Lab Course on Kitaev's Honeycomb Lattice Model: An Exactly Soluble Quantum Spin Liquid

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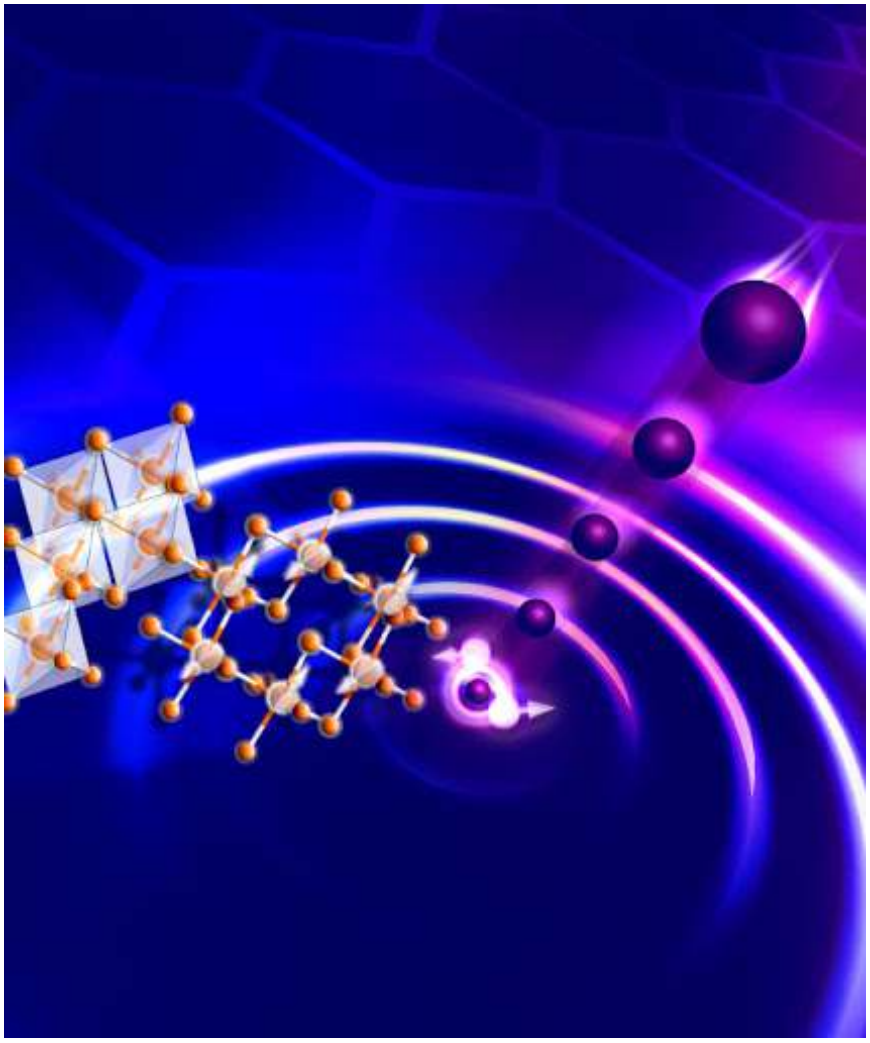

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Title image of the previous page is taken from http://www.sci-news.com /physics/quantum-spin-liquid-new-quantum-state-matter-03754.html

1 Organization and Preliminary Reading

The objective of this Lab Course is to learn about Quantum Spin Liquids (QSL) in frustrated magnets via gaining an in-depth understanding of the celebrated Kitaev honeycomb lattice model [1]. The minimal prerequisites for this Lab Course are the Quantum Mechanics and Statistical Physics lectures but additional experience in the Theory of Phase Transitions and Many-Body Theory are highly beneficial. Note, to carry out the Lab Course you should know and be able to use *second quantization*.

The Lab Course runs over two days. We expect that you go over the preliminary reading before. On the first day, we will start with a discussion of your questions at 9am in Room PHY 3225. Then you will be guided by these notes through the exact solution. There are a number of concrete Problems, which you are supposed to solve during the two days. These are mainly analytical calculations supplemented by basic numerics, e.g via Mathematica (or your preference). Throughout the day there will be time for questions and discussions. At the end, we expect you to compile a protocol with details of the solutions and a summary of your understanding (to be handed in one week after the Lab Course). We will later provide feedback on the protocol.

