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RKKY interaction in non-centrosymmetric superconductors

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1 Introduction

- relevancy of superconductors for spintronics
- latest advances in experimental set-ups
- unconventional superconductors (e.g. high T_c SC [**balatsky2006impurity**], he also has an explanation of it incl. sources on page 4)
- state of the art regarding RKKY in superconductors
- state of the art regarding non-centrosymmetric superconductors
- Atousa's work (thesis)

The interest in unconventional superconductors is rising because of the recent experimental advances in ???. They allow to characterize ??? in more detail. This deepens the knowledge about the spin-state of the cooper pairs, especially of the spin-triplet state. Spin-triplet superconductors the spin as well as the charge degree of freedom exhibit superfluid behavior leading to a variety of new phenomena in comparison to spin-singlet superconductors. Among them are several phases of superconductivity, which is already observed [**mackenzie2003superconductivity**], and an expected collective motion of spin or orbital moments with preserved cooper pairs. Additionally, the state of broken time reversal symmetry (TRS) in spin-triplet superconductors is characterized by the fact that all Cooper pairs within a single superconducting domain have the same sign of their orbital moments. This allows to describe the TRS state with chirality, which might be used as a quantum bit if it can be externally controlled.

previous work on RKKY in unconventional superconductors [**aristov˙dn˙rkky˙nodate**]:

1.1 Structure

1. Introduction
2. Theory: SWT, BCS, Non-centrosymmetric SC, RKKY, ... (everything that is known entirely)
3. Results: normal metal, SOC, SC, SOC+SC (state clearly what is known surely and what is new, present own calculations to prove the correctness of the method)

2 Theoretical Background

Hier schon den Hamiltonian einführen und dann später nur noch Lösung und Basistransformation?

2.1 Normal Metals

- density of states
- van-Hoove singularity
- spin orbit coupling (different types)
- preference of spin orientation due to spin orbit coupling
- Dzyaloshinskii-Moriya interaction

2.2 Spin Orbit Coupling

What is this?
Which types are there?

2.2.1 Rashba type

The Rashba type of SOC was formulated in 1960 [**rashba1960properties**] and its general form reads

$$H_\gamma = \sum_{\sigma,\sigma',\langle i,j\rangle} \gamma\, \mathbf{n}\,(\mathbf{d}_{i,j} \times \vec{\sigma}_{\sigma,\sigma'})\, c^\dagger_{i,\sigma} c_{j,\sigma'} \tag{2.1}$$

with σ, σ' being spin-indices and $\vec{\sigma}$ the Pauli-matrix vector. There are many different types of SOC and for the moment the type is not specified in any way. The different forms can be realized by choosing the interaction vector $\mathbf{d}_{i,j} = \hat{x}(\delta_{i+\hat{x},j} - \delta_{i-\hat{x},j}) + \hat{y}(\delta_{i+\hat{y},j} - \delta_{i-\hat{y},j}) + \hat{z}(\delta_{i+\hat{z},j} - \delta_{i-\hat{z},j})$ and the spin orbit field direction vector $\mathbf{n}$ accordingly.
For an out of plane SOC field $\mathbf{n} = \hat{z}$ in the framework used here. Consequently, the Rashba type SOC can be rewritten in k-space as

$$H_\gamma = \sum_{\sigma,\sigma',k} \gamma(k_y\hat{x} - k_x\hat{y}) c^\dagger_{k,\sigma} c_{k,\sigma'} \tag{2.2}$$

2.3 Superconductors

- it is a phase of materials, add link to explanatory video
- expelling of magnetic fields (higgs mechanism, mexican hat)
- complete loss of electrical resistivity
- type one and type two
- conventional vs. unconventional [**klam˙ludwig˙unconventional˙2010**, **balatsky2006impurity**]
- density of states [**sudbo˙asle˙superconductivity˙2004**] p.93
- LDOS comparison normal metal and superconductor

2.3.1 BCS Theory

- cooper pairs
- graph with Fermi-surface
- different pairing mechanisms
- retarding effect
- coherence length
- proof of lower energy (reference DeltaT just for fun?)
- calculation of critical temperature [**sigrist˙manfred˙introduction˙nodate**] [**sudbo˙asle˙superconductivity˙2**

BCS theory is applicable for even frequency superconductors, which are the ones treated here.

