The Kitaev model

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Outline

- Kitaev model and motivations for studying it

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- Mapping spin-1/2's to Majorana fermions

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- Large-S model and spin wave theory

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- Effects of quenching
- Large-S model and spin wave theory
- Outlook

Kitaev model

Kitaev, Ann. Phys. 321 (2006) 2

Some observations:

- A two-dimensional quantum spin model which is completely solvable
- Reduces to a problem of non-interacting Majorana fermions
- Excitations have Abelian or non-Abelian statistics
- Model has topological order

Majorana fermions

A Majorana fermion operator m is one which anticommutes with all other fermion operators and is Hermitian. We can normalize it so that $m^2 = 1$

Two different Majorana operators satisfy $\{m_1, m_2\} = 0$

Two such operators can be combined to give a single Dirac fermion operator:

$$d = \frac{1}{\sqrt{2}}(m_1 + i\,m_2) \quad \text{and} \quad d^\dagger = \frac{1}{\sqrt{2}}(m_1 - i\,m_2)$$

so that $d^2 = d^{\dagger 2} = 0$ and $\{d, d^\dagger\} = 1$

If the operators m_1 and m_2 are associated with widely separate points, so that the interaction between the Majoranas is negligible, then it is very difficult to disturb a state which contains a single Dirac fermion $d^\dagger d = 1$

To manipulate that Dirac fermion, one might try to couple an external field operator $\phi(\vec{r})$ to $d^\dagger d = 1 + i m_1 m_2.$
But it is difficult to have a term like this since it is non-local

Majorana fermions $\cdots$

Majorana fermions separated by large distances from each other provide a robust way of storing information

They may occur in certain situations such as in a fractional quantum Hall system with filling fraction equal to $5/2,$ at the core of half-vortices in layered $p-$wave superconductors (such as Sr_2RuO_4), at the interface of a ferromagnetic insulator and a superconductor on the surface of a topological insulator, and perhaps in $p-$wave condensates of spin-polarized ^{40}K and ^{6}Li atoms in optical traps

Read and Green, Phys. Rev. B 61 (2000) 10267;
Ivanov, Phys. Rev. Lett. 86 (2001) 268;
Stern, von Oppen and Mariani, Phys. Rev. B 70 (2004) 205338;
Tewari, Zhang, Das Sarma, Nayak and Lee, Phys. Rev. Lett. 100 (2008) 027001

Majorana fermions $\cdots$

Spin-1/2's can be written in terms of Majorana fermions in many ways, all of which satisfy the anticommutation relations at the same site j and the commutation relations between different sites j and k

- Can use three Majorana fermions (Shastry) to write $\sigma_j^x = - i b_j^y b_j^z$, $\sigma_j^y = - i b_j^z b_j^x$ and $\sigma_j^z = - i b_j^x b_j^y$, where the b_j^a are Majorana fermions

- Can use four Majorana fermions (Kitaev) to write $\sigma_j^x = i c_j c_j^x$, $\sigma_j^y = i c_j c_j^y$ and $\sigma_j^z = i c_j c_j^z$, where the c_j and c_j^a are Majorana fermions, and the physical states are those which satisfy $c_j c_j^x c_j^y c_j^z = 1$

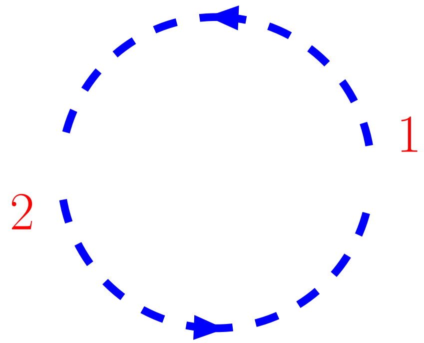
Both these representations increase the dimension of the Hilbert space, giving some redundant states

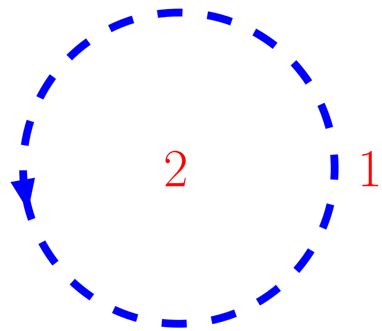
This is the route Kitaev used to solve his model. We will follow a different route which involves Majorana fermions but does not introduce any redundant states

Feng, Zhang and Xiang, Phys. Rev. Lett. 98 (2007) 087204; Lee, Zhang and Xiang, Phys. Rev. Lett. 99 (2007) 196805; Chen and Nussinov, J. Phys. A 41 (2008) 075001

Quantum statistics

In quantum mechanics, statistics refers to the change of the wave function of two particles when they are exchanged (for identical particles), or when one is taken around the other in a loop in two dimensions (for any two particles)





If the wave function has only component and it picks up a phase under the above processes, the statistics is called Abelian