The goal of the preliminary reading is to familiarise yourself with the basic concept of QSLs. You should address, for example, the following questions: How are QSLs different from long-range ordered magnets? Why are QSL of current research interest? What is the fractionalization of spin quantum numbers? What are the entanglement properties of QSLs and why are they potentially useful for quantum computation? You can find qualitative introductions to Quantum Spin Liquids (QSLs) in Refs. [2, 3]. A longer review, which would take several days to fully read and understand, is Ref. [4]. For this Lab course of particular interest are the sections 1, 2 (especially the Toric code), 3 until 3.5 and the section 4 until 4.4. Note, we do not expect you to fully understand all the technical details but please write down the basic questions which come up in the preparation.

QSLs are strongly correlated quantum phases, which are generically hard to describe theoretically. Traditionally, research has invented a number of approximate mean-field theories for QSLs or elaborate numerical methods, which unfortunately suffer from finite size restrictions. A key development was the advent of exactly soluble models with QSL ground states. The first and most important one is the one studied here – the Kitaev honeycomb lattice model [1]. Its physics is summarised in a number of recent overview articles Refs. [5, 6, 7]. Note, we do not expect you do go over these reviews in detail beforehand as you are going to learn about the technical content in this Lab Course, but we recommend to consult them afterward.

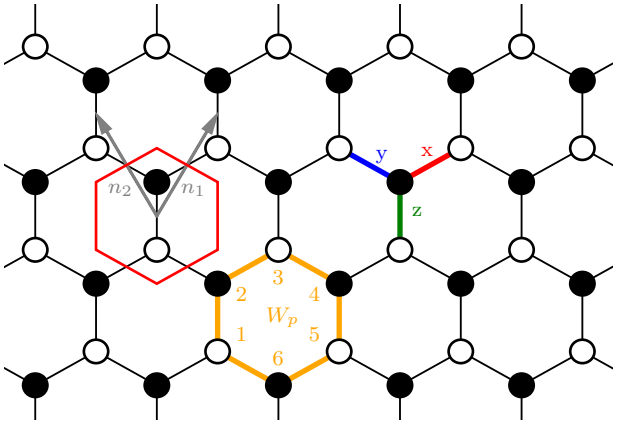

Figure 1: The honeycomb lattice with the 3 inequivalent bond directions x, y, z. The two sublattices A and B have solid and open circles as vertices respectively. The first Brillouin zone is highlighted in red and lattice vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ are drawn in grey. The plaquette operator W_p is highlighted orange.

2 Kitaev's Honeycomb Lattice Model

Kitaev's honeycomb model is one of the rare exactly solvable interacting quantum models in 2D. [1] Nowadays it serves as a representative for a complete class of quantum spin liquids (QSL) where Majorana fermions are coupled to a $\mathbb{Z}_2$ gauge field. [8] The model is defined on a honeycomb lattice which consists of a hexagonal Bravais lattice (lattice vectors $\boldsymbol{n_1} = (\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $\boldsymbol{n_2} = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$) and a two sided unit cell, which also includes three inequivalent bonds x, y and z, see fig. 1. On the vertices of the honeycomb lattice are spin-1/2, interacting via competing nearest-neighbor Ising exchanges, captured by the Hamiltonian

$$H = -K^x \sum_{\text{x-bonds}} \sigma_i^x \sigma_j^x - K^y \sum_{\text{y-bonds}} \sigma_i^y \sigma_j^y - K^z \sum_{\text{z-bonds}} \sigma_i^z \sigma_j^z. \tag{1}$$

The crucial ingredient for the exact solubility is that the direction α of the Ising interaction $\sigma_i^\alpha \sigma_j^\alpha$ is set by the bond type $\alpha = \alpha_{i,j}$, where $\alpha_{i,j}$ is meant to be understood as a function depending on the two neighboring sites i and j and returning the type of bond between them. In the literature the symbol $\langle i, j \rangle_\alpha$ is often used to specify the bond type α between sites i and j. Note, the strong bond-dependence of the Ising interaction is essentially a type of spin-orbit coupling.

Although this seems like a very academic Hamiltonian and not related to any real system, an important research achievement was made in Ref.[9] which established that several materials actually exhibit Kitaev-like interac-

tions and some of them even in leading order. Promising Kitaev candidate materials have strongly correlated electrons with spin orbit coupling. Examples include Iridates and $\alpha-\mathrm{RuCl}_3$, see Refs. [5, 6, 7] for details. Establishing the existence of a (Kitaev) QSL in a material is one of the primary goals in correlated quantum matter research.