2.4 RKKY interaction

- phenomenological explanation
- follow paper that discovered it?
- does there exist a good book about this?

The concept of the Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction was firstly discussed by M. Rudermann and C. Kittel as an explanation for the broadened lines of nuclear spin resonance [**rudermann˙ma˙indirect˙1954**]. It was introduced as the indirect exchange coupling between magnetic moments in a metal via the direct hyperfine interaction with the conduction electrons. T. Kasuya and K. Yosida expanded this theory to localize inner d-electron interactions [**yosida1957magnetic**, **kasuya1956theory**].
The derivation of different characteristics of the RKKy-interaction takes a non-magnetic metal with two impurity spins, which do not directly interact with each other, as a starting point. The spin of the conduction electrons of the metal is assumed to interact locally and directly with the impurity spins, which leads to the general expression for the RKKY interaction:

$$H_{RKKY} = \sum_{i=1}^{2} J\vec{S}_i\vec{s}_i \tag{2.3}$$

The itinerant spins can be expressed via fermionic creation and annihilation operators $c^{[\dagger]}$ and transformed into k-space. Based on that expression, the effect of the RKKY-interaction onto the system can be studied via perturbation theory.
To first order in perturbation the correction to the groundstate energy is zero, because the electron system is not spin-polarized. to second order in perturbation, there is a contribution due to the fact that excited states are taken into account. If those excited states correspond to particle-hole excitations, their contribution is not vanishing. When using the formalism of spinors and the Pauli matrice, the energy correction to the groundstate energy to second order in perturbation theory reads

$$E_0^{(2)} = \frac{-J^2\hbar^2}{2N^2} \sum_{\substack{k,q \\ i,j}} \Theta_{k,k+q} e^{-iq(r_i - r_j)} \frac{\langle f|\vec{S}_i \cdot \vec{S}_j|f\rangle}{\epsilon(k+q) - \epsilon(k}$$

where Θ is the Heaveside-stepfunction, $\epsilon(k)$ is the energy of the unperturbed system, N the total number of particles and $|f\rangle$ is the spin state of the itinerant electrons.
Therefore the coupling constant J is

$$J_{ij}^{RKKY} = \frac{J^2\hbar^2}{2N^2} \sum_{k,q,m_s} \sum_{i,j=1}^{2} \Theta_{k,k+q} e^{-iq(r_i - r_j)} \frac{\langle f|\vec{S}_i \cdot \vec{S}_j|f\rangle}{\epsilon(k+q) - \epsilon(k} \tag{2.4}$$

which shows an oscillatory behavior as a function of the separation $(r_i - r_j)$ of the impurity spins. The oscillatory nature of this interaction can also be understood based on the electron density between the two impurity spins. When treating the impurity spins as ferromagnetic layers that enclose a non-magnetic layer representing the normal metal, it becomes clear that the wave function of the electron depends on the free plane-wave and a reflected wave. The probability of finding an electron at a certain position is therefore $|\Pi(x)|^2 = |exp(ikx) + Rexp(-ikx)|^2 = 1 + R^2 + 2Rcos(2kx)$ with the reflection coefficient R. Therefore the spin-density of the electrons odes also vary proportional to $cos(x)$. Since the electrons are the carries of the spin information that facilitate the indirect interaction between the fixed spins, this interaction is also of oscillatory nature.
Find a graph to show oscillatory behavior. And a graph to schematically show what kind of interaction we are talking about.

3 Methods

The subject of RKKY interaction in non-centrosymmetric superconductors is approached analytically as well as numerically. Both approaches have the goal of determining the energy spectrum

of the system in dependency on the system parameters.

