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MASTER'S THESIS

«Perturbed Kitaev model: excitation spectrum and long-ranged spin correlations»

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Contents

Chapter 1

Introduction

1.1 Magnetic states of matter

Proprieties of ferromagnetics and anti-ferromagnetics are well-known. Ground states of this type are characterized by a local order parameter. It means that at zero-temperature an average of a spin operator is non-zero and quantum fluctuations of such spin are relatively weak. So, in such systems we can speak about the orientations of spins. The ferromagnetic order means that all spins are almost parallel to each other. The anti-ferromagnetic order means that a half of spins are parallel to one direction and another half of spins are parallel to the opposite direction. Elementary excitations of such systems are called magnons. They describe deviation of spins from the average direction like phonons describe a deviation of atoms from their average positions. Magnons also obey Bose statistics. There is a difference in a form of a spectrum of such excitations: in a ferromagnet matter the energy is quadratically depend on the momentum, in a anti-ferromagnetic this dependence is linear. There are systems with other orders and they have almost the same low-energy physic: the excitations are also magnons with different types of a spectrum.

There are several examples of states which have an essentially another description of magnetic properties. They are valence bonds [2], and spin liquids. Spin liquid has no any order parameter (for example the average of the spin like it was in case of ferromagnetics). Such behaviour can be related with strong quantum fluctuations which make ordered phase unstable.

Quantum fluctuations are enhanced in systems with small spins. For example, if the spin is $s = \frac{1}{2}$ then the average of s^2 is $\frac{3}{4}$. Quantum fluctuations are especially important in low-dimensional systems.

Another example of a mechanism which can destroy an order is the frustration [16]. For, example we can imagine that spins are situated at the triangle lattice with the nearest-neighbour anti-ferromagnetic interaction. In this case Neel type state is not possible due to frustration.

There is no a general theory of spin-liquids but there are several examples, for review see ref.[4]. Exactly solvable 1-dimensional XY model is known since Jordan and Wigner [6], while first 2-dimensional generalization was proposed recently by Kitaev [8]. There are a lot of experiments where people try to find evidence of spin-liquid in real materials.

1.2 Importance of the model and an overview of results

Kitaev model is also important for the theory of quantum computation. A lot of people try to find a mater which properties can be described by Kitaev model and use it for qubits. Properties of real matter depend also on perturbations to Kitaev model which exist in every material. So it is important to understand properties of Kiteav model with perturbations. In this thesis we present an analysis of such properties. We analyse which spin-spin correlation can be created by perturbation and how perturbations can change low-energy spectrum.

In the Second chapter of this Thesis we describe pure Kitaev model, in the Third chapter we develop a theory of a spin-spin correlation functions in the infra-red limit and calculate corrections to the low-energy Hamiltonian, also we show the importance of the time-reversal symmetry. In the Fourth chapter we demonstrate an application of our results for different types of perturbations.

Chapter 2

Pure Kitaev model

2.1 Hamiltonian

Kitaev model [8] describes a system of interacting spins with $s = \frac{1}{2}$. Spins are situated in sites of the honeycomb lattice. Such lattices has 3 types of edges which are called as x, y and z, see Fig. (2.1). In the system only nearest-neighbours spins interact. Spins which are situated on, for example, a x edge interact with each other using the x component of spins only. The Hamiltonian of the model is:

$$H = \sum_{\langle i,j\rangle \in \alpha\beta(\gamma)} K_\gamma \sigma_i^\gamma \sigma_j^\gamma \tag{2.1}$$

Here $\langle i, j\rangle$ is an edge which has a type γ, as indicated by the notation $\langle i, j\rangle \in \alpha\beta(\gamma)$. Here $\alpha\beta(\gamma)$ has three possible values: $xy(z)$, $zx(y)$ and $yz(x)$. This model is exactly solvable and can be solved using a representation of Pauli matrices via Majorana fermions.

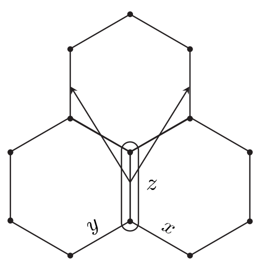


Figure 2.1: The lattice of the model, which has 3 different types of edges: x,y and z. Translations vectors are also presented

2.2 Majorana fermions representation

One can consider a fermion operator ψ and also consider its "real" and "imaginary" parts:

$$a = \psi + \psi^\dagger \quad b = i(\psi^\dagger - \psi) \tag{2.2}$$

Operators a and b have the following anti-commutation relations:

$$\{a, a\} = 2 \quad \{b, b\} = 2 \quad \{a, b\} = 0 \tag{2.3}$$

Operators a and b describe particles which are called Majorana fermions.

For any site i we introduce four Majorana fermions. We will call them as b_i^x,b_i^y, b_i^z and c_i. Let us consider operators:

$$\tilde{\sigma}_i^\alpha = i b_i^\alpha c_i \tag{2.4}$$

We also would like to consider the subspace of the Hilbert space where each vector is an eigenvector of the operator $D_i = b_i^x b_i^y b_i^z c_i$ for any i with an eigenvalue equal to 1.The operator $\tilde{\sigma}_i^\alpha$ commute with D_j for any j. It means that this space is invariant under an action of $\tilde{\sigma}_i^\alpha$. Below we consider only a projection of these operators on this subspace. In this assumption we can calculate commutation relations of these operators:

$$\begin{gathered}[\tilde{\sigma}_i^\alpha, \tilde{\sigma}_j^\beta] = -\delta_{ij}[b_i^\alpha c_i, b_i^\beta c_i] = \delta_{ij}(b_i^\alpha b_i^\beta - b_i^\beta b_i^\alpha) = \\ -\delta_{ij}(b^\alpha b^\beta - b^\beta b^\alpha) b_i^\gamma c_i b_i^\gamma c_i = i b_i^x b_i^y b_i^z c_i \delta_{ij} \varepsilon^{\alpha\beta\gamma} \tilde{\sigma}_i^\gamma = i \varepsilon^{\alpha\beta\gamma} \tilde{\sigma}_i^\gamma\end{gathered} \tag{2.5}$$

The last step was done as operators act on eigenfunctions of D_i. So we can represent Pauli matrices using these Majorana fermions. The Hamiltonian has the following form:

$$H = \sum_{\langle i,j \rangle \in \alpha\beta(\gamma)} -i K_\gamma (i b_i^\gamma b_j^\gamma) c_i c_j \tag{2.6}$$

One can note that in the initial problem a dimension of the Hilbert space is 2^N, where N is a number of sites in the lattice. The space where lives Majorana fermions has dimension 4^N because each 2 Majorana fermions are equivalent to an ordinary fermion. So after our choice of the subspace we have also the Hilbert space with the size 2^N.

We would like to introduce a new operator for an edge $\langle i, j \rangle$ which has the type

γ, this operator $u_{ij} = ib_i^\gamma b_j^\gamma$. u_{ij} is an integral of motion, because it commutes with the Hamiltonian. However, it is a not "physical" variable. The "physical" integral of motion is a flux. Let's consider a honeycomb cell, see Fig.(2.2), and the operator:

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z = u_{21} u_{23} u_{43} u_{45} u_6 u_{61} \tag{2.7}$$

It is also an integral of motion, and it can be represented through Pauli matrices. This operator has eigenvalues ± 1. If in some state $W_p = -1$ we will say that there is a flux in the cell p in this state. In the work [9] it was shown that there is an energy gap between states with fluxes and without them. So in the ground state there is no fluxes and all $W_p = 1$.