Problem 1: Competing Ising exchanges
Find and draw the classical configuration of the ground state in the three limits $(K^x, K^y, K^z) = (1, 0, 0)$, $(K^x, K^y, K^z) = (0, 1, 0)$ *and* $(K^x, K^y, K^z) = (0, 0, 1)$. *Explain why for general couplings the interactions of the Kitaev system are frustrated. Compare this to the isotropic AFM Ising model on the honeycomb and triangular lattice.*

3 Solution and Phase Diagram

The exact solution of the model proceeds in a number of steps, which we will now explain in detail.

3.1 Flux Sectors

The first remarkable observation is that there is a large number of constants of motion in this model. For each plaquette p, the plaquette operator

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z \tag{2}$$

which is the product of all spins along the six corners of the plaquette with their spin components corresponding to the outwards pointing bond direction, commutes with the Hamiltonian and with each other. Therefore they are static. As $W_p^2 = 1$, the eigenvalues are $w_p = \pm 1$. We call these operators flux operators and associate $w_p = +1$ with a flux free plaquette and $w_p = -1$ with a plaquette that has flux, very similar as it is done in the Toric code model.

Problem 2: Flux operators as constants of motion
Show that $[W_p, H] = 0$ *and* $W_p^2 = 1$. *Convince yourself that* $[W_p, W_{p'}] = 0$.

The constants of motion allow to block diagonalize the full Hilbert space $\mathcal{L}$ into smaller flux sectors $\mathcal{L}_{\{w_1,\ldots,w_N\}}$

$$\mathcal{L} = \bigoplus_{\{w_1,\ldots,w_N\}} \mathcal{L}_{\{w_1,\ldots,w_N\}} \tag{3}$$

where $\{w_1, ..., w_N\}$ is a set of numbers determining the flux for each plaquette. In a system with N unit cells and periodic boundary conditions there are $2N$ spins leading to a 2^{2N}-dimensional Hilbert space $\mathcal{L}$. There are 2^N different flux sectors, such that the dimension of each flux sector $\mathcal{L}_{\{w_1,...,w_N\}}$ is 2^N. Observe that each sector still has an exponentially large number of degrees of freedom but it turns out that these can be described by free Majorana fermion excitations.

3.2 Mapping Spins to Majorana Fermions

Majorana fermions b^μ, first proposed in high energy-physics, can be obtained by splitting ordinary complex fermions f_σ into real and imaginary parts

$$\begin{aligned} f_\uparrow &= \frac{1}{2}(b^0 + \mathrm{i}b^3) \\ f_\downarrow &= \frac{1}{2}(\mathrm{i}b^1 - b^2). \end{aligned} \tag{4}$$

Note that while the complex fermions do posses spin, Majorana fermion have four components μ but no spin degree of freedom. Majoranas are also known as real fermions, since $b^{\dagger\mu} = b^\mu$. They fulfill the usual fermionic anticommutation relation $\{b^\mu, b^\nu\} = 2\delta_{\mu,\nu}$.

We can obtain a representation of the spin operators in terms of Majorana fermions, which is better known as "Kitaev's representation of spins"

$$\sigma^\alpha = \mathrm{i}cb^\alpha, \tag{5}$$

where we have defined $b^0 \equiv c$, since in our model it is convenient to have a separate notation for the 0^{th} component of the so called 'matter' Majoranas. It is convenient to think of eq. (5) as a parton description, as you have read it in ref. [4]. A schematic image of this decomposition is given in the left panel of fig. 3.

Problem 3: Majorana representation
Show that Majoranas are indeed fermions, i.e. $\{b^\mu, b^\nu\} = 2\delta_{\mu,\nu}$. *Calculate* $(b^\mu)^2$ *and interpret the result. Using these properties show that Kitaev's representation of spins fulfills the standard spin-*$1/2$ *algebra* $\{\sigma^\alpha, \sigma^\beta\} = 2\delta_{\alpha,\beta}$.