3.1 Bogoliubov-de Gennes transformation

make vectors orthonormal
formulate transformation matrix and check that it is unitary, since fermionic nature of operators has to be preserved
transformation matrix is transformation between original particle operators and new quasi-particles operators

The Bogoliubov-de Gennes method (BdG) was developed by Pierre-Gilles de Gennes [**de2018superconductivity**, **zhu2016bogoliubov**] and is based on the BCS - theory. It is based on a set of coupled Schrödinger equations and enables to solve those, which allows to study more detailed and complicated superconducting systems. The main idea is that the coupled equations can be solved by introducing effective new quasi-particles, which contain all information about the system. Therefore the BdG is a complementary approach to the Ginzburg-Landau theory [**cyrot1973ginzburg**].
As first step, the system of coupled Schrödinger equations are formulated in matrix form. The focus is set onto a 4x4 matrix here, whose eigenvalue problem can be formulated as

$$\begin{bmatrix} \epsilon_k \sigma_0 & \mathbf{A}(k) \\ \mathbf{A}^\dagger(k) & -\epsilon_k \sigma_0 \end{bmatrix} \begin{pmatrix} \mathrm{a} \\ \mathrm{b} \end{pmatrix} = E_k \begin{pmatrix} \mathrm{a} \\ \mathrm{b} \end{pmatrix} \tag{3.1}$$

where $\mathbf{A}(k)$ is a 2x2 matrix with $\mathbf{A}(k)\mathbf{A}^\dagger(k) = |\mathbf{A}(k)|^2 \sigma_0$, k momentum index, σ_0 the unit matrix in Pauli matrix formulation and E_k are the eigenvalues of the matrix. The eigenvector two dimensional components $\mathbf{a}$ and $\mathbf{b}$ have to be determined.
The notation in the following is close to the notation of Ghanbari [**ghanbari˙rkky˙nodate**].
Based on Eq. **??**, the two components of the eigenvectors can be related via

$$\mathbf{b} = \frac{\mathbf{A}^\dagger(k)}{|\mathbf{A}(k)|^2}(E_k - \epsilon_k)\mathbf{a} \tag{3.2}$$

and therefore the first two eigenvectors can be written as

$$\Psi_1 = \begin{pmatrix} \mathbf{a}_1 \\ \frac{\mathbf{A}^\dagger(k)}{|\mathbf{A}(k)|^2}(E_k - \epsilon_k)\mathbf{a}_1 \end{pmatrix}, \quad \Psi_2 = \begin{pmatrix} \mathbf{a}_2 \\ \frac{\mathbf{A}^\dagger(k)}{|\mathbf{A}(k)|^2}(E_k - \epsilon_k)\mathbf{a}_2 \end{pmatrix}$$

The remaining two eigenvectors for the four dimensional matrix can be obtained in the same way from

$$\mathbf{a} = -\frac{\mathbf{A}(k)}{(E_k + \epsilon_k)}\mathbf{b}$$

and consequently read

$$\Psi_3 = \begin{pmatrix} -\frac{\mathbf{A}(k)}{(E_k+\epsilon_k)}\mathbf{b}_3 \\ \mathbf{b}_3 \end{pmatrix}, \quad \Psi_2 = \begin{pmatrix} -\frac{\mathbf{A}(k)}{(E_k+\epsilon_k)}\mathbf{b}_4 \\ \mathbf{b}_4 \end{pmatrix}$$

These eigenvectors have to be orthonormal in order to form a unitary transformation, which is needed to transform the operators without loss of information about the system. The condition for orthonormality reads $\langle \Psi_i | \Psi_j \rangle = \delta_{ij}$, where δ is the Dirac-Delta function, and takes the following form for the proposed eigenvectors

$$|\mathbf{a}_1|^2 = |\mathbf{a}_2|^2 = \frac{|\mathbf{A}(k)|^2}{|\mathbf{A}(k)|^2 + (E_k - \epsilon_k)^2}$$
$$|\mathbf{b}_3|^2 = |\mathbf{b}_4|^2 = \frac{(E_k + \epsilon_k)^2}{|\mathbf{A}(k)|^2 + (E_k + \epsilon_k)^2}$$

These factors are used as normalization for the components of the eigenvectors.
The transformation matrix P is comprised of the four eigenvectors as columns. The vector part of the components is chosen in accordance with the requirement that P is unitary and is therefore

$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}_3 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{b}_4 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