What about u_{ij} ? Firstly, $u_{ij} = -u_{ji}$ so we want to fix that i is from the even sublattice (2,4,6 on Fig.(2.2)) and j is from the odd one. Secondly, in this problem there is a gauge transformation, in a vertex i, we can change all signs of Majorana operators. The spin variables are quadratic in terms of fermion operators, so they do not change their signs. So this transform does not change W_p and H and also it does not change operator $D_j = b_i^x b_i^y b_i^z c_i$ so we still live in the same subspace. But u_{ij} changes the sign under this transform. Using this transforms we can made all $u_{ij} = 1$ in the ground state, so the Hamiltonian which describes low-energy excitations above the ground state has the following form:

$$H = \sum_{\langle i,j \rangle} -iK_\gamma c_i c_j \tag{2.8}$$

2.3 Diagonalization of the Hamiltonian

We see that the Hamiltonian (2.8) is quadratic and has translation invariance so we can use Fourier transform to diagonalize it. The lattice as was discussed above has 2 sub-lattices,

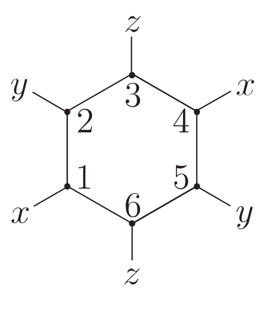


Figure 2.2

odd and even and two translation vectors $\mathbf{n}_1 = \{\frac{1}{2}, \frac{\sqrt{3}}{2}\}$ and $\mathbf{n}_2 = \{-\frac{1}{2}, \frac{\sqrt{3}}{2}\}$. Let two sites which are connected by z-edge will constitute a unit-cell, see Fig.(2.1). So each vertex can be parametrized by $\mathbf{r}$-a vector of a unit cell and by an index λ which describes the parity. Then the Hamiltonian has the following form:

$$H = \frac{1}{4} \sum_{\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta} U^{\alpha,\beta}(\mathbf{r}_{2,1}) c_{\mathbf{r}_1,\alpha} c_{\mathbf{r}_2,\beta} \tag{2.9}$$

Here $\mathbf{r}_{1,2} = \mathbf{r}_1 - \mathbf{r}_2$. Here:

$$U^{\alpha,\beta}(\mathbf{r}) = 2 \begin{pmatrix} 0 & i(\delta_{\mathbf{r},0} K_z + \delta_{\mathbf{r},-\mathbf{n}_1} K_x + \delta \mathbf{r}, -\mathbf{n}_2 K_y) \\ -i(\delta_{\mathbf{r},0} K_z + \delta_{\mathbf{r},\mathbf{n}_1} K_x + \delta \mathbf{r}, \mathbf{n}_2 K_y) & 0 \end{pmatrix} \tag{2.10}$$

Then we can do the Fourier transform:

$$c_{\mathbf{r},\lambda} = \frac{\sqrt{2}}{\sqrt{N}} \sum_{\mathbf{p}} c_{\mathbf{p},\lambda} e^{i(\mathbf{p},\mathbf{r})} \tag{2.11}$$

$$U^{\alpha,\beta}(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{p}} A^{\alpha,\beta}(\mathbf{p}) e^{i(\mathbf{p},\mathbf{r})} \tag{2.12}$$

$$A^{\alpha,\beta}(\mathbf{p}) = \begin{pmatrix} 0 & f(\mathbf{p}) \\ f^{\dagger}(\mathbf{p}) & 0 \end{pmatrix} \tag{2.13}$$

Where $f(\mathbf{p}) = 2i(K_z + K_x e^{i(\mathbf{p},\mathbf{n}_1)} + K_y e^{i(\mathbf{p},\mathbf{n}_2)})$ Note, that $c_{\mathbf{q},\lambda} = c^{\dagger}_{-\mathbf{q},\lambda}$ and there are the following commutation relations $\{c_{\mathbf{p},\alpha}, c_{\mathbf{q},\beta}\} = \delta_{\mathbf{p},-\mathbf{q}} \delta_{\alpha,\beta}$. So we have:

$$H = \frac{1}{2} \sum_{\mathbf{p},\alpha,\beta} A^{\alpha\beta}(\mathbf{p}) c_{-\mathbf{p},\alpha} c_{\mathbf{p},\beta} \tag{2.14}$$

Note that due to the identity $c^{\dagger}_{\mathbf{r},\lambda} = c_{\mathbf{r},\lambda}$ only a half of operators are "independent" as $c^{\dagger}_{-\mathbf{p},\lambda} = c_{\mathbf{p},\lambda}$.

2.4 Spectrum and Green functions

The Hamiltonian (2.14) has the spectrum $\varepsilon(\mathbf{p}) = \pm|f(\mathbf{p})|$. It has 2 conic points if $K_\alpha + K_\beta > K_\gamma$. Below we will study this case. For simplicity we will consider only the isotropic model, where $K_z = K_x = K_y$ but our results are also applicable for any case with conic points. Conic points, in isotropic case, are located at points $\mathbf{K}_{1,2} = \begin{pmatrix} \pm\frac{2\pi}{3} \\ \frac{2\pi}{\sqrt{3}} \end{pmatrix}$.

Green functions and their Fourier transform have the following form:

$$G_{\alpha,\beta}(\mathbf{r},t) = \langle T c_{\mathbf{r},\alpha}(t) c_{0,\beta}(0)\rangle \tag{2.15}$$

$$G_{\alpha,\beta}(\mathbf{p},\varepsilon) = 2i \begin{pmatrix} \frac{\varepsilon}{\varepsilon^2-|f(\mathbf{p})|^2+i0} & \frac{f(\mathbf{p})}{\varepsilon^2-|f(\mathbf{p})|^2+i0} \\ \frac{f^\dagger(\mathbf{p})}{\varepsilon^2-|f(\mathbf{p})|^2+i0} & \frac{\varepsilon}{\varepsilon^2-|f(\mathbf{p})|^2+i0} \end{pmatrix} \tag{2.16}$$

We can calculate the behaviour of Green functions in the infra-red limit: $Kt \gg 1$, $r \gg 1$ and $|\sqrt{3}Kt - r| \gg 1$. The last conditions mean that we are not very close to light cone. The behaviour of the Green function is determined by the behaviour of the spectrum near conic points. Function f has the following form near conic points $f(\mathbf{K}_{1,2} + \delta\mathbf{p}) \approx \sqrt{3}K(\delta p_y \pm i\delta p_x)$. In this limit Green functions have the following form:

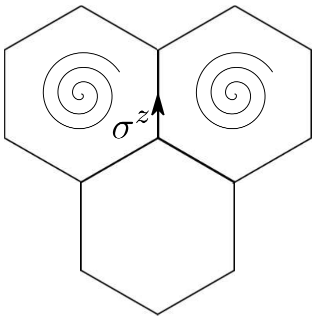
$$G_{\alpha,\beta}(\mathbf{r},t) = \frac{1}{2\pi(3(Kt)^2 - r^2)^{\frac{3}{2}}} \begin{pmatrix} -\sqrt{3}Kt(e^{i(\mathbf{K_1},\mathbf{r})}+e^{i(\mathbf{K_2},\mathbf{r})}) & ir(e^{i(\mathbf{K_1},\mathbf{r})+i\alpha}+e^{i(\mathbf{K_2},\mathbf{r})-i\alpha}) \\ ir(e^{i(\mathbf{K_2},\mathbf{r})+i\alpha}+e^{i(\mathbf{K_1},\mathbf{r})-i\alpha}) & -\sqrt{3}Kt(e^{i(\mathbf{K_1},\mathbf{r})}+e^{i(\mathbf{K_2},\mathbf{r})}) \end{pmatrix} \tag{2.17}$$

Here α is the angle between x axes and $\mathbf{r}$.