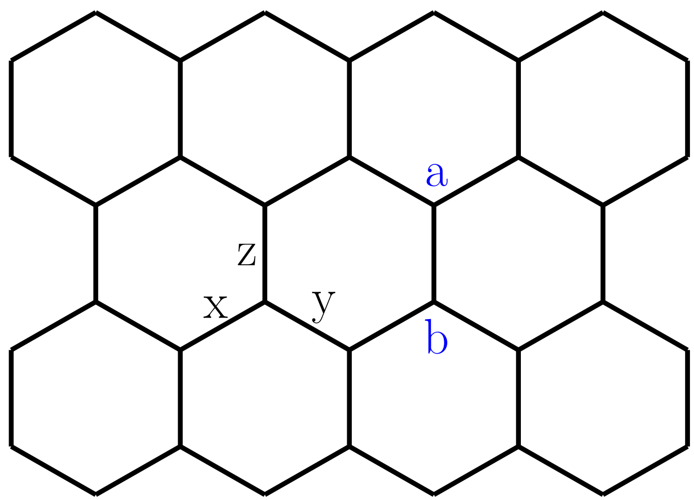
If the wave function has n components and it gets multiplied by a $n \times n$ unitary matrix under the above processes, and the unitary matrices for different pairs of particles do not commute with each other, the statistics is called non-Abelian. This is more robust since finite-dimensional matrices satisfying some group properties are more tightly constrained than phases

Kitaev model

The model has spin-1/2's on a honeycomb lattice, with highly anisotropic couplings between nearest neighbors. The Hamiltonian is

$$H = \sum_{j+l=\text{even}} \left(J_1\, \sigma^x_{j,l}\sigma^x_{j+1,l} + J_2\, \sigma^y_{j-1,l}\sigma^y_{j,l} + J_3\, \sigma^z_{j,l}\sigma^z_{j,l+1} \right)$$

Can assume that all couplings $J_i \geq 0$



Jordan-Wigner transformation

The Kitaev model can be solved exactly by mapping it to Majorana fermions by a Jordan-Wigner transformation, even though it is a model in two dimensions

$$a_{\vec{n}} = \left[\prod_{\vec{m}=-\infty}^{\vec{n}-1} \sigma^z_{\vec{m}} \right] \sigma^y_{\vec{n}} \; (\sigma^x_{\vec{n}}) \text{ for even (odd) numbered chains,}$$

$$b_{\vec{n}} = \left[\prod_{\vec{m}=-\infty}^{\vec{n}-1} \sigma^z_{\vec{m}} \right] \sigma^x_{\vec{n}} \; (\sigma^y_{\vec{n}}) \text{ for even (odd) numbered chains,}$$

depending on whether $\vec{n}$ lies on the A or B sub-lattice

These operators satisfy the anticommutation relations

$$\{ a_{\vec{m}} , a_{\vec{n}} \} = \{ b_{\vec{m}} , b_{\vec{n}} \} = 2\, \delta_{\vec{m}\vec{n}}, \text{ and } \{ a_{\vec{m}} , b_{\vec{n}} \} = 0$$

The string of $\sigma^z_{\vec{m}}$'s is chosen to go along the x and y bonds, towards the right (left) on even (odd) numbered chains

Jordan-Wigner transformation

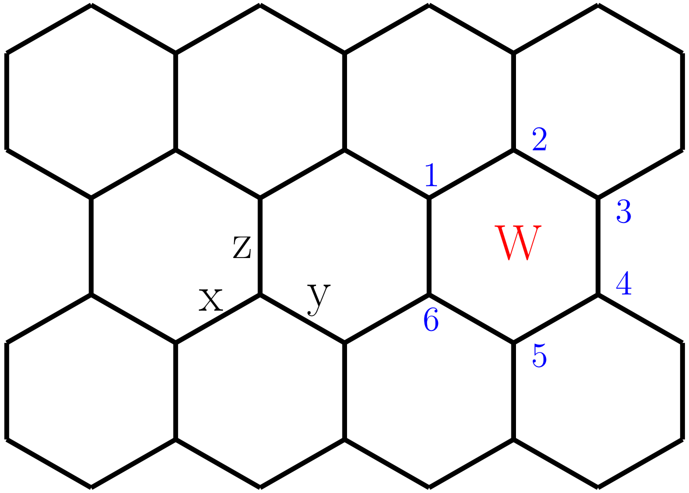
$$H = \sum_{j+l=\mathrm{even}} \left(J_1\, \sigma^x_{j,l}\sigma^x_{j+1,l} + J_2\, \sigma^y_{j-1,l}\sigma^y_{j,l} + J_3\, \sigma^z_{j,l}\sigma^z_{j,l+1} \right)$$

The xx and yy interactions become local and quadratic in the Majorana fermions under the Jordan-Wigner transformation

The zz interaction would normally become non-local and quartic in the fermions

But in this model, this remains local and only couples fermions on nearest neighbor sites due to a large number of conserved quantities

Conserved quantities



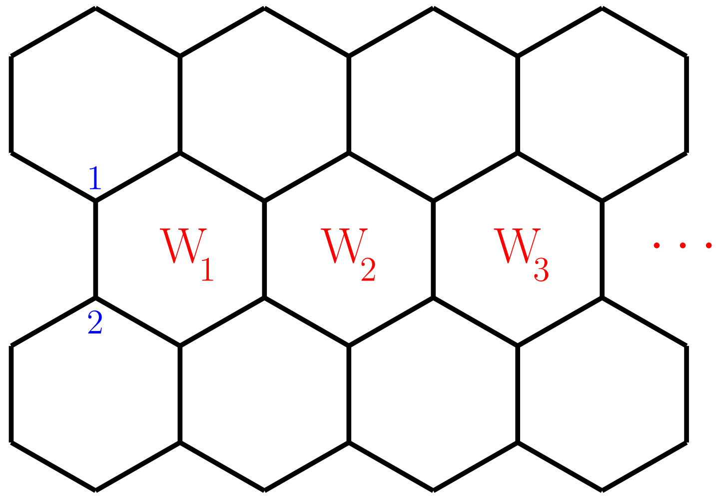
The model has a conserved quantity W associated with each hexagon:

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

Hence there are $2^{N/2}$ decoupled sectors corresponding to the values of $W = \pm 1$ in the $N/2$ different hexagons (the number of sites is N)

Because of these conserved quantities, the zz interactions become local in terms of the Majorana fermions

Kitaev model $\cdots$



If $1/2$ lies on an even/odd numbered chain, then $\sigma_1^z \sigma_2^z \sim a_1 \, b_1 \, W_1 \, W_2 \, W_3 \, \cdots$

In any particular sector with some given values of W_i, the zz interaction reduces to a product of two fermion operators. The ground state turns out to lie in a sector in which all the $W_i = 1$. In that sector, we find that

$$H = i \sum_{\vec{n}} \left[J_1 \, b_{\vec{n}} \, a_{\vec{n}-\vec{M}_1} + J_2 \, b_{\vec{n}} \, a_{\vec{n}+\vec{M}_2} + J_3 \, b_{\vec{n}} \, a_{\vec{n}} \right],$$

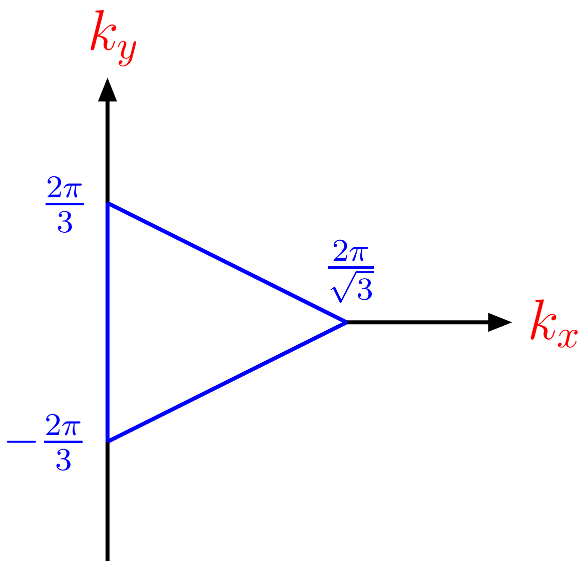
where $\vec{M}_1 = \frac{\sqrt{3}}{2}\hat{i} + \frac{3}{2}\hat{j}$ and $\vec{M}_2 = \frac{\sqrt{3}}{2}\hat{i} - \frac{3}{2}\hat{j}$

Brillouin zone

Define the Fourier transforms

$$a_{\vec{n}} = \sqrt{\frac{4}{N}} \sum_{\vec{k}} [\, a_{\vec{k}}\, e^{i\vec{k}\cdot\vec{n}} + a^{\dagger}_{\vec{k}}\, e^{-i\vec{k}\cdot\vec{n}}\,],$$
$$b_{\vec{n}} = \sqrt{\frac{4}{N}} \sum_{\vec{k}} [\, b_{\vec{k}}\, e^{i\vec{k}\cdot\vec{n}} + b^{\dagger}_{\vec{k}}\, e^{-i\vec{k}\cdot\vec{n}}\,],$$

where $\vec{k}$ runs over only half the Brillouin zone which looks as follows:



Hamiltonian

The Hamiltonian of the Kitaev model is

$$
\begin{aligned}
H &= \sum_{\vec{k}} \begin{pmatrix} a^{\dagger}_{\vec{k}} & b^{\dagger}_{\vec{k}} \end{pmatrix} H_{\vec{k}} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}, \\
H_{\vec{k}} &= 2\left[J_3 \;+\; J_1 \cos(\vec{k}\cdot\vec{M}_1) \;+\; J_2 \cos(\vec{k}\cdot\vec{M}_2)\right]\sigma^3 \\
&\quad + 2\left[J_1 \sin(\vec{k}\cdot\vec{M}_1) \;-\; J_2 \sin(\vec{k}\cdot\vec{M}_2)\right]\sigma^1,
\end{aligned}
$$

where $\vec{M}_1 = \frac{\sqrt{3}}{2}\hat{i} + \frac{3}{2}\hat{j}$ and $\vec{M}_2 = \frac{\sqrt{3}}{2}\hat{i} - \frac{3}{2}\hat{j}$