With this, the P can be written as

$$\mathbf{P} = \begin{bmatrix} \mathbf{u}_k & \mathbf{v}_k \\ -\mathbf{v}_k^\dagger & \mathbf{u}_k \end{bmatrix}$$

with the components

$$\mathbf{u}_k = \frac{E_K + \epsilon_k}{\sqrt{(e_k + \epsilon_k)^2 + |\mathbf{A}(k)|^2}} \sigma_0 \,, \quad \mathbf{v}_k = \frac{-\mathbf{A}(k)}{\sqrt{(e_k + \epsilon_k)^2 + |\mathbf{A}(k)|^2}} \tag{3.3}$$

The new quasi-particle operators that diagonalize the originally coupled set of Schrödinger equations are defined as $c' = \mathbf{P}c$.

3.2 Schrieffer-Wolff transformation

The RKKY-interaction is a second-order in perturbation phenomenon. In order to calculate analytically the correction to the energy spectrum of the unperturbed system, the so-called Schrieffer-Wolff transformation (SWT) is going to be used [**schrieffer1966relation**]. This method is based on a unitary transformation from the eigenbasis of the unperturbed system H_0 towards the basis of the effective Hamiltonian $\tilde{H} = H_0 + H_{RKKY}$.
The interaction strength of the perturbation is denoted by J and the unitary matrix U is defined as $U = e^{iS}$. This leads to a unitary transformation of the total Hamiltonian of

$$\begin{aligned} \tilde{H} &= UHU^\dagger = e^{iS} H e^{-iS} \\ &= H_0 + H_{RKKY} + i[S, H_0] + i[S, H_{RKKY}] + O(J^3) \end{aligned} \tag{3.4}$$

The expansion in the second line is going to be cut at $O(J^3)$, so that the effective Hamiltonian is determined up to $O(J^2)$. Choosing the unitary matrix such that $H_{RKKY} + i[S, H_0] = 0$ leads to an effective Hamiltonian of $\tilde{H} = H_0 + i[S, H_{RKKY}]$.
In order to get an explicit expression for $\tilde{H}$, the following ansatz is made

$$\begin{aligned} S = \sum_{k,k',\alpha,\beta} & (A_{k,k',\alpha,\beta} d^\dagger_{k,\alpha} d^\dagger_{k,-\beta} + B_{k,k',\alpha,\beta} d^\dagger_{k,\alpha} d_{k',-\beta} \\ & + C_{k,k',\alpha,\beta} d_{k',\alpha} d_{k',-\beta} + D_{k,k',\alpha,\beta} d^\dagger_{k,-\beta} d_{k',-\alpha}) \end{aligned} \tag{3.5}$$

where $d^{[\dagger]}$ are the annihilation [creation] operators for particles in the system of interest. The coefficients are explicitly determined by the requirement $H_{RKKY} + i[S, H_0] = 0$, which enables to calculate the missing commutator in Eq. (**??**).

3.3 Numerical Approach

More details here, see Lina's thesis and compare with original.pdf again, re-do 2D derivation, it looks like it's not necessary to cite Nambu basis.
it would be really cool to actually get the self consistency thing running

- Hamiltonian
- partial transformation to k-space
- degrees of freedom

- density of states
- self-consistency equation for gap

In addition to the analytical approach, the two dimensional Hamiltonian is diagonalized numerically in *python*. The formulation of the Hamiltonian is done in a spin basis with the structure of a Nambu-basis [**original.pdf**] How can I cite this? Who wrote this?. The boundary conditions are chosen to be hard-wall for the x-direction and periodic for the y-direction. Consequently, the real-space Hamiltonian has to be partially Fourier-transformed by

$$c_{\vec{i},\sigma} = \frac{1}{N_y}\sum_{k_y} c_{i_x,k_y,\sigma} e^{i(k_y i_y)}$$