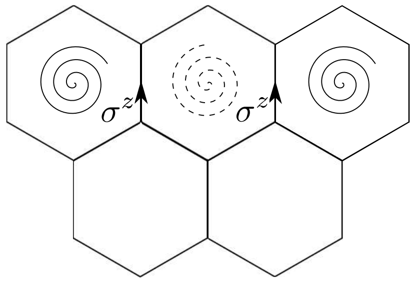
We see from (2.16) that diagonal elements are odd functions of the energy so in the $(\mathbf{r}, t)$ representation they are also odd functions of time. But off-diagonal term are even functions. This difference will be important in our analysis.

2.5 Fluxes

In the previous section we discussed elementary excitations above the ground state which can be created by an operator c_i. But c_i is not a "physical" operator since all observable should be represented through Pauli matrices, using fermion representation : $\sigma_i^\alpha = ib_ic_i$. Let $\langle i,j\rangle \in \alpha\beta(\gamma)$ then we have that $\{\sigma_i^\gamma, u_{ij}\} = 0$ it means what the action of the spin operator changes the sign of u_{ij}. If we apply a spin operator to the ground state then we change one u_{ij}. It is equivalent to the change of two W_p where p has the edge $\langle i,j\rangle$ see Fig. (2.3a). If we apply other spin operator we can create other pair of fluxes or annihilate one fluxe and create anew see Fig.(2.3b).



(a) Two fluxes created by one spin



(b) Two fluxes created by two spin

Figure 2.3

Properties of fluxes are important for understanding of properties of spin correlations functions. Firstly, we consider a spin average $\langle\sigma_i^\alpha\rangle$. After action of spin operator: $\sigma_i^\alpha|0\rangle$ we obtain a state with 2 fluxes. The projection of this state on the ground state is zero as there is no fluxes in the ground state. So this average is zero. Secondly, we can consider the spin-spin correlation function: $\langle\sigma_i^\alpha(t)\sigma_j^\beta(0)\rangle$. It will not be zero if the operator $\sigma_i^\alpha\sigma_j^\beta$ does not create fluxes. It is true only if $\alpha = \beta$ and $i = j$ or i and j are neighbours, which are connected by α edge.

On the one hand, we see that correlation functions in this model are strictly local, they are exactly zero for non-neighbour spins. On the other hand, we know that spectrum has conic points and we expect a power-low decay of correlation functions. This paradox is due to the exact integrability of the model. We can remove it if we add some perturbations to the Hamiltonian.

An analysis of the model with perturbations is important because there are perturbations in real materials and we need to understand their properties. Below we will show how perturbations affect on the low-energy physics: how does spin-spin correlation function looks-like. We also found how perturbations can change the low-energy spectrum.

Chapter 3

Perturbed model

3.1 Types of perturbations

The most part of our results presented below were published in the ref. [11]

The general form of the Perturbed Kitaev model has the following form:

$$H = H_K + V \tag{3.1}$$

Where H_K is the Hamiltonian of the pure model and $V = \sum V_i$. Here i is a number of a site and V_i is some local perturbation. For example:

$$V_H = \sum_{\langle i,j \rangle} J(\vec{\sigma}_i, \vec{\sigma}_j) \quad \text{Heisenberg interaction} \tag{3.2}$$

$$V_\Gamma = \sum_{\langle i,j \rangle} \Gamma_{ij}^{\gamma} (\sigma_i^\alpha \sigma_j^\beta + \sigma_j^\alpha \sigma_i^\beta) \quad \text{pseudodipolar interaction} \tag{3.3}$$

$$V_h = \sum_i (\vec{h}, \vec{\sigma}_i) \quad \text{magnetic field} \tag{3.4}$$

$$V_{DM} = \sum_{\langle\langle i,j \rangle\rangle} (\vec{D}_{ij}, [\vec{\sigma}_i, \vec{\sigma}_j]) \quad \text{DM interaction} \tag{3.5}$$

First two types of perturbations are present almost in any magnetic material. The third example describes an external magnetic field, this case was studied in ref. [15],[10]. The last term is a next-nearest-neighbours Dzyaloshinskii-Moriya interaction. Below we will show why this term is important in the theory of perturbed Kitaev model.

3.2 Flux analysis

First, we assume that the ground state of the perturbed model is similar to the ground state of the pure model and we can use perturbation theory. Then for the spin-spin correlation function we have:

$$S_{ij}^{\alpha\beta} = \langle T\sigma_i^\alpha(t)\sigma_j^\beta(0)\rangle = \sum_n \frac{(-1)^n}{n!} \sum_{k_1,\ldots,k_n} \int d\tau_1 \ldots d\tau_n \langle T\sigma_i^\alpha(t)\sigma_j^\beta(0)V_{k_1}(\tau_1)\ldots V_{k_n}(\tau_n)\rangle \quad (3.6)$$

Analysis of correlation functions in the pure model shows us that for a non-zero result the operator under the average should not create fluxes. We can apply this result for perturbations which were described above. Fig.(3.1) shows different patterns created by these perturbations. A magnetic field and DM create the same pattern as a single spin. Heisenberg interaction creates 4 fluxes, if we apply such perturbation after a spin operator we will destroy 2 fluxes created by spin and create 2 other fluxes. So we can think what it moves fluxes. To destroy two pairs of fluxes we should move one pair of fluxes to the other one. So we should apply n times perturbation, where n is the distance between spins which enter in the correlation function. Thus, such correlations decay exponentially. They are not so interesting for us because this decay is connected with the flux's behaviour and we expect power-law correlation in this model, like in the case of magnetic field perturbation.

We expect that the non-zero second term in the perturbation series will appear in the case of DM interaction. In the case of Heisenberg and pseudodipolar interaction the analysis of flux patterns show that we obtain non-zero result in the fourth order of perturbation theory. But it was shown that fourth term vanishes and the first non-zero term comes in the 8-th order, for details see ref. [14]. So the flux analysis is not sufficient for perturbation theory. Below we will show that the consideration of the time-reversal symmetry is also necessary for this analysis.

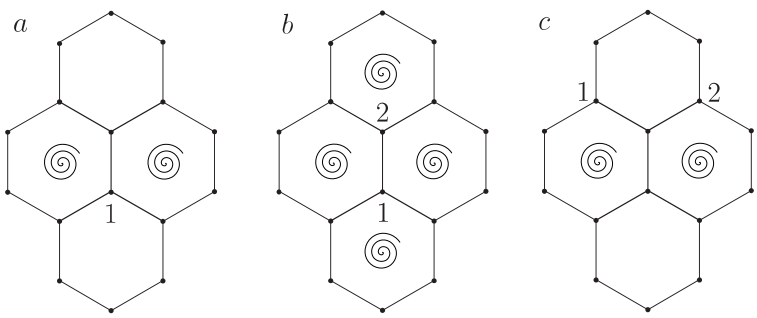


Figure 3.1: Flux patter created by different perturbations: a) magnetic field: σ_1^z b) Heisenberg interaction: $\sigma_1^x\sigma_2^x$ or $\sigma_1^y\sigma_2^y$. c) DM interaction: $\sigma_1^y\sigma_2^x$

3.3 Spin-spin correlation function

In this Section we will show how to calculate the spin-spin correlation function. First, we would like to consider a simple model:

$$H = H_K + \sum_{i \in even, \alpha} V_i^\alpha \tag{3.7}$$

Here a perturbation $V_{i,\alpha}$ is a product of spins which creates the same pattern of flux like the spin σ_i^α. We are interested in the spin-spin correlation function: $S_{i,j}^{\alpha\beta}(t) = \langle T\sigma_i^\alpha(t)\sigma_{j,\mu}^\beta(0)\rangle$. Below we will show that such correlation function in the infra red limit: $r \gg 1$ and $Kt \gg 1$ and $|r - \sqrt{3}Kt| \gg 1$, (r is a distance between i and j) can be expressed through the correlation function of bilinear form of fermion operators:

$$S_{i,j}^{\alpha\beta}(t) = \langle TQ_i^\alpha(t)Q_j^\beta(0)\rangle_0 \tag{3.8}$$

$$Q_i^\alpha = \frac{i}{2}\sum_{c_a, c_b \in C_i^\alpha} V_{i,ab}^\alpha c_a c_b \tag{3.9}$$

