^{+}}{i} = c$$

 \circ We need to be able to project the full 4-D space of states L of the 2 fermions back to the physical space of the spin states L .

• This is done with the 'projection' operator

$$D = -b^{x}b^{y}b^{z}c$$
 where $|\psi\rangle \in L \Leftrightarrow D|\psi\rangle = |\psi\rangle$

and

$$\tilde{\sigma}^x = ib^x c$$
 $\tilde{\sigma}^y = ib^y c$ $\tilde{\sigma}^z = ib^z c$

represent the Pauli spin operators on this extended space





The Fermionic picture

Matrix representation: $a_1 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ $a_2 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

• 4 Majorana operators $b^{x_i} b^{y_i} b^z$, c:

$$b^{x} = -\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \quad b^{y} = \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & i \\ 0 & -i & 0 & 0 \end{bmatrix} \quad b^{z} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad c = \begin{bmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix}$$

• Stabilizer $D = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Quadratic Hamiltonian

o Recall that

$$H = -J_{x} \sum_{xx-links} \sigma_{j}^{x} \sigma_{k}^{x} - J_{y} \sum_{yy-links} \sigma_{j}^{y} \sigma_{k}^{y} - J_{z} \sum_{zz-links} \sigma_{j}^{z} \sigma_{k}^{z}$$

 The diagonalization of the Hamiltonian is re-expressed as the diagonalization of

 $H(\sigma_j^{\alpha}) = H(\{ib_j^{\alpha}c_j\})$

accompanied by the constraint $D_j |\psi\rangle = |\psi\rangle$.

• Using this transformation we have $\sigma_j^{\ \alpha}\sigma_k^{\ \alpha} = -i\hat{u}_{jk}c_jc_k$ with $\hat{u}_{jk} = ib_j^{\ \alpha}b_k^{\ \alpha}$ to finally obtain

$$\widetilde{H} = \frac{i}{4} \sum_{j,k} \widehat{A}_{j,k} c_j c_k \quad \text{where} \quad \widehat{A}_{j,k} = \begin{cases} 2J_{\alpha} \widehat{u}_{j,k}, \\ 0, \end{cases} \quad \text{otherwise.} \end{cases}$$

Quadratic Hamiltonian

- The operators \hat{u}_{jk} commute with the Hamiltonian and with each other.
- Similarly to before we use these to break the space up into sectors
 ~ ~

$$\widetilde{L}=\bigoplus_{u}\widetilde{L}_{u}$$

• To restrict the Hamiltonian to the sector we want we replace the operators by the eigenvalues by 'removing hats' to get

$$\widetilde{H} = \frac{i}{4} \sum_{j,k} A_{j,k} c_j c_k$$

• This type of Hamiltonian can be solved exactly. In fact, so can any Hamiltonian that can be written as

$$H = \sum_{jk} \left(\alpha_{jk} a_j a_k^{+} + \alpha_{jk}^{*} a_j^{+} a_k + \beta_{jk} a_j a_k + \beta_{jk}^{*} a_j^{+} a_k^{+} \right)$$

Lieb, Schultz and Mattis, Annals of Physics, 16, pages 407-466 (1961)

Spectral Properties

• Discrete or gapped spectrum implies local excitations

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





Spectral Properties





• Examine finite size effects of the spectrum of the system without external magnetic field.



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- Study (B) phase with external magnetic field beyond the perturbative limit.



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- Isolate and examine non-abelian anyons.



- Examine finite size effects of the spectrum of the system without external magnetic field.
- Study (B) phase with external magnetic field beyond the perturbative limit.
- Isolate and examine non-abelian anyons.
- Examine phase-transition between abelian (A) and non-abelian phase (B).



$$H = -J_{x} \sum_{xx-links} \sigma_{j}^{x} \sigma_{k}^{x} - J_{y} \sum_{yy-links} \sigma_{j}^{y} \sigma_{k}^{y} - J_{z} \sum_{zz-links} \sigma_{j}^{z} \sigma_{k}^{z} + \sum_{n} B_{x} \sigma_{n}^{x} + B_{y} \sigma_{n}^{y} + B_{z} \sigma_{n}^{z}$$

External Magnetic Field

• Spin Hamiltonian can be represented as sparse Matrix, e.g.



 Lower energy eigensolutions via the ARPACK library with LAW (Linear Algebra Wrapper) library to perform matrix multiplication



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- Choose valid lattice configuration and label lattice sites







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Hardware

- Currently calculating jobs for 20 and 24 and 28 spin lattice configurations
- Hamilton is a shared memory machine belonging to ICHEC (Irish Centre for High-End Computing),
- 32 Intel Itanium 2 processors and 256GB of RAM.



Hardware

- Plans to write code that will run on a distributed memory cluster.
- o Walton has
 - 948 AMD Opteron cpus.
 - 2.1 TB memory.
 - 474 separate servers connected with gigabit Ethernet.
- This would allow > 32 spins to be analysed.





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