This is a system of non-interacting Majorana fermions

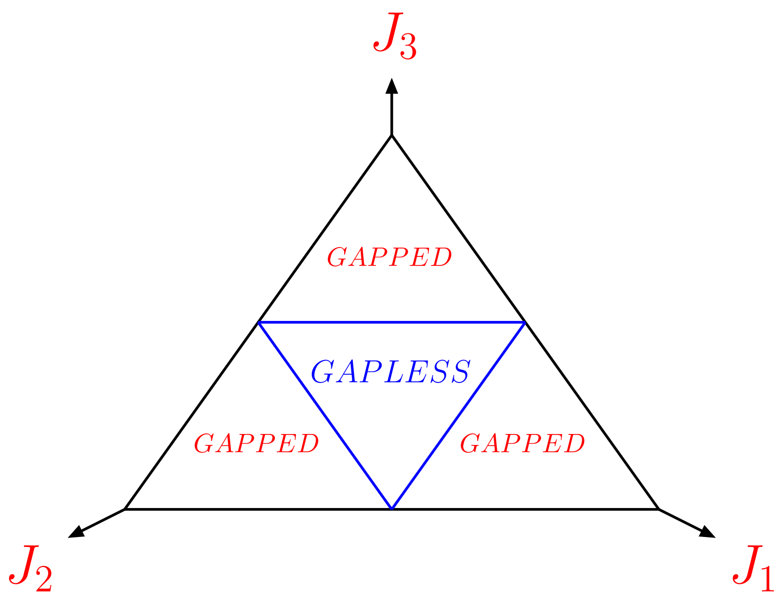
Depending on the values of $J_1,\; J_2,\; J_3,$ there may or may not be a gap between the ground state and the first excited state

Phase diagram of Kitaev model

If $J_1 < J_2 + J_3, \quad J_2 < J_3 + J_1$ and $J_3 < J_1 + J_2,$ the system is gapless at one value of $(k_x, k_y),$ with a massless Dirac spectrum around that point: $E \; = \; \pm \; v \sqrt{\delta k_x^2 \; + \; \delta k_y^2}$

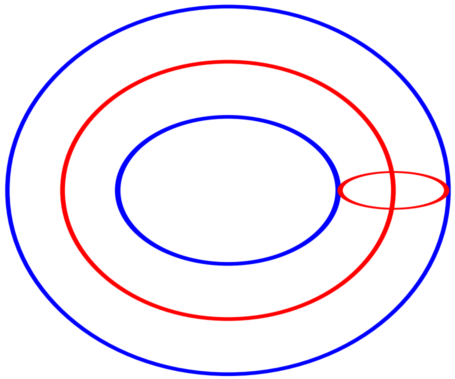
For all other values of $(J_1, \; J_2, \; J_3),$ the system is gapped

The phase diagram can be shown in terms of points in an equilateral triangle satisfying $J_1 \; + \; J_2 \; + \; J_3 \; = \; 1$ (the value of J_i is the distance from the opposite side)



Topological order

On the surface of a torus, in the thermodynamic limit, the energy spectrum is independent of the product of the W_i along the two loops shown in red



The two loop variables can take the values ± 1 independently.
Hence all energy levels have a degeneracy of 4

This is a signature of topological order

Recall: fractional quantum Hall states also have topological order. On a surface of genus g, ($g = 0$ and 1 for a sphere and a torus respectively), the ground state for a quantum Hall state with filling fraction $1/3$ has a degeneracy of 3^g

Quantum statistics

Back to the Kitaev model on the plane: the ground state lies in the sector in which all the hexagonal quantities $W_i = 1.$ This is called a vortex-free state

If $W_i = -1$ on any hexagon, it is called a vortex. The lowest energy state in a sector with one vortex is separated from the ground state by a finite gap; this is true in all the phases. The fermionic spectra can be gapped or gapless

In the gapped phases, the different particles (fermions and vortex) have Abelian statistics. Taking any particle around any other, or exchanging two identical particles, only multiplies the wave function by $\pm\ 1$

Difficult to discuss statistics for a gapless system as exchanging two particles or taking one around the other produces low-energy excitations no matter how slowly the exchange is done, so the initial and final states are quite different

Adding a magnetic field at each site, $\sum_i\ (h_x \sigma_i^x\ +\ h_y \sigma_i^y\ +\ h_z \sigma_i^z),$
produces a gap, and makes it possible to discuss statistics.
It also allows a vortex to move from one hexagon to another
since the W_i do not commute with the magnetic field term

Quantum statistics $\cdots$

Taking a fermion around a vortex gives a phase factor of -1

But taking one vertex around another produces non-Abelian statistics which is described by the fusion rules of the conformal field theory of the Ising model in two dimensions

If $1,$ ϵ and σ denote the vacuum, Majorana fermion and vortex operators respectively, then the fusion rules are given by

$$\epsilon \times \epsilon = 1, \quad \epsilon \times \sigma = \sigma, \quad \sigma \times \sigma = 1 + \epsilon$$

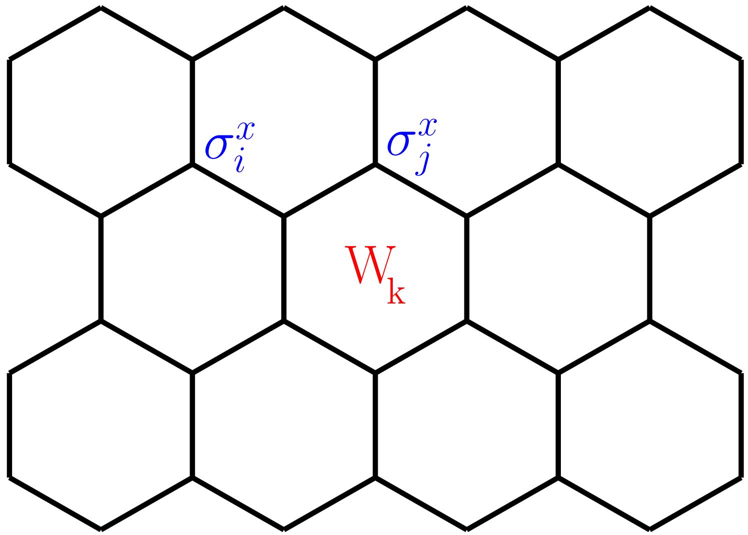
These relations describe various coalescing and splitting processes, and they can also be used to find what happens when two particles are exchanged (if they are identical) or if one is taken around the other