Back to the Kitaev model we continue by representing every spin operator in eq. (1) by two Majorana operators. Note that eq. (5) gets an additional sites index i. The Kitaev Hamiltonian in terms of Majorana fermions reads

$$H = \mathrm{i}\sum_{\alpha,\langle i,j\rangle_\alpha} K_\alpha \hat{u}_{\langle i,j\rangle_\alpha} c_i c_j \quad \text{with bond operators} \quad \hat{u}_{\langle i,j\rangle_\alpha} = \mathrm{i}b_i^\alpha b_j^\alpha. \tag{6}$$

At this point the Kitaev Hamiltonian is still quartic in operators which is generally not soluble.

Remarkably, all bond operators do commute with the Hamiltonian and among each other, therefore they reduce the Hamiltonian to a quadratic form. We can connect the bond operators to the flux operator of eq. (2) by the product of all link variables,

$$W_p = \hat{u}_{2,1}\hat{u}_{2,3}\hat{u}_{4,3}\hat{u}_{4,5}\hat{u}_{6,5}\hat{u}_{6,1} \tag{7}$$

which explains the name flux operators. A particle moving around a plaquette p picks up a phase $w_p = \pm 1$. Note, that many different configurations of the bond operators map to the same flux configuration, which shows that we are dealing with Majoranas coupled to a Z_2 gauge field.

Problem 4: Majorana Fermion Hamiltonian
Here and in the following it is useful to adopt the notation $i \in A$ sublattice and $j \in B$ sublattice. Derive eq. (6) from eq. (1) and convince yourself that the bond operators $\hat{u}_{\langle i,j\rangle_\alpha}$ and the Hamiltonian eq. (6) are hermitian. Furthermore convince yourself that $\hat{u}_{\langle i,j\rangle_\alpha} = -\hat{u}_{\langle j,i\rangle_\alpha}$ and that the bond operator has eigenvalues $u_{\langle i,j\rangle_\alpha} = \pm 1$. Finally, show that eq. (7) holds.

What happens to the Hilbert space when we introduce Kitaev's representation of spins in terms of Majoranas? Previously we had $2N$ spin-1/2 leading to the 2^{2N} dimensional *physical Hilbert space*. Each Majorana has a nominal dimension of $\sqrt{2}$, originating from the fact the two Majoranas can be combined to a single complex fermion with dimension 2 (occupied or not occupied). Therefore we are now dealing with an artificially enlarged Hilbert space of dimension 4^{2N}. We need to differentiate between states which are present in the physical Hilbert space and states we have added artificially by representing the spins in terms of Majoranas.

From the spin-1/2 algebra follows that $-\mathrm{i}\sigma^x\sigma^y\sigma^z = 1$ which translates in terms of Majoranas to $D_j = b_j^x b_j^y b_j^z c_j$ which has however eigenvalues ± 1. Hence a state that is also part of the physical Hilbert space $|\Phi_{\mathrm{phys}}\rangle$ needs to satisfy $D_j|\Phi_{\mathrm{phys}}\rangle = |\Phi_{\mathrm{phys}}\rangle$. As we will see, the operators D_j play the role of a gauge operator i.e. it changes the gauge. For a given set of eigenvalues of the bond operators $\{u_{\langle i,j\rangle_\alpha}\}$ the associated Hilbert space is not gauge invariant. Applying the operator D_i changes the values of $u_{\langle i,j\rangle_\alpha}$ on the links connecting i with its adjacent vertices j. To obtain a physical Hilbert space where to action of D_j is trivial we must symmetrize over all possible gauge transformations by the projection

$$P|\Phi\rangle = \prod_i \frac{1+D_i}{2}|\Phi\rangle = |\Phi_{\mathrm{phys}}\rangle. \tag{8}$$

However, one can show that for all practical purposes this projection does not influence the calculation of expectation values up to an overall phase factor coming from fermion parity. [10, 11] In short, (almost all) matrix elements calculated in physical or unphysical states are equivalent (up to finite size corrections). Therefore, we ignore the projection operator in the remainder of the notes, e.g. in sec. 5.