That allows to express the Hamilton operator of the system as

$$H = H_0 + \frac{1}{2}\sum_{k_y} W_{k_y}^\dagger H_{k_y} W_{k_y} \tag{3.6}$$

where W_{k_y} is the vector containing B_{i_x,k_y} for all positions in x-direction i_x of the system. B_{i_x,k_y} contains the Nambu-basis for one position i_x, which has the form

$$\Psi_{i_x}^\dagger = \left(c_{i_x,\uparrow}^\dagger, c_{i_x,\downarrow}^\dagger, c_{i_x,\uparrow}, c_{i_x,\downarrow}\right) \tag{3.7}$$

The matrix H_{k_y} is of dimension $4N_x \times 4N_x$, where N_x is the number of lattice sites in x-direction. The SOC term H_{SOC} transforms under the partial Fourier transformation as

$$\begin{aligned}
H_{SOC} &= i\gamma \sum_{\langle i,j\rangle,\alpha,\beta} c_{i,\alpha}^\dagger \mathbf{n}\cdot(\mathbf{d}_{i,j}\times\vec{\sigma})\, c_{j,\beta} \\
&= \frac{i\gamma}{N} \sum_{\substack{i_x,j_x,\vec{\delta} \\ k_y,k_y',\alpha,\beta}} c_{i_x,k_y,\alpha}^\dagger \left(\vec{\delta}\cdot\mathbf{y}\sigma_x - \vec{\delta}\cdot\mathbf{x}\sigma_y\right) c_{i_x+\vec{\delta}\cdot\mathbf{x},k_y',\beta}\, e^{-ik_y i_y}\, e^{ik_y'(i_y+\vec{\delta}\cdot\mathbf{y})} \\
&= i\gamma \sum_{i_x\vec{\delta},k_y,\alpha,\beta} c_{i_x,k_y,\alpha}^\dagger \left(\vec{\delta}\cdot\mathbf{y}\sigma_x - \vec{\delta}\cdot\mathbf{x}\sigma_y\right) c_{i_x+\vec{\delta}\cdot\mathbf{x},k_y,\beta}\, e^{ik_y\vec{\delta}\cdot\mathbf{y}} \\
&= \gamma \sum_{i_x,k_y,\alpha,\beta} \Big[c_{i_x,k_y,\alpha}^\dagger (i\sigma_y)_{\alpha\beta} c_{j_x,k_y,\beta}(\delta_{j_x,i_x+1} - \delta_{j_x,i_x-1}) - c_{i_x,k_y,\alpha}(\sigma_x)_{\alpha\beta} c_{j_x,k_y,\beta}\delta_{i_x j_x} 2\sin(k_y a)\Big]
\end{aligned}$$

where $\vec{\delta}$ is the distance between two nearest-neighbors on a square lattice with lattice constant a. Therefore, there are local and nearest-neighbor terms in the SOC, although the original term contained only nearest neighbor terms. Terms local in x-direction arise due to the transformation because the nearest-neighbor in y-direction has a different k_y-value, but the same i_x-value.
The components of H_{k_y} can be expressed by the following $4x4$ matrix

$$H_{i_x,j_x,k_y} = \tag{3.8}$$
$$\begin{bmatrix}
\epsilon^\uparrow(k_y) & \xi_{i_x}^\uparrow(k_y,-\gamma) & V_{i_x,k_y}^\uparrow(\delta_{i_x,j_x+1}-\delta_{i_x,j_x-1}) & U_{i_x,k_y}^* \delta_{i_x,j_x} \\
\xi_{i_x}^\downarrow(k_y,+\gamma) & \epsilon^\downarrow(k_y) & -U_{i_x,k_y}^* \delta_{i_x,j_x} & -(V_{i_x,k_y}^\downarrow)^*(\delta_{i_x,j_x+1}-\delta_{i_x,j_x-1}) \\
(V_{i_x,k_y}^\uparrow)^*(\delta_{i_x,j_x+1}-\delta_{i_x,j_x-1}) & -U_{i_x,k_y}\delta_{i_x,j_x} & -\epsilon^\uparrow(k_y) & -\xi_{i_x}^\uparrow(k_y,-\gamma) \\
U_{i_x,k_y}\delta_{i_x,j_x} & -V_{i_x,k_y}^\downarrow(\delta_{i_x,j_x+1}-\delta_{i_x,j_x-1}) & -\xi_{i_x}^\downarrow(k_y,+\gamma) & -\epsilon^\downarrow(k_y)
\end{bmatrix}$$