The fact that the last fusion rule is the sum of two terms means that we need a two-dimensional wave function to describe a state with two vortices, and the exchange of two vortices changes the wave function by a unitary matrix

Spin correlation functions

Consider the two-spin correlation function $\langle \sigma_i^a \sigma_j^b \rangle$ in some eigenstate of the Kitaev Hamiltonian H

If i and j are not nearest neighbors, one can find a hexagon invariant W_k which commutes with σ_i^a and anticommutes with σ_j^b



Here W_k anticommutes with σ_j^x because W_k contains the term σ_j^z

Spin correlation functions $\cdots$

Since we can choose every eigenstate of H to also be an eigenstate of W_k, with eigenvalue ± 1, we have
$\langle \sigma_i^a \sigma_j^b \rangle = \langle W_k \sigma_i^a \sigma_j^b W_k \rangle = \langle \sigma_i^a W_k \sigma_j^b W_k \rangle = - \langle \sigma_i^a \sigma_j^b \rangle$,
which implies that $\langle \sigma_i^a \sigma_j^b \rangle = 0$

A similar argument shows that if i and j are nearest neighbors, and the bond joining them has, say, an xx interaction, then $\langle \sigma_i^a \sigma_j^b \rangle = 0$ if either a or b is different from x

Thus, $\langle \sigma_i^a \sigma_j^b \rangle \neq 0$ only if i and j are nearest neighbors and $a = b$ is equal to the type of bond which joins i and j

Thus the two-spin correlation functions are extremely short-ranged and of a very special type

Baskaran, Mandal and Shankar, Phys. Rev. Lett. 98 (2007) 247201

Spin correlation functions $\cdots$

We can also consider correlation functions in time

In the gapless phase, the ground state correlation functions fall off as powers:

$$\langle 0|\sigma_i^a(t)\sigma_{i'}^{a'}(0)|0\rangle \ \sim \ \frac{1}{t^\alpha}$$

for large times t if $i,\ i'$ and $a,\ a'$ satisfy the constraints discussed before, and

$$\langle 0|\sigma_i^a(t)\sigma_{i'}^{a'}(t)\sigma_j^b(0)\sigma_{j'}^{b'}(0)|0\rangle \ \sim \ \frac{1}{(t^2 \ + \ |i-j|^2)^2}$$

if $t^2 \ + \ |i-j|^2$ is large

Spin correlation functions $\cdots$

Instead of considering correlation functions of spins, we can consider correlations of the Majorana fermions. In general, these will involve correlations of spins with strings of σ_i^z joining them

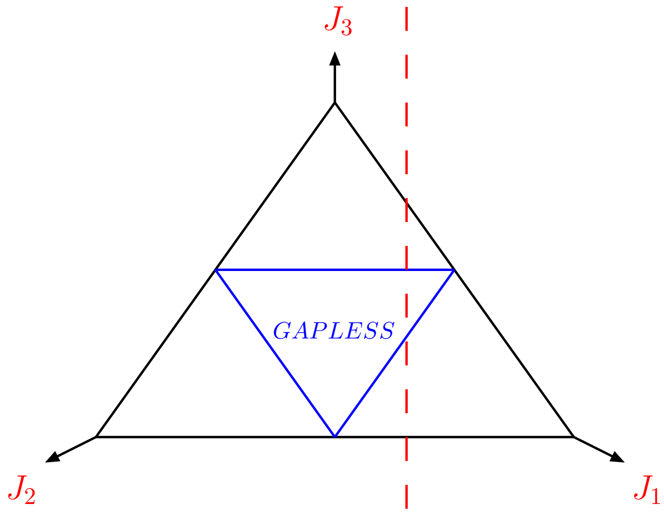
We can consider expectation values of an operator like $O_{\vec{r}} \;=\; i\, a_{\vec{n}}\, b_{\vec{n}+\vec{r}}$. This commutes with all the hexagon invariants W_i, otherwise its expectation value would be zero. In the gapless phase, we again expect this value to fall off as a power for large $\vec{r}$

One of our studies involved looking at these correlations and how they vary if the coupling parameters J_i change with time

For $J_3 \;\rightarrow\; \pm\; \infty$, nearest-neighbor spins form Ising antiferromagnetic (ferromagnetic) dimers on the vertical (zz) bonds. These correspond to $\langle O_{\vec{r}} \rangle \;=\; \pm\; \delta_{\vec{r},\vec{0}}$

Quenching in the Kitaev model

Let us hold $J_1,\ J_2$ fixed, and vary J_3 in time as $Jt/\tau,$ from $t = -\infty$ to $t = \infty$ (as shown by the red dotted line). Then the system will pass through the gapless region for some time