C_i is the set of fermions which can be determined in the next way. Let us consider a product of operators $\sigma_i^\alpha V_i^\alpha$. If $i \in odd$ then instead V_i^α we will write $V_{i+\alpha}^\alpha$, $i+\alpha$ means the vertex connected with i by an α-type edge. Then the operator $\sigma_i^\alpha V_i^\alpha$ does not create fluxes. So we can present this operator in the following way:

$$\sigma_i^\alpha V_i^\alpha = A_i c_1^{(i)} \dots c_{n_i}^{(i)} U_i \tag{3.10}$$

In the RHS there is also a dependence on α, but we did not write it for brevity. Here U_i is a product of some first integrals u_{cd}. A_i is a constant and set of $c_1^{(i)} \dots c_{n_i}^{(i)}$ is C_I. Constant $V_{i,ab}^\alpha$ determined by the following correlation functions:

$$V_{i,ab}^\alpha = \int_{-\infty}^0 \langle c_a(0)c_b(0)\sigma_i^\alpha(0)V_i^\alpha(\tau)\rangle + \int_0^\infty \langle V_i^\alpha(\tau)\sigma_i^\alpha(0)c_a(0)c_b(0)\rangle \tag{3.11}$$

This coefficient can be expressed through correlation function of spins operators only. For example, when $V_i^\alpha = h^\alpha(\sigma_i^\alpha + \sigma_{i+\alpha}^\alpha)$ then $Q_i^\alpha = i\gamma_i h^\alpha V_h c_i c_{i+\alpha}$ where $\gamma_i = 1$ if i belongs to odd sub-lattice and -1 if i belongs to the even sublattice. Here $V_h = 2\int_0^\infty \langle\sigma_i^z(\tau)\sigma_i^z(0)\rangle d\tau$.

To obtain Eq.(3.8 we consider the second term of perturbation theory which has the following form (below all average are calculated over the ground state of the pure model):

$$S_{i,j}^{\alpha\beta}(t) = \langle T\sigma_i^\alpha(t)\sigma_j^\beta(0)\rangle = -\int d\tau_1 d\tau_2 \langle T\sigma_i^\alpha(t)V_i^\alpha(\tau_1)V_j^\beta(\tau_2)\sigma_j^\beta(0)\rangle \qquad (3.12)$$

We work in the infra-red limit. As states with flux has energy $\propto K$ then they can not live long, compared to t, so time τ_1 is close to t and τ_2 to 0. Here we consider only one term in the above average when $t > \tau_1 > \tau_2 > 0$. We call this term as $S_{ij}^I(t)$ Other terms can be considered in the same way. Then we obtain:

$$S_{ij}^I(t) = -\int_0^t d\tau_1 \int_0^{\tau_1} d\tau_2 \langle T\sigma_i^\alpha(t)V_i^\alpha(\tau_1)V_j^\beta(\tau_2)\sigma_j^\beta(0)\rangle \qquad (3.13)$$

It is convenient to introduce operator $\tilde{V}_i^\alpha$ via the definition:

$$V_i^\alpha \tilde{V}_i^\alpha = [H, V_i^\alpha] \qquad (3.14)$$

For example when $V_i^\alpha = \sigma_i^\alpha$ then $\sigma_i^\alpha \tilde{V}_i^\alpha = K\sum_\gamma \sigma_{i+\gamma}^\gamma[\sigma_i^\gamma, \sigma_i^\alpha] = 2K\sum_{\gamma\neq\alpha}\sigma_{i+\gamma}^\gamma\sigma_i^\gamma\sigma_i^\alpha$ so $\tilde{V}_i^\alpha = 2K\sum_{\gamma\neq\alpha}\sigma_{i+\gamma}^\gamma\sigma_i^\gamma$ up to sign this operator has the form: $\tilde{V}_i^\alpha = 2K\sum_{\gamma\neq\alpha} ic_{i+\gamma}c_i$. This form demonstrates general properties of the operator $\tilde{V}_\alpha^i$. First, it does not create fluxes. Second, it is quadratic form over fermion operators and each term contains fermions from both sublattice. Using this operator, we can rewrite the time average in the following form:

$$S_{ij}^I(t) = -\int_0^t d\tau_1 \int_0^{\tau_2} \langle e^{iHt}\sigma_i^\alpha V_i^\alpha e^{-(H+\tilde{V}_i^\alpha)(t-\tau_1)} e^{-(H+\tilde{V}_j^\beta)\tau_2} V_j^\beta \sigma_j^\beta\rangle \qquad (3.15)$$

Using the fermions representation from Eq. (3.10) we can rewrite this average (up to sign as $V_j^\beta\sigma_j^\beta = \pm\sigma_j^\beta V_j^\beta$, at the end of our computation we restore this sign). Also, one can note that $U_i = U_j = 1$

$$S_{ij}^I(t) = -\int_0^t d\tau_1 \int_0^{\tau_2} \langle e^{iHt}A_i c_1^{(i)}\dots c_{n_i}^{(i)} e^{-(H+\tilde{V}_i^\alpha)(t-\tau_1)} e^{-(H+\tilde{V}_j^\beta)\tau_2} A_j c_1^{(j)}\dots c_{n_j}^{(j)}\rangle \qquad (3.16)$$

This average under the integral corresponds to the potential which is turned for some part of time only. A similar problem was studied in ref. [12], but there is a difference: in our problem Fermi-energy is zero and Fermi-surface is just two conic points. So the density of states is zero and we avoid a problem related with "orthogonality catastrophe", which was described in ref. [1].

Since $G(\mathbf{r}, t) \approx |\max\{r, Kt\}|^{-2}$ the leading order at large t and r of the irreducible part of this average contains only two "non-local" Green functions ("non-local" means that this function contain operator from C_i^α and other one from C_j^β) while other functions are "local". Typical diagram is shown in Fig.(3.2). These diagrams can be summed up, and the result reads:

$$S_{ij}^I(t) = -\frac{1}{4}\sum_{c_a,c_b;c_f,c_g}\langle Tc_a(t)c_b(t)c_e(0)c_g(0)\int_0^t d\tau_1\int_0^{\tau_1}d\tau_2\langle c_a(t)c_b(t)\sigma_i^\alpha(t)V_i^\alpha(\tau_1)\rangle \times\langle V_j^\beta(\tau_2)\sigma_j^\beta c_p(0)c_q(0)\rangle \quad (3.17)$$

Here $c_a, c_b \in C_i^\alpha$ and $c_f, c_g \in C_j^\beta$. Here we have used identity $c_a^2 = 1$ to express fermion average through spin operators. Function under the average is oscillating with frequency $\propto K$. Since $Kt \gg 1$ we can change the limits of integration (0 and τ_1) on infinity. This terms describe case $t > \tau_1 > \tau_2 > 0$. After summation of all cases we obtain answer Eq. (3.8).