3.3 Ground state properties

To find the ground state of the Kitaev model we must calculate in principle the ground states of all different flux sectors and then compare their energies to find the one with lowest energy. Fortunately Lieb's theorem [12] states that if gapped gauge fluxes exist the ground state on the honeycomb lattice is always flux free. We can therefore focus on the flux-free sector and work with the gauge where $u_{\langle i,j\rangle_\alpha} = \delta_{\langle i,j\rangle_\alpha}$. The system is then translationally invariant and momentum is a good quantum number. The honeycomb lattice itself is however not a Bravais lattice and therefore not translational invariant, it must be split into two sublattices (A and B), see fig. 1. We split the site index i into the position of the unit cell $\boldsymbol{r}$ and a variable λ associated with the sublattice. We can then introduce Fourier transforms

$$c_{\boldsymbol{q},\lambda} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\boldsymbol{r}} c_{\boldsymbol{r},\lambda}. \tag{9}$$

Applying this to the Hamiltonian, using the conventions from fig. 1 we find

$$H = \frac{\mathrm{i}}{2} \sum_{\boldsymbol{q}} \begin{pmatrix} c_{-\boldsymbol{q},A} & c_{-\boldsymbol{q},B} \end{pmatrix} \begin{pmatrix} 0 & S(-\boldsymbol{q}) \\ -S(\boldsymbol{q}) & 0 \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{q},A} \\ c_{\boldsymbol{q},B} \end{pmatrix} \tag{10}$$

where $S(\boldsymbol{q}) = K_z + K_x \mathrm{e}^{\mathrm{i}\boldsymbol{q}\boldsymbol{n}_1} + K_y \mathrm{e}^{\mathrm{i}\boldsymbol{q}\boldsymbol{n}_2}$.

We now continue by introducing complex fermions as they are more convenient to work with. We fuse Majoranas of the sublattices A and B to one complex matter fermion

$$f^\dagger_{\boldsymbol{q}} = \frac{1}{2}(c_{\boldsymbol{q},A} - \mathrm{i}c_{-\boldsymbol{q},B}) \quad \text{and} \quad f_{\boldsymbol{q}} = \frac{1}{2}(c_{\boldsymbol{q},A} + \mathrm{i}c_{-\boldsymbol{q},B}). \tag{11}$$

to obtain

$$H = \sum_{\boldsymbol{q}} \begin{pmatrix} f_{\boldsymbol{q}} \\ f^\dagger_{-\boldsymbol{q}} \end{pmatrix}^\dagger \begin{pmatrix} \xi_{\boldsymbol{q}} & -\Delta_{\boldsymbol{q}} \\ -\Delta^*_{\boldsymbol{q}} & -\xi_{-\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} f_{\boldsymbol{q}} \\ f^\dagger_{-\boldsymbol{q}} \end{pmatrix}. \tag{12}$$

This Hamiltonian can be thought of as a superconductor with a momentum dependent gap $\Delta_{\boldsymbol{q}} = \mathrm{i}\mathfrak{Im}S(\boldsymbol{q})$ and a normal state dispersion $\xi_{\boldsymbol{q}} = \mathfrak{Re}S(\boldsymbol{q})$. It can be diagonalized by a standard Bogoliubov transformation

$$\begin{pmatrix} f_{\boldsymbol{q}} \\ f^\dagger_{-\boldsymbol{q}} \end{pmatrix} = \begin{pmatrix} \cos\theta_{\boldsymbol{q}} & \mathrm{i}\sin\theta_{\boldsymbol{q}} \\ \mathrm{i}\sin\theta_{\boldsymbol{q}} & \cos\theta_{\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} a_{\boldsymbol{q}} \\ a^\dagger_{-\boldsymbol{q}} \end{pmatrix} \tag{13}$$

such that the diagonalized Hamiltonian is given by

$$H = 2\sum_{\boldsymbol{q}} |S(\boldsymbol{q})|(a^\dagger_{\boldsymbol{q}} a_{\boldsymbol{q}} - \frac{1}{2}). \tag{14}$$

Problem 5: Ground state solution and dispersion
Carry out the calculation described in this section step by step until eq. (14). Start by deriving eq. (10) from eq. (6) (remember that you have to split into two different sublattices in order to Fourier transform). To get eq. (12) you must use the properties $S^*(\boldsymbol{q}) = S(-\boldsymbol{q})$ *and* $(c_{\boldsymbol{q}})^* = c_{-\boldsymbol{q}}$*. Find the equation determining* $\theta_{\boldsymbol{q}}$*.*

From eq. (14) the excitation spectrum can be read off. Visualize the excitation spectrum over the first Brillouin zone in Mathematica with `ContourPlot` *and* `Plot3D` *(you might as well use a different program with similar functions). The ground state features two different phases: A gapped phase A and a gapless phase B. Find conditions on the parameters* K^α *to determine which phase the system is in and visualize the phase diagram for* $K^x + K^y + K^z = 1$ *and* $K^\alpha > 0$ *(hint, use the ternary plot function).*