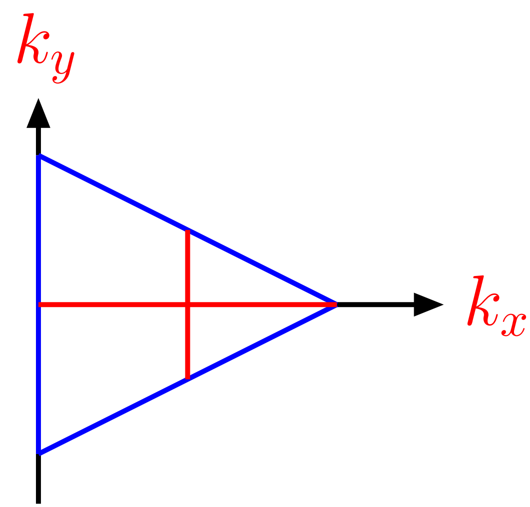


We expect that if we start with the ground state of the system at $t \to -\infty$ and the variation of J_3 is adiabatic, i.e., $\tau \to \infty$, then we will end up with the ground state of the system at $t \to \infty$. The question is, how close do we get to the final ground state if τ is large but not infinite?

Sengupta, Sen and Mondal, Phys. Rev. Lett. 100 (2008) 077204;
Mondal, Sen and Sengupta, Phys. Rev. B 78 (2008) 045101

Scaling of defect density

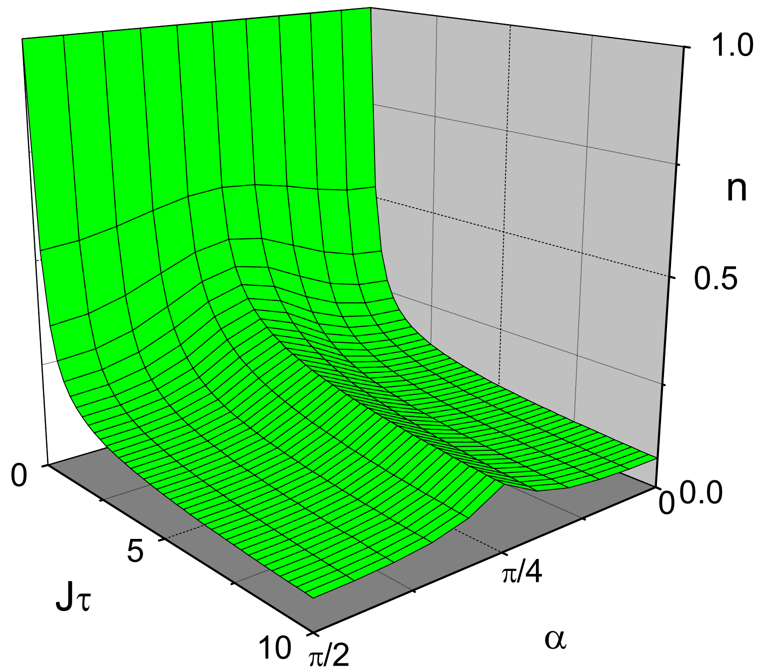
As J_3 is varied through the gapless region, the energy of the low-lying excitations typically vanishes on some lines in half the Brillouin zone as indicated in red



Using the Landau-Zener result for the transition probability from the ground state to the excited state of a two-level system, we showed that the quenching produces defects in the final state (i.e., deviations from the ground state) whose density scales as $n \sim 1/\sqrt{\tau}$

The reason that $n \to 0$ as a power of τ rather than exponentially is that we are passing through a gapless region. So no matter how large τ is, there are states with sufficiently low energies $(\Delta E \lesssim 1/\tau)$ which get excited

Plot of defect density



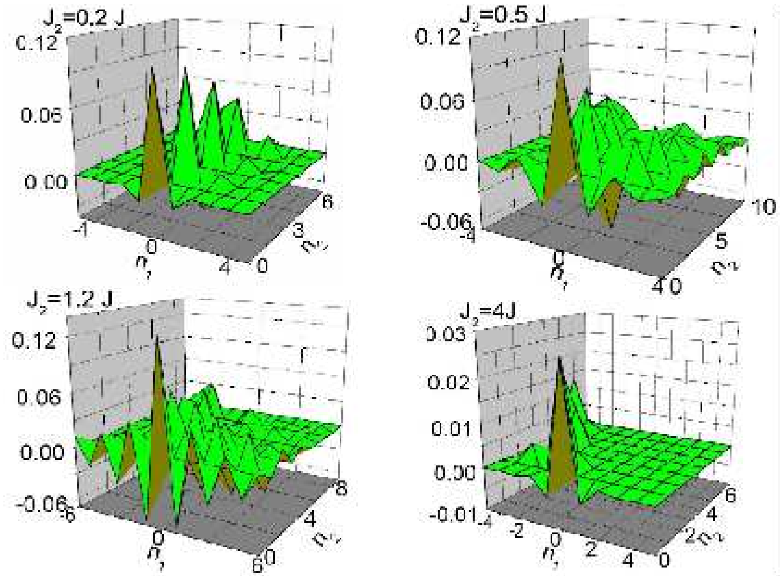
n versus $J\tau$ and $\alpha = \tan^{-1}(J_2/J_1)$