The answer from Eq.(3.8,3.9) can be generalized for a general form of a perturbation. Let us imagine that instead V_i^α we have several perturbations $(V_{i_1}, \ldots, V_{i_1k})$ which together can cancel flux created by σ_i^α. Then we obtain:

$$\sigma_i^\alpha V_{i_1}\ldots V_{i_k} = A_i c_1^{(i)}\ldots c_{n_i}^{(i)}U_i \quad (3.18)$$

We can define C_i in the same way as in Eq. (3.9). Then for the correlation-function we have the expression like Eq. (3.10) but with other V_{ab} in Eq.(3.9):

$$V_{ab} = \sum_{k=0}^{n}\sum_{\zeta=\langle i_1\ldots i_n\rangle\in S^n}\xi_{ab,\zeta,k}\int_0^t d\tau_1\int_0^{\tau_1}d\tau_2\ldots\int_0^{\tau_{k-1}}d\tau_k\int_{-\infty}^0 d\tau_k\ldots\int_{-\infty}^{\tau_{n-1}}d\tau_n \langle V_{i_1}(\tau_1)\ldots V_{i_k}(\tau_k)c_a(0)c_b(0)\sigma_i^\alpha(0)V_{i_{k+1}}(\tau_{k+1})\ldots V_{i_n}(\tau_n)\rangle \quad (3.19)$$

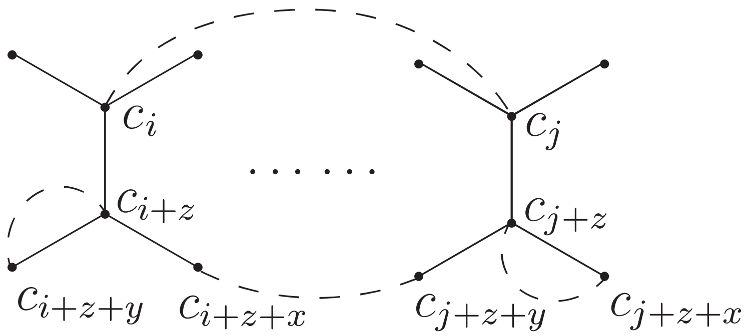


Figure 3.2: the leading-order digram for the spin-spin correlation function in the presence of DM interaction

Here ζ is a permutation of $1\dots n$. And $\xi_{ab,\zeta,k}=\pm 1$ is determined by the following expression: $c_a c_b V_{i_1}\dots V_{i_k}=\xi_{ab,\zeta,k}V_{i_1}\dots V_{i_k}c_a c_b$. In the terms where $k=0$ all $\tau_i<0$ and in the terms where $k=n$ all $\tau_i>0$.f The application of this results will be presented. In the next section we show how using the same analysis one can obtain a correction to the low-energy Hamiltonian.

3.4 Correction to the low-energy Hamiltonian

Let us consider the following Hamiltonian:

$$H=H_k+\sum_i V_{i,1}+V_{i,2} \tag{3.20}$$

Here $V_{i,1}$ and $V_{i,2}$ are some products of spins. Let operator $V_{i,1}V_{i,2}$ does not create fluxes. For example, one can consider the case when $V_{i,1}=h_i^z\sigma_i^z$ -magnetic field and $V_{i,2}=\sigma_{i+y}^y\sigma_{i+x}^x$ -one of the terms in the DM interaction. The perturbations in the model can change the low-energy Hamiltonian. To find the correction we consider perturbation theory to the Green function:

$$G_{ij}(t)=\sum_n\frac{(-i)^n}{n!}\sum_{m_i,\xi_i}\int d\tau_1\dots d\tau_n\langle Tc_i(t)c_j(0)V_{m_1,\xi_1}(\tau_1)\dots V_{m_n,\xi_n}(\tau_n)\rangle \tag{3.21}$$

In the above average, the operator should not create fluxes, otherwise this term is equal to zero. So we should combine perturbations in pairs with following condition: one term in pair turns on fluxes and other one turns off. So we have:

$$\begin{aligned}G_{ij}(t)=\sum_n\frac{(-i)^{2n}}{n!2^n}\sum_{m_i,\xi_i,\zeta_i}\int d\tau_1\dots d\tau_n\\ \langle Tc_i(t)c_j(0)V_{m_1,\xi_1}(\tau_1)V_{m_1,\zeta_1}(\tau_2)\dots V_{m_n,\xi_n}(\tau_{2n-1})V_{m_n,\zeta_n}(\tau_{2n})\rangle\end{aligned} \tag{3.22}$$

We consider one of the possible time-ordering. In our case $\tau_i>\tau_j$ when $i>j$. Then:

$$\begin{aligned}\delta G_{ij}(t)=\sum_n\frac{(-i)^{2n}}{2^n}\sum_{m_i,\xi_i,\zeta_i}\int_{-\infty}^{\infty}d\tau_1\int_{-\infty}^{\tau_1}d\tau_2\dots\int_{-\infty}^{\tau_{2m-1}}d\tau_{2m}\\ \langle Tc_i(t)c_j(0)V_{m_1,\xi_1}(\tau_1)V_{m_1,\zeta_1}(\tau_2)\dots V_{m_n,\xi_n}(\tau_{2n-1})V_{m_n,\zeta_n}(\tau_{2n})\end{aligned} \tag{3.23}$$

We can apply the same argument as previous, where we have proceeded from Eq.(3.16) to Eq.(3.17), and obtain for the average the following expression:

$$\delta G_{ij}(t) = \sum_n \frac{(-i)^n}{2^{2n}} \sum_{m_i,\xi_i,\zeta_i,(p_i,q_i)} \int_{-\infty}^{\infty} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2 \ldots \int_{-\infty}^{\tau_{2m-1}} d\tau_{2m}$$
$$\langle T c_i(t) c_j(0) c_{p_1}(\tau_1) c_{q_1}(\tau_1) \ldots c_{p_n}(\tau_{2n-1}) c_{q_n}(\tau_{2n-1})\rangle$$
$$\langle c_{p_1}(\tau_1) c_{q_1}(\tau_1) V_{m_1,\xi_1}(\tau_1) V_{m_1,\zeta_1}(\tau_2)\rangle \ldots \langle c_{p_n}(\tau_{2n-1}) c_{q_n}(\tau_{2n-1}) V_{m_n,\xi_n}(\tau_{2n-1}) V_{m_n,\zeta_n}(\tau_{2n})\rangle \quad (3.24)$$

Here c_{p_i} and c_{q_i} are fermion operators, which are present in the product $V_{m_i,1}V_{m_i,2}$ like fermions c_a and c_b from Eq.(3.9) are present in the product $\sigma_i^\alpha V_i^\alpha$. After summation over all cases (with other orders of times in pairs and other orders of pairs) and after changing limits of integration we can obtain:

$$G_{ij}(t) = \sum_n \frac{(-i)^n}{n!} \int d\tau_1 \ldots d\tau_n \langle T c_i(t) c_j(0) V_{\tau_1} \ldots V_{\tau_n}\rangle \quad (3.25)$$

It is a perturbation series, where V has the following form:

$$V = -\frac{i}{4} \sum_m \sum_{c_p,c_q} V_{m,pq} c_p c_q \quad (3.26)$$

$$V = \int_0^{\infty} d\tau \langle V_{m,1}(\tau) V_{m,2}(0) c_p(0) c_q(0)\rangle + \int_{-\infty}^{0} \langle c_p(0) c_q(0) V_{m,2}(0) V_{m,1}(\tau) d\tau + (1 \leftrightarrow 2) \quad (3.27)$$

This perturbation describes a correction to the low-energy Hamiltonian. This result can be also generalized for more general case. Let us imagine that there are several terms in perturbation which togeter do not create fluxes. Such situation leads to a correction to the low-energy Hamiltonian. For example, in the case of a magnetic field operators σ_i^x,σ_i^y,σ_i^z together do not create fluxes so they lead to a correction to the low-energy Hamiltonian. In general case a correction can lead to the shift of conic point like in the case with DM interaction or a magnetic field along z axes or it can change the structure of the spectrum and create a gap, like in the general situation with a magnetic field. The time-reversal symmetry plays here the crucial role.