4 Relation to the Toric Code

4.1 Motivation

The last chapter has shown that two phases exist in the Kitaev model. Most of Kitaev's original paper [1] is actually dedicated to the gapless phase B. It can be shown that by adding an additional term breaking time reversal symmetry the Hamiltonian of the model remains exactly solvable. The B phase becomes gapped and the Majorana system resembles a $p_x + ip_y$ superconductor, which exhibits topologically non-trivial excitations, called *non-Abelian anyons*. These are distinct from the anyons appearing in the Toric code model, which are *Abelian anyons*, meaning that fusion of two anyons always leads one definite other anyon. In non-Abelian phases fusion can lead to various different anyons.

In this lab course we will not further explore the B phase but rather focus our understanding on the nature of the A phase. An important conceptual point is that the gapped A phase of the Kitaev model can be mapped to the Toric code model, therefore displaying the same topological order and anyonic excitations.

Let us focus on the phase A_z, which occurs when $|K^x| + |K^y| < |K^z|$. Since we are interested in properties of the phase, we set $|K^x|, |K^y| \ll |K^z|$

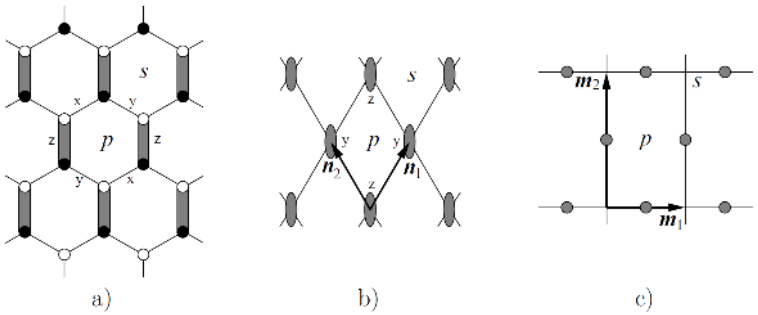

Figure 2: Mapping to the Toric code. Strong z-bonds in the Kitaev model (a) become effective spins (b), which are associated with the bonds of new lattice (c). Taken from ref. [1].

(as qualitative properties cannot change inside the phase) and we may apply perturbation theory.

4.2 Perturbation theory

We split the Hamiltonian eq. (1) into a main part H_0 and a perturbation V:

$$\begin{aligned} H_0 &= -K^z \sum_{\text{z-bonds}} \sigma_i^z \sigma_j^z \\ V &= -K^x \sum_{\text{x-bonds}} \sigma_i^x \sigma_j^x - K^y \sum_{\text{y-bonds}} \sigma_i^y \sigma_j^y \end{aligned} \tag{15}$$

We assume w.l.o.g. $K^z > 0$.

The starting point for the perturbation theory is to determine the Eigenstates of the unperturbed system $K^x = K^y = 0$, which correspond to the classical states of Problem 1. In the ground state each two spins connected by a z-bond are aligned ($\uparrow\uparrow$ or $\downarrow\downarrow$) leading to the ground state energy $E_0 = -NK^z$. The aligned pairs of spins can be interpreted as an effective new spin. The goal of the following paragraph is then to explain, at least on a qualitative level, that the low energy model for these effective spins is precisely the Toric code.

The excited states have n pairs along z-bonds of spins which are not aligned ($\uparrow\downarrow$ or $\downarrow\uparrow$) and have an energy $E_n = 2nK^z + E_0$. As a next step we determine contributions of V to the lowest non-vanishing order to the low energy manifold. A first order process, i.e. applying V once to the ground state, is not possible within the low energy sector as we get two excitations (misaligned spins) at the end of the bonds on which we applied V. The same happens to higher processes. In order to end up with the ground state again we have to move the two excitations once around an entire plaquette and then annihilate them with each other. Therefore the lowest non-vanishing