The defect density is maximum when $\alpha = \pi/4,$ i.e., when $J_1 = J_2$ because this is when the system stays in the gapless phase for the longest time

Defect correlation functions

We can compute the correlation function $\langle O_{\vec{r}} \rangle$, where $O_{\vec{r}} = i b_{\vec{0}} a_{\vec{0}+\vec{r}}$ and
$\vec{r} = \sqrt{3}(n_1 + n_2/2)\,\hat{x} \; + \; (3n_2/2)\,\hat{y}$

This gives an idea of the ‘shape’ and ‘size’ of the defects



Plot of $\langle O_{\vec{r}} \rangle$ versus $\vec{r}$ for several values of J_2/J_1 for $J\tau = 5$

The ‘shape’ of the defects changes with J_2/J_1 and the ‘size’ is of the order of $\sqrt{\tau}$

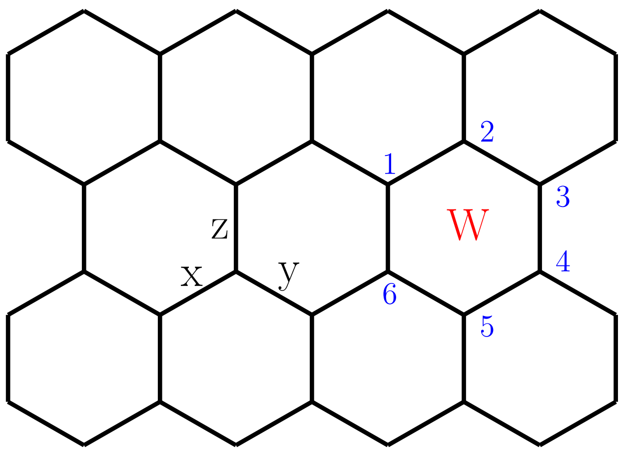
Large-S Kitaev model

Do the various features of the spin-1/2 Kitaev model survive for higher spins?

Baskaran, Sen and Shankar, Phys. Rev. B 78 (2008) 115116

The Hamiltonian is

$$H = \frac{1}{S} \sum_{j+l=\mathrm{even}} (J_1 \, S^x_{j,l} S^x_{j+1,l} + J_2 \, S^y_{j-1,l} S^y_{j,l} + J_3 \, S^z_{j,l} S^z_{j,l+1})$$



The conserved quantities on each hexagon survive:

$$W = e^{i\pi \, (S_1^y + S_2^z + S_3^x + S_4^y + S_5^z + S_6^x)}$$

Large-S Kitaev model $\cdots$

$$H = \frac{1}{S} \sum_{j+l=\mathrm{even}} (J_1 \, S^x_{j,l} S^x_{j+1,l} + J_2 \, S^y_{j-1,l} S^y_{j,l} + J_3 \, S^z_{j,l} S^z_{j,l+1})$$

The most interesting situation arises if $J_1 = J_2 = J_3$

Then there are continuous families of classical ground states, for instance, all the spins on the A sublattice pointing in some direction and all the spins on the B sublattice pointing in the opposite direction

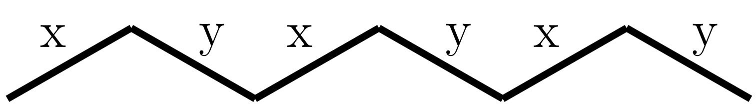
Apart from these continuous families, there is also a discrete set of ground states in which pairs of nearest neighbor spins on, say, a xx bond point along the $\pm \hat{x}$ direction

The number of such discrete states is equal to the number of dimer coverings of the honeycomb lattice which is 1.175^N times 1.414^N (due to the choice of $\pm$), which gives 1.662^N discrete classical ground states

Dimer coverings

Now we consider the correction to the energy at the next order in $1/S$. This is done by looking at the spin wave spectrum around different classical ground states, calculating the zero point energy of the spin waves, and finding the ground state for which this is the minimum

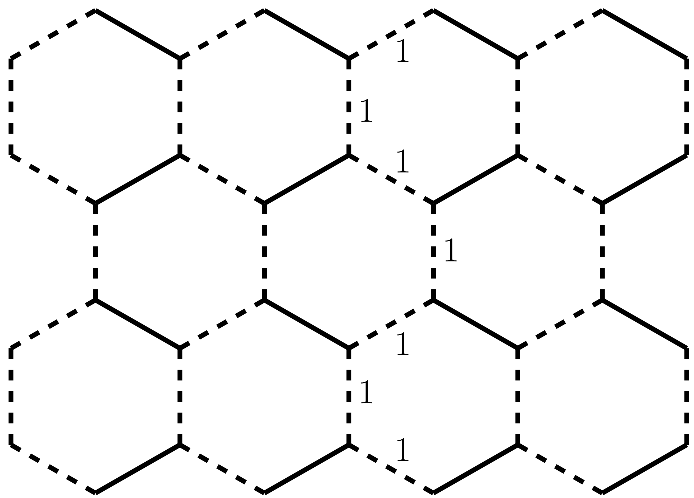
We did this calculation only around the discrete set of classical ground states (the dimer coverings) because a similar calculation for a one-dimensional version of the Kitaev model showed that those have a lower zero point energy than the continuous family of ground states



Classical ground states in which the spins point only along the $\pm\ \hat{x}$ or $\pm\ \hat{y}$ directions have a lower spin wave zero point energy than ground states with spins pointing in other directions