3.5 Time-reversal symmetry

One can note that expressions in Eq.(3.9, 3.27) have almost the same structure:

$$V=\int_0^\infty \langle V_1(\tau)V_2(0)\rangle d\tau-\int_{-\infty}^0 \langle V_2^\dagger(0)V_1^\dagger(\tau)\rangle \tag{3.28}$$

Here V_1 and V_2 are some products of spins multiplied by the coefficients, so V_i may be non-hermitian. For example in Eq. (3.9) $V_1=V_i^\alpha$ and $V_2=\sigma_i^\alpha c_a c_b$. There are two such terms in Eq.(3.27). Let $V_\alpha=\eta_\alpha C_\alpha B_\alpha$, where $\alpha=1,2$ and η is some constant. C_α is a product of some fermion operators c_i and B_α is a product of b_i. B_α satisfies the following condition : $B_1B_2=bU$, where U is a product of first integrals and b is some constant. We also would like to use operators $\tilde{V}_\alpha$ which are defined like in eq .(3.14). Then, using commutation relations, we can obtain (up to a sign) the following results:

$$\pm V=\eta_1\eta_2\int_0^\infty \langle e^{iH\tau}C_1C_2B_1B_2e^{-i(H+\tilde{V}_2)\tau}\rangle-\eta_1^*\eta_2^*\int_{-\infty}^0 \langle e^{-i(H+\tilde{V}_2)\tau}B_2^\dagger B_1^\dagger C_2^\dagger C_1^\dagger e^{-iH\tau}\rangle \tag{3.29}$$

As $B_1B_2=bU$ we obtain that:

$$\pm V=\eta_1\eta_2 b\int_0^\infty \langle TC_1(\tau)C_2(\tau)e^{-i\int_0^\tau \tilde{V}_2(\tau')d\tau'}\rangle-\eta_1^*\eta_2^*b^*\int_{-\infty}^0 \langle TC_2^\dagger(\tau)C_1^\dagger(\tau)e^{-i\int_\tau^0 \tilde{V}_2(\tau')d\tau'}\rangle \tag{3.30}$$

One can note that sets of diagrams which represent averages under integrals are the same, but diagrams has different dependence on time. To make them the same we should do several manipulations: 1) change orders of c_i in the operator $C_2^\dagger C_1^\dagger$ to obtain operator C_1C_2, it leads to the factor $(-1)^{\frac{N(N-1)}{2}}$, where N is a number of fermions in the operator C_1C_2 2)We should make the change of variables in the second term: $\tau\to-\tau$, and 3) use the parity of Green functions. After these manipulations we obtain the same set of diagrams with same arguments but signs of terms can be different. This difference is related with 1) and the parity of Green functions. From Eq.(2.16) one can find that the G_{11} and G_{22} are odd functions and $G_{12}$and G_{21} are even. As a result, the difference in sign will be $(-1)^{m+\frac{N(N-1)}{2}}$ where m is a number of odd functions. We note that this parity depends only on a number of fermions from different sublattices and does not depend on the structure of a diagram. For a diagram which have N fermion operators, where the number of operators from the second sublattice is N_2, we obtain that $m\equiv(\frac{N}{2}-N_2)(mod\ 2)$. For V we have the following expression:

$$\pm V = (\eta_1\eta_2 b - \eta_1^*\eta_2^* b^*(-1)^{N_2}) \int_0^\infty \langle TC_1(\tau)C_2(\tau)e^{-i\int_0^\tau \tilde{V}_2(\tau')d\tau'}\rangle \tag{3.31}$$

For the last step we will use a time reversal symmetry of fermion operators. To define an action of the time-resersal symmetry on these fermion operators, we can look at parity of Green functions. G_{11} and G_{22} are odd functions of time. G_{12} and G_{21} are even functions. We see that time-reversal symmetry should change sign of fermion operators from one sublattice, only, for example the second one i.e. $Tc_{\mathbf{r},1}T^{-1} = c_{\mathbf{r},1}$ and $Tc_{\mathbf{r},2}T^{-1} = -c_{\mathbf{r},2}$. Than we have:

$$b^*\eta_1^*\eta_2^* V_1 V_2 = (-1)^{N_2} b\eta_1\eta_2 T V_1 V_2 T^{-1} \tag{3.32}$$

as V_1 and V_2 is a product of spins then $TV_1V_2T^{(-1)} = (-1)^\zeta V_1V_2$ so we have:

$$\pm V = \eta_1\eta_2 b(1 - (-1)^\zeta) \int_0^\infty \langle TC_1(\tau)C_2(\tau)e^{-i\int_0^\tau \tilde{V}_2(\tau')d\tau'}\rangle \tag{3.33}$$

We conclude that $\zeta = 0 \Leftrightarrow V = 0$

We can apply this rule to Eq.(3.9) to obtain following relations:

$$\begin{aligned} TV_i^\alpha\sigma_i^\alpha c_a c_b T^{-1} &= (-1)^{\zeta_{ab}+\zeta_V+1} V_i^\alpha \sigma_i^\alpha c_a c_b \\ Tc_a c_b T^{-1} = (-1)^{\zeta_{ab}} c_a c_b &\quad TVT^{-1} = (-1)^{\zeta_V} V \end{aligned} \tag{3.34}$$

Non-zero contributions to Q comes from the terms where $\zeta_{ab} + \zeta_V = 0$. So if V_i^α is even with respect to the time reversal symmetry then $\zeta_{ab} = 0$. It means what c_a and c_b should be from the same sublattice. If V is odd then c_a and c_b should be from different sublattices. This difference will be seen in the different behaviour of the correlation functions. For example, a magnetic field leads to an oscillation term in the correlation function in opposite to DM interaction. Applying this result for Eq.(3.27) we obtain following relations:

$$\begin{aligned} TV_1V_2c_pc_qT^{(-1)} &= (-1)^{\zeta_V+\zeta_{pq}} V_1V_2c_pc_q \\ TV_1V_2T^{(-1)} = (-1)^{\zeta_V} &\quad Tc_pc_qT^{-1} = (-1)^{\zeta_{pq}} c_pc_q \end{aligned} \tag{3.35}$$

Let V_1V_2 is even under the time reversal symmetry then c_p and c_q should be from different sublatices and in Fourier domain we obtain only off-dioganal term, like in pure Kitaev model, see Eq.(2.14). Such correction leads to a shift of conic points. In opposite case, V_1V_2 is odd under this symmetry and we obtain that c_p and c_q are from the same sublattice. In the Fouirer representation we obtain diagonal terms which leads to a gap in the spectrum.

Our conclusions about correlation function and correction to the Hamiltonian can be generalized for situations when fluxes can be turned off by several operators.

Chapter 4

Experimental data and application of the results

4.1 Proximate candidates for Kitaev spin liquid

Spin liquid's properties and topological excitations make Kitaev model interesting for investigation. So a lot of people try to find materials which can be described by this model.

They have investigated several matters in search for Kitaev ground states: Na_2IrO_3,$\alpha-RuCl_3$ and $\alpha - Li_2IrO_3$. These materials have almost the same crystal structure which is shown in Fig.(4.1) and strong spin-orbit coupling. It is important, because, electrons on the last orbital of the Iridium due to strong spin-orbit coupling create a state which can be described by full momentum $j = \frac{1}{2}$. The effective low-energy Hamiltonian of the system can be written in terms of spins Eq.(4.1)