with the short-hand notation

$$\begin{aligned}
\epsilon^\sigma(k_y) &= (-2t\cos(k_y))(\delta_{i_x,j_x+1} + \delta_{i_x,j_x-1}) - \mu\delta_{i_x,j_x} + J\vec{S}_{i_x}\vec{\sigma}_{\sigma\sigma}\delta_{i_x,i} \\
\xi_{i_x}^\sigma(k_y,\pm\gamma) &= \left(-2\gamma\sin(k_y a)(\sigma_x)_{\sigma-\sigma} + J\vec{S}_{i_x}\vec{\sigma}_{\sigma,-\sigma}\delta_{i_x,i}\right)\delta_{i_x,j_x} \pm \gamma(\delta_{j_x,i_x+1} - \delta_{j_x,i_x-1})
\end{aligned} \tag{3.9}$$

This Hamiltonian fulfills the relation $H_{i_x,j_x,k_y} = H_{j_x,i_x,k_y}^\dagger$, which is imposed by complex conjugating Eq. (**??**).
All sites i_x containing an impurity spin are selected by $\delta_{i_x,i}$.

This matrix describes the on-site as well as nearest-neighbor interaction of the system and the SOC is already of Rashba-type, which can be seen in the fact that triplet pairing is only considered for the case of equal spins [**frigeri2004superconductivity**]. Explain. Since there are many zero-entries in each H_{k_y} and their amount grows with system size, it is advisable to use a sparse-matrix format.
When looking at the eigenvalue equations of H_{k_y}, one finds that if E_{n,k_y} is an eigenvalue of H_{k_y} then $-E_{n,-k_y}$ is also an eigenvalue of H_{k_y}. The eigenvector of $-E_{n,-k_y}$ is found to be the complex conjugate of the eigenvector of E_{n,k_y}, when additionally the momentum is reversed. This symmetry can be exploited when diagonalizing the Hamiltonian numerically.
The diagonalized Hamiltonian can be expressed by the diagonal matrix D, which contains all eigenvalues, when the original basis W is transformed into a new basis Γ. This new basis is the eigenbasis of the Hamiltonian and defined by the relation

$$\Gamma_{k_y}^\dagger = W_{k_y}^\dagger P_{k_y} = \left(\gamma_{k_y,1}, \gamma_{k_y,2}, \dots \gamma_{k_y,4N_x}\right) \tag{3.10}$$

where P_{k_y} contains all eigenvectors as columns. The components of these eigenvectors can be labeled as $\left(u_{1,n,k_y}, v_{1,n,k_y}, w_{1,n,k_y}, x_{1,n,k_y}, u_{2,n,k_y}, \dots x_{N_x,n,k_y}\right)^T$, which leads to the definition of each single entry of the eigenbasis-vector as

$$\gamma_{k_y,n}^\dagger = \sum_{i_x} \left(c_{i_x,k_y,\uparrow}^\dagger u_{i_x,n,k_y} + c_{i_x,k_y,\downarrow}^\dagger v_{i_x,n,k_y} + c_{i_x,-k_y,\uparrow} w_{i_x,n,k_y} + c_{i_x,-k_y,\downarrow}^\dagger x_{i_x,n,k_y}\right) \tag{3.11}$$

Using the symmetry of the eigenvectors, which can be written as
$\left(w_{1,n,k_y}^*, x_{1,n,k_y}^*, u_{1,n,k_y}^*, v_{1,n,k_y}^*, w_{2,n,k_y}^*, \dots v_{N_x,n,k_y}^*\right)^T$ and therefore the eigenbasis-vector components can also be defined as

$$\gamma_{-k_y,n}^\dagger = \sum_{i_x} \left(c_{i_x,-k_y,\uparrow}^\dagger w_{i_x,n,k_y}^* + c_{i_x,-k_y,\downarrow}^\dagger x_{i_x,n,k_y}^* + c_{i_x,k_y,\uparrow} u_{i_x,n,k_y}^* + c_{i_x,k_y,\downarrow} v_{i_x,n,k_y}^*\right) \tag{3.12}$$