order is a 4^{th}-order process and will lead to an effective Hamiltonian

$$H_{\text{eff}} \propto \frac{K^{x2}K^{y2}}{K^{z3}} \sum_p Q_p \tag{16}$$

where

$$\begin{aligned} Q_p &\propto \sigma^x_{p_2}\sigma^x_{p_3}\sigma^y_{p_3}\sigma^y_{p_4}\sigma^x_{p_5}\sigma^x_{p_6}\sigma^y_{p_6}\sigma^y_{p_1} && (17)\\ &\propto \sigma^x_{p_2}\sigma^z_{p_3}\sigma^y_{p_4}\sigma^x_{p_5}\sigma^z_{p_6}\sigma^y_{p_1} && (18)\\ &= \sigma^y_{p_1}\sigma^x_{p_2}\sigma^z_{p_3}\sigma^y_{p_4}\sigma^x_{p_5}\sigma^z_{p_6} && (19)\\ &\propto \sigma^y_{\text{left}(p)}\sigma^z_{\text{top}(p)}\sigma^y_{\text{right}(p)}\sigma^z_{\text{bottom}(p)}. && (20) \end{aligned}$$

We have used the algebraic property $\sigma^x_i\sigma^y_i \propto \sigma^z_i$ and that $\sigma^y_i\sigma^x_{i+1}$ acts as $\sigma^y_{(i,i+1)}$ on the effective spin, consisting of the spins located at i and $i+1$. Furthermore we have used the conventions from fig. 1 and 2 implying $\text{left}(p) = (p_1, p_2)$, $\text{top}(p) = p_3$ etc.

After this transformation we have two kind of plaquettes: For one of them σ^z operators act on the right and left sites and σ^y operators act on the top and bottom sites, for the other kind it is exactly reversed. A suitable spin rotation can transform these interactions in a star operator with only σ^z terms and a plaquette operator with only σ^x terms. These are exactly the star and plaquette operators appearing in the Hamiltonian of the Toric code model. We thus have established an exact mapping between the gapped A phase of the Kiteav-Honeycomb model and the Toric code model. Therefore the Kitaev model also hosts (abelian) anyons.

> **Problem 6: Excitations of the Toric code**
> *If time on the first day permits, follow the original Kitaev paper [1] and identify the e- and m-particles of the Toric code as excitations of the Kitaev honeycomb model.*

5 Spin Correlation Functions

In this section, you will learn how to use the exact solution for the calculation of physical observables. You will see that the fractionalization of spin flips into static flux and mobile Majorana excitations leads to highly unusual behaviour for the correlation functions, which serve as a characteristic signature of the Kitaev QSL phase.

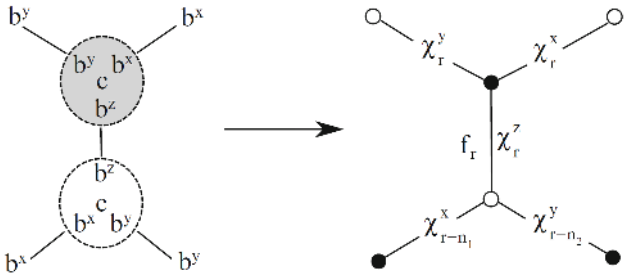

Figure 3: Kitaev's representation of spins in terms of Majoranas is shown on the left, while on the right formalism of complex bond fermions is shown. Taken from ref. [13].

5.1 Bond fermions

For the calculation of matrix elements it useful to introduce the concept of bond fermions, see fig. 3. Conceptually they are similar to complex matter fermions introduced in eq. (11) but here we transform the Majoranas b_i^α into bond fermions

$$\begin{aligned} &\chi^\dagger_{\langle i,j\rangle_\alpha} = \frac{1}{2}(b_i^\alpha - \mathrm{i}b_j^\alpha) \quad \text{and} \quad \chi_{\langle i,j\rangle_\alpha} = \frac{1}{2}(b_i^\alpha + \mathrm{i}b_j^\alpha) \quad \text{such that} \\ &\hat{u}_{\langle i,j\rangle_\alpha} = 2\chi^\dagger_{\langle i,j\rangle_\alpha}\chi_{\langle i,j\rangle_\alpha} - 1. \end{aligned} \tag{21}$$

The bond variables $\hat{u}^\dagger_{\langle i,j\rangle_\alpha}$ are simply related to the occupation number of these bond fermions. Note, in a slightly different notation $\boldsymbol{r}$ is the unit cell coordinate in which site i lies $\chi^\alpha_{\boldsymbol{r}} = \chi_{\langle i,j\rangle_\alpha}$. It is also convenient to find the corresponding equations for eq. (11) in real space

$$f^\dagger_{\boldsymbol{r}} = \frac{1}{2}(c_{\boldsymbol{r},A} - \mathrm{i}c_{\boldsymbol{r},B}) \quad \text{and} \quad f_{\boldsymbol{r}} = \frac{1}{2}(c_{\boldsymbol{r},A} + \mathrm{i}c_{\boldsymbol{r},B}). \tag{22}$$