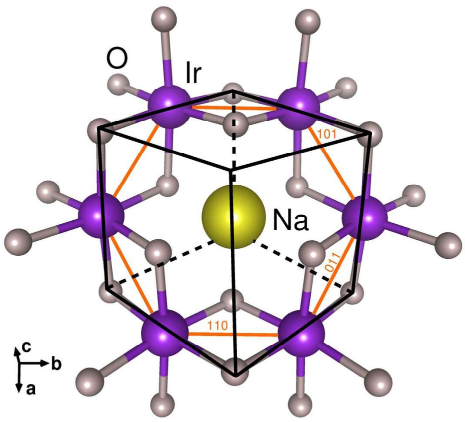
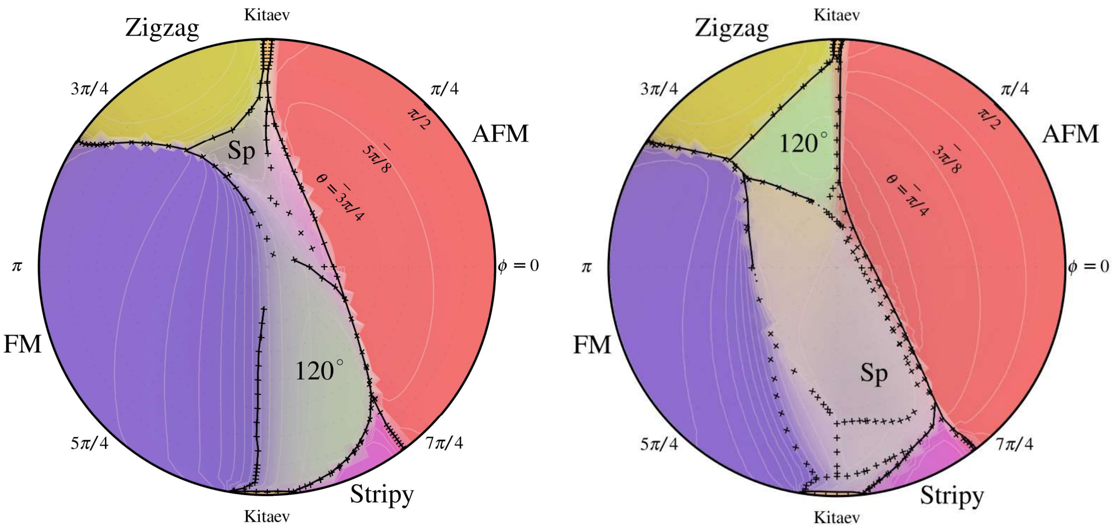


Figure 4.1

$$H = \sum_{\langle i,j\rangle \in \alpha\beta(\gamma)} J(\vec{\sigma}_i, \vec{\sigma}_j) + K\sigma_i^\gamma \sigma_j^\gamma + \Gamma(\sigma_i^\alpha \sigma_j^\beta + \sigma_i^\beta \sigma_j^\gamma) \tag{4.1}$$

It is important to understand how properties of the ground state depend on the parameters of this Hamiltonian. Numerical investigation of this question was done in Ref.[13].

Authors used an exact diagonalization for the system which consists of 24 spins and the result diagrams are present at Fig. (4.2). They show several types of the ground state. The figures show projection of upper and lower semisphere $J^2 + K^2 + \Gamma^2 = 1$ on the plane J, K here $\phi = \arctan(\frac{K}{J})$.



(a) $\Gamma > 0$ (b) $\Gamma > 0$

Figure 4.2: The phase of ground state obtained by exact diagonalyzation. Figure was taken from Ref. [13]

Unfortunately, we see that the phases with Kitaev spin-liquid like ground state are small in size. It can be due to finite-size effect, however.

In ref. [18] the constants in the Hamiltonian (4.1) were calculated from first-principles, also it was shown that an interaction of non-nearest neighbours can be important, for-example, DM interaction which was mentioned in the previous section. In the table below we show typical values of J,Γ and K.

	K	J	Γ	D
Na_2IrO_3	-16.2	1.6	2.1	0.17
α-$RuCl_3$	-7.5	-2.2	8.0	0.44
α-Li_2IrO_3	-13.0	-4.6	11.6	0.44

Here D describes the strength of DM interaction, its specific definition will be presented-below.

4.2 Magnetic field

Here we reproduce the result obtained in ref.[15]. According to our analysis, instead of a correlation function of spins we can consider a correlation function of operators Q_i^α. In presence of a magnetic field $V = \sum_i (\vec{h}, \vec{\sigma}_i)$, a bilinear operator is given by the following formula:

$$Q_i^\alpha = i\gamma_i h^\alpha V_h c_i c_{i+\alpha} \tag{4.2}$$

Here $\gamma_i = \pm 1$ for site i in the even/odd sublattice, $V_h = 2\int_0^\infty \langle \sigma_i^z(\tau)\sigma_i^z(0)\rangle$.

The spin-spin correlation function acquires the form:

$$S_{ij}^{\alpha\beta}(\mathbf{r},t) = \frac{h^\alpha h^\beta V_h^2}{\pi^2(r^2 - 3K^2t^2)}\Bigg\{ r^2 \sin\left[\frac{2\pi}{3}(\mathbf{e}_x, \mathbf{n}_\beta + \mathbf{r} - \phi_x)\right] \sin\left[\frac{2\pi}{3}(\mathbf{e}_x, \mathbf{n}_\alpha - \mathbf{r} - \phi_x)\right] - \\ -3K^2t^2 \cos\left[\frac{2\pi}{3}(\mathbf{e}_x, (\mathbf{n}_\alpha - \mathbf{n}_\beta - \mathbf{r}))\right] \cos\left[\frac{2\pi}{3}(\mathbf{r}, \mathbf{e_x})\right]\Bigg\} \tag{4.3}$$

Here, for simplicity, i and j are from even sublattice. To obtain formula with spin operators from odd sublatice one should use identity $Q_{i+\alpha}^\alpha = Q_i^\alpha$. Also, we use the following notations: $\mathbf{n}_x = 2\mathbf{n}_1$, $\mathbf{n}_y = 2\mathbf{n}_2$ and $\mathbf{n}_z = 0$. $\mathbf{e}_x$ is a unit vector along the x axes and ϕ_x are an angle between $\mathbf{r}$ and x axes.

This correlation function on can be used to calculate a structure factor. It is not zero in the vicinity of the points: $\mathbf{q}_0 = (0,0)$, $\mathbf{q} = \pm 2\mathbf{e}_x$, only. When $\boldsymbol{q}$ lies in the vicinity of $\mathbf{q}_0$ we have:

$$S^{\alpha,\beta}(\mathbf{q},\omega) - S^{\alpha\beta}(0,0) = \frac{h^\alpha h^\beta V_h^2 \theta(\omega^2 - 3K^2q^2)}{8\sqrt{\omega^2 - 3K^2q^2}}\left\{q^2 + (2\omega^2 - 3K^2q^2)\cos\left(\frac{2\pi}{3}(\mathbf{e}_x, \mathbf{n}_\alpha - \mathbf{n}_\beta)\right)\right\} \tag{4.4}$$

If $\boldsymbol{q}$ lies in the vicinity of $\mathbf{q}_\pm$ we have:

$$S^{\alpha\beta}(\mathbf{q}_\pm + \delta\mathbf{q},\omega) - S^{\alpha\beta}(\mathbf{q}_\pm, 0) = \frac{h^\alpha h^\beta V_h^2 \theta(\omega^2 - 3K^2\delta q^2)}{4}\sqrt{\omega^2 - 3K^2\delta q^2} e^{\mp i\frac{2\pi}{3}(\mathbf{e}_x, \mathbf{n}_\alpha - \mathbf{n}_\beta)} \tag{4.5}$$

Corrections for the Hamiltonian can lead to some shift of conic points, this results was obtained in [10]. In the ref. [8] was mentioned a model with a magnetic field. It has a gap in the spectrum which is proportional to $h_x h_y h_z$. It satisfies our criteria: we have three perturbations $h_x\sigma_x$, $h_y\sigma_y$ and $h_z\sigma_z$, their product does not create fluxes and it is odd under the time-reversal symmetry so it leads to a gap in the spectrum.