Dimer coverings $\cdots$

For each dimer covering, there is a set of self-avoiding walks (SAWs) covering the lattice such that none of bonds appearing on the SAW is a dimer. For instance, a SAW is shown by 1's below



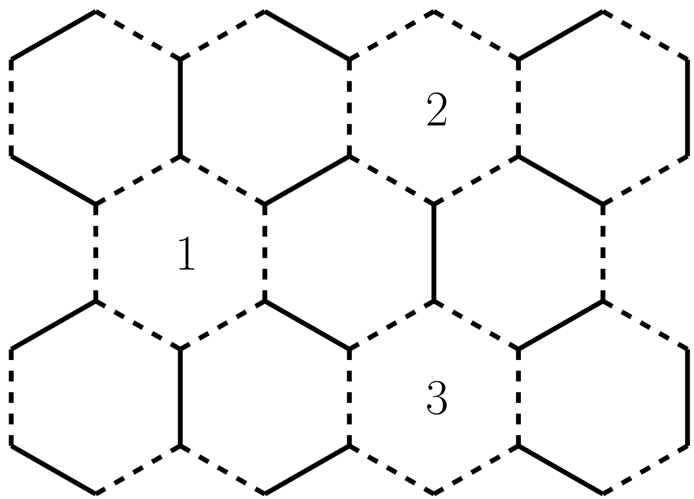
To do a spin wave analysis, we make a Holstein-Primakoff transformation from a large spin to a harmonic oscillator. For a spin pointing in the $\hat{z}$ direction, we define $S^z = S - (p^2 + q^2)/2$, $S^x = \sqrt{S}\, q$ and $S^y = \sqrt{S}\, p$

We then write the spin Hamiltonian up to second order in the p's and q's

Spin wave analysis

We then find that, to this order, there is no interaction between spins lying on different SAWs. Thus we only have to study the spin waves on separate SAWs, each of which can either form an infinitely long chain or a finite closed loop

The zero point energy turns out to be the lowest if all the SAWs are closed loops forming hexagons

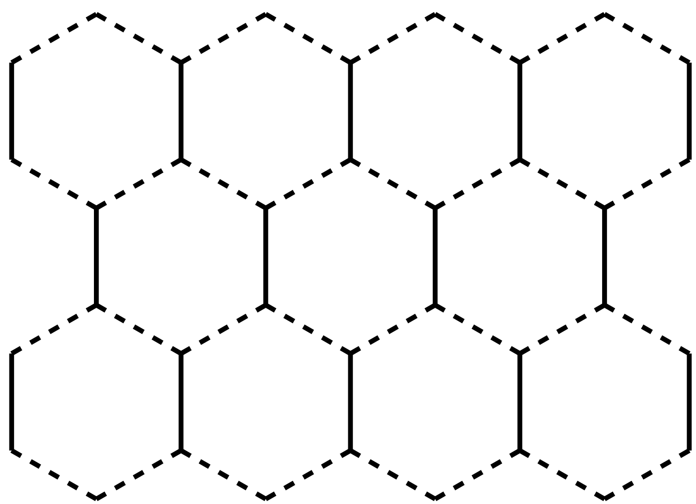


We find that pairs of spins in groups of three dimers can still point in 2 different ways without changing the zero point energy. This gives $2^{N/3} \sim 1.260^N$ different dimer coverings with the same zero point energy. This is still exponentially large although it is smaller than the number of classical ground states $\sim 1.662^N$

Spin wave analysis $\cdots$

$$H = \frac{1}{S} \sum_{j+l=\text{even}} (J_1\, S^x_{j,l} S^x_{j+1,l} + J_2\, S^y_{j-1,l} S^y_{j,l} + J_3\, S^z_{j,l} S^z_{j,l+1})$$

What happens if the three couplings are not equal? If J_3 is larger than the other two, the classical ground states are those in which pairs of spins on each zz bond form antiferromagnetic dimers. The number of such states is $2^{N/2}$ if the number of sites is N



The degeneracy between this discrete set of classical ground states is not broken by the zero point energy of the spin waves

Generalizations of Kitaev model

The Kitaev model involves three anticommuting matrices at each site, and a coordination number of three

This can be extended to a model obtained by replacing each point of the honeycomb lattice by a triangle

Yao and Kivelson, Phys. Rev. Lett. 99 (2007) 247203

or to a lattice in three dimensions

Mandal and Surendran, Phys. Rev. B 79 (2009) 024426

The model can be generalized to have four anticommuting matrices (like the Dirac matrices) at each site, and a coordination number of four such as a square lattice

Yao, Zhang and Kivelson, Phys. Rev. Lett. 102 (2009) 217202

or more complicated lattices

Wu, Arovas and Hung, arXiv:0811.1380

Outlook

Effect of disorder and doping on the Kitaev model

Higher spin Kitaev models: a Jordan-Wigner transformation naturally leads to Majorana fermion operators for half-odd-integer spins and hard core boson operators for integer spins

The spin-1/2 Kitaev chain is completely solvable and is known to be gapless, while preliminary studies of the spin-1 model shows that it has a small gap. The integer spin chain has N conserved quantities while the half-odd-integer spin chain has $N/2$ conserved quantities