Using the representations of eq. (21) and eq. (22) we can rewrite the spin operator

$$\sigma^\alpha_{\boldsymbol{r},A} = \mathrm{i}\left(f^\dagger_{\boldsymbol{r}} + f_{\boldsymbol{r}}\right)\left((\chi^\alpha_{\boldsymbol{r}})^\dagger + \chi^\alpha_{\boldsymbol{r}}\right). \tag{23}$$

5.2 2-Point Correlator

We now use the bond fermion formalism to understand the behaviour of the most basic correlation function

$$S^{\alpha\beta}_{ij} = \langle \sigma^\alpha_i \sigma^\beta_j \rangle \tag{24}$$

Problem 7: 2-Point Correlator
Calculate the correlator $S_{ij}^{\alpha\beta}$ in the ground state. Start by convincing yourself that it is ultra-short ranged (hint, use the fact that the spin operator eq. (23) does not commute with the bond operators and inserts fluxes). Then express the correlation function as a sum over the 1^{st} Brillouin zone and plot the behaviour in the ternary phase diagram for $K_x + K_y + K_z = 1$. Discuss the results and compare the behaviour to that of a general unfrustrated magnet at low and high temperature.

5.3 Dirac Points

Problem 8: Dirac cones
Using your results from Problem 5 derive the effective low energy Majorana Hamiltonian and the band structure in the vicinity of the K and the K′-point. You may assume that $K^x = K^y = K^z$ and use Mathematica. Note however that your findings are generic within the gapless B phase. What is the difference to the case of graphene?

5.4 4-Point Correlator

A peculiar feature of the Kitaev model are the ultra-short-ranged spin correlations, which arise because of the flux selection rules. Since the isotropic B phase is gapless, one would also expect long-range correlations. Indeed, operators which do not excite fluxes show the expected critical behaviour of the Dirac phase as we discuss in the following.

Problem 9: 4-Point Correlator
Derive the 4-Point correlator $C_4^\alpha(\boldsymbol{r}, \boldsymbol{r'})$ for $\boldsymbol{r} \neq \boldsymbol{r'}$

$$\begin{aligned} C_4^\alpha(\boldsymbol{r}, \boldsymbol{r'}) &= \langle \sigma^\alpha_{\boldsymbol{r},A} \sigma^\alpha_{\boldsymbol{r},B} \sigma^\alpha_{\boldsymbol{r'},A} \sigma^\alpha_{\boldsymbol{r'},B} \rangle - \langle \sigma^\alpha_{\boldsymbol{r},A} \sigma^\alpha_{\boldsymbol{r},B} \rangle \langle \sigma^\alpha_{\boldsymbol{r'},A} \sigma^\alpha_{\boldsymbol{r'},B} \rangle \\ &= -\left| \frac{1}{N} \sum_{\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}(\boldsymbol{r}-\boldsymbol{r'})} \frac{\mathfrak{Re} S(\boldsymbol{q})}{|S(\boldsymbol{q})|} \right|^2 . \end{aligned} \tag{25}$$

and evaluate it numerically to plot $C_4^\alpha(\boldsymbol{r}, \boldsymbol{r'})$ against $\boldsymbol{r} - \boldsymbol{r'} = \Delta r(\boldsymbol{n_1} - \boldsymbol{n_2})$ on a log-log scale inside the gapped A and the gapless B phase.

By taking the thermodynamic limit show analytically that $C_4^\alpha(\boldsymbol{r}, \boldsymbol{r'}) \propto 1/r^4$ in the B phase (choose $K^x = K^y = K^z = 1$ for simplicity) and therefore decays algebraically. After you have transferred the sum to

an integral you need to introduce a soft cut-off by weighting the integrand with $\exp(-a^2p^2r^2)$ *and extend the integral to* ∞*. The main contribution of this integral comes from the Dirac points such that you can use your results from section 5.3. Note that for some angles of* $\boldsymbol{q}$ *with respect to the lattice or* $\boldsymbol{r}-\boldsymbol{r}'$ *the lowest order* $1/r^4$ *disappears and the decay is of higher order. You do not need to consider these special cases.*

Finally, interpret the results. What kind of behavior would you expect in the gapped A phase?

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