4.3 DM interaction

The second-neighbours DM interaction has the following form:

$$V = \sum_{\langle\langle i.j\rangle\rangle\in\gamma} (\vec{D}_\gamma, [\vec{\sigma}_i, \vec{\sigma}_j]) \tag{4.6}$$

This interaction depends on the direction of the line which connects i and j. This directions also named as x,y and z. Name x has a direction which is perpendicular to a x-type edge. Not all terms are important for our treatment. Only terms which contain D^x_x, D^y_y and D^z_z can create the same pattern of fluxes, like spin. Below we call these constant as D^x, D^y and D^z respectively. We define a vector $\mathbf{D} = (D^x, D^y, D^z)$, and D in the table is $D = |\mathbf{D}|$. Let consider a case when there is DM interaction only. In this case Q operators from 3.9 has the following form:

$$Q^\gamma_i = Q^{\alpha\beta(\gamma)}_i = iD^\gamma(Ac_{i+\alpha}c_{i+\beta} + Bc_ic_{i+\gamma+\alpha} - Bc_ic_{i+\gamma+\beta} + Cc_{i+\gamma+\alpha}c_{i+\gamma+\beta}) \tag{4.7}$$

Here A,B and C are some local correlation functions of spins. For the correlation function we have:

$$S^{\alpha\beta}_{ab}(\mathbf{r}, t) = \frac{3D^\alpha D^\beta}{4\pi^2(r^2 - 3K^2t^2)^{\frac{3}{2}}}\left[((A-C)^2 + 4B^2)\hat{\sigma}_0 + 4B(A-C)\hat{\sigma}_1\right](\hat{\sigma}_1 r^2 - \hat{\sigma}_0 3K^2t^2) \tag{4.8}$$

Here $\hat{\sigma}_0$ is the identity matrix in the space of sublattices, and $\hat{\sigma}_1$ is the first Pauli matrix. The structure factor has the following form:

$$S^{\alpha\beta}_{ab}(\mathbf{q}, \omega) - S^{\alpha\beta}_{ab}(0, 0) = \frac{3D^\alpha D^\beta \theta(\omega^2 - 3K^2q^2)}{16\sqrt{\omega^2 - 3K^2q^2}}\left[((A-C)^2 + 4B^2)\hat{\sigma}_0 + 4B(A-C)\hat{\sigma}_1\right]$$
$$\times(\hat{\sigma}_1(2\omega^2 - 9K^2q^2) - \hat{\sigma}_0(2\omega^2 - 3K^2q^2)) \tag{4.9}$$

The correction to the low energy Hamiltonian can shift conic points but can not change a structure of the spectrum. In the previous part we have seen that the form of the spectrum can be changed by a magnetic field, but the spectral gap was small as third power of the field.

4.4 DM interaction and magnetic field

In the presence of both DM interaction and a magnetic field we can obtain the changes of the structure of the spectrum and this correction is bilinear on both D and h.

In this case the Hamiltonian has the following form in the Fourier space:

$$H = \sum_{\mathbf{q}\in BZ/2} \begin{pmatrix} c^\dagger_{\mathbf{q},1} & c^\dagger_{\mathbf{q},2} \end{pmatrix} \begin{pmatrix} \Delta(\mathbf{q}) & f(\mathbf{q})+\delta(\mathbf{q}) \\ f^\dagger(\mathbf{q})+\delta(\mathbf{q})^\dagger & -\Delta(\mathbf{q}) \end{pmatrix} \begin{pmatrix} c_{\mathbf{q},1} \\ c_{\mathbf{q},2} \end{pmatrix} \tag{4.10}$$

For the infra-red asymptotic we need to know the value of $\Delta(\mathbf{q})$ at conic points. Let $\Delta = |\Delta(\mathbf{K}_1)| = |\Delta(\mathbf{K}_2)|$. Δ is a value of gap in the spectrum. The most interesting feature of Δ is that $\Delta \propto |(\mathbf{D}, \mathbf{h})|$. The behaviour of the correlation function change when $\mathbf{r} \gg l = \frac{\Delta}{\sqrt{3}K}$ ($\sqrt{3}K$ is a speed of waves in the free problem.) In the limit $r \gg l \gg Kt$ and $D^\alpha \gg h^\alpha$ we have:

$$S^{\alpha\beta}_{ab} = -\zeta_a\zeta_b \frac{D^\alpha D^\beta \tilde{C}}{4\pi^2 l^2 r^2} e^{-\frac{2r}{l}} \tag{4.11}$$

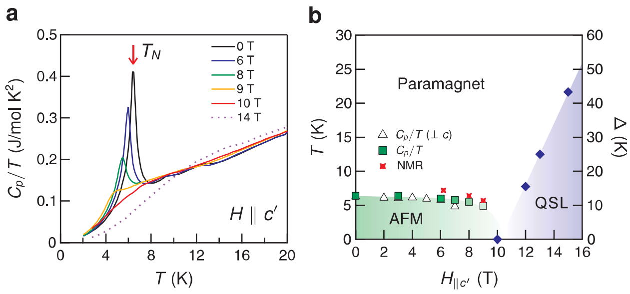
Here $\zeta_a = 1$ if a is even and -1 if a is odd.

One can note the difference between Eq. (4.3) and Eq.(4.8), in the first expression there is a oscillated term. The reasons of this difference is the time reversal symmetry of a perturbation. It was mentioned in the previous chapter.

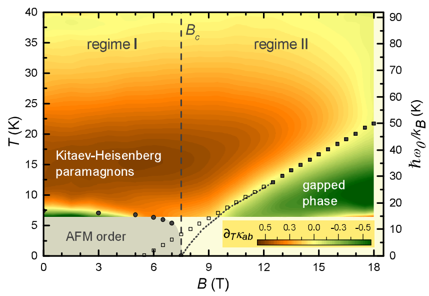
4.5 Application of the results

About a year ago several papers about experiments in $\alpha - RuCl_3$ see ref.[3],[5]. In both works was investigated $\alpha - RuCl_3$ in presence of a magnetic field. Without the field it has Neel order in the ground state. If the magnetic field is strong and is applied to destroy order, there will be phase transition at $h \approx 8T$. After this transition there is a gap in the spectrum of magnetic excitations which increase linearly with the field. Results of measurements are presented at Fig.(4.3)

In ref.[13] nuclear spin-lattice relaxation rate was measured. Using this data, the authors computed the gap in the spectrum. In ref.[5] heat conductivity in the plane of layers was measured. On the figure you can see the derivative of this thermal conductivity over the



(a) Figures are taken from ref.[13]. a) Heat capacity b) gap dependence on the field



(b) Figures are taken from ref.[[5]]. Derivative of the heat conductivity by temperature

Figure 4.3

temperature. According to author's theory the minimum of conductivity is reached when $T = \Delta$ where Δ is a size of the gap. Both works shows similar results about a size of the gap and this effect is similar to one we found in the previous section.

The presence of the gap in this material was also detected by several works. In ref. [17] a microwave absorption measurements was done. Authors measured the absorption rate on different frequencies. They founded the energy of excitation with $\vec{q} = 0$.

Unfortunately, the gap was found only in clean crystals. Ordinary, there are two phase transitions with temperatures $T_{N,1} = 7K$ and $T_{N,2} = 14K$ in this material. In clean structure there is only one at $T_{N,1}$. Detail investigation of this transition which done by a muon spin rotation/relaxation in work [19]. It was shown that in the $\alpha - RuCl_3$ there are several phase transitions in the vicinity of $T_{N,1}$ which have different spin order.

In the work [7] thermal Hall conductivity was measured. Authors compared their results with results predicted by theory, where heat are carried by neutral-charged Majorana mode. They obtained good agreement. Above results shows that $\alpha - RuCl_3$ is a good candidate for Kitaev spin liquid.

4.6 Conclusion

In our work we show how to find correlation function and correction to the low-energy Hamiltonian. We show how time reversal symmetry affects qualitatively the behaviour of the model: the behaviour of correlation function and gap in the spectrum. Our theory may help in search of materials with Kitaev spin liquid's properties.

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