which also follows from the relation $W_{-k_y} = P_{-k_y}\Gamma_{-k_y}$. It follows directly, that $\gamma_{-k_y,n}^\dagger = \gamma_{k_y,n}$, which implies that not all $\gamma_{k_y,n}$ operators are independent of each other for all k_y-values what restores the correct amount of degrees of freedom.
The diagonal Hamiltonian can now be written in terms of the new operators and reads

$$H = H_0 + \frac{1}{2}\sum_{n,k_y>0} E_{n,k_y}\gamma_{n,k_y}^\dagger\gamma_{n,k_y} + \frac{1}{2}\sum_{n,k_y<0} E_{n,k_y}\gamma_{n,k_y}^\dagger\gamma_{n,k_y} + K$$

where the sum was split into a $k_y < 0$, $k_y > 0$ and $k_y = 0$ part. The latter is going to be treated in detail later and simply denoted by K for now. Substituting $E_{n,k_y} \to -E_{n,k_y}$ in the sum over $k < 0$ allows to use the relation $\gamma_{-k_y,n}^\dagger = \gamma_{k_y,n}$ in the $k < 0$ term. When renaming $k_y \to -k_y$ and apply the relation $\gamma_{-k_y,n}^\dagger = \gamma_{k_y,n}$ a second time, the Hamiltonian reads

$$H = H_0 - \frac{1}{2}\sum_{n,k_y>0} E_{n,k_y} + \sum_{n,k_y>0} E_{n,k_y}\gamma_{k_y,n}^\dagger\gamma_{k_y,n} + K$$

In order to evaluate the $k_y = 0$ term, the problem that this mode does not have a negative partner has to be resolved. That is done by apply the relation $\gamma_{-k_y,n}^\dagger = \gamma_{k_y,n}$ and using that the eigenvalues of $H - k_y$ are $-E_{n,k_y}$, since the Hamiltonian then is

$$H = H_0 - \frac{1}{2}\sum_{n,k_y>0} E_{n,k_y} + \frac{1}{2}\sum_{n,k_y>0} E_{n,k_y}\gamma_{n,k_y}^\dagger\gamma_{n,k_y} + \frac{1}{2}\sum_{n} E_{n,0}\gamma_{n,0}^\dagger\gamma_{n,0}$$

Here, the Fermi-Dirac distribution may be used again, since all γ-operators in $\sum_{n,k_y>0}$ are independent in this formulation of the Hamiltonian.
It is possible that for the $k_y = 0$ mode, $H_{k_y} = H_{-k_y}$ holds true. In that case, it also holds that if $E_{n,0}$ is an eigenvalue then so is $-E_{n,0}$. Consequently, the eigenvalues can be sorted such that the first $2N_x$ ones are negative and the last $2N_x$ ones are positive. If one of the eigenvalues is zero,

then there is a pair of eigenvalues equaling zero and the first and second half of the eigenvalues is going to contain one of them each. The final expression for the Hamiltonian is therefore

$$H = H_0 - \frac{1}{2}\sum_{n,k_y>0} E_{n,k_y} - \frac{1}{2}\sum_{E_{n,0}\geq 0} E_{n,0} + \sum_{n,k_y>0} E_{n,k_y}\gamma^\dagger_{n,k_y}\gamma_{n,k_y} + \sum_{E_{n,0}\geq 0} E_{n,0}\gamma^\dagger_{n,0}\gamma_{n,0} \tag{3.13}$$

where all operators are independent of each other.

3.3.1 Self-consistency equation

One of the most interesting observables of a superconductor is the gap-order parameter. It is defined in the context of the BCS theory explained in Sec. **??** and reads

$$\Delta_{i_x} = \frac{V_{i_x}}{N}\sum_{k_y}\langle c_{i_x,k_y,\uparrow}c_{i_x,-k_y,\downarrow}\rangle$$

In the eigenbasis Γ_{k_y} of the Hamiltonian, the gap expression transforms into

$$\begin{aligned}
\Delta_{i_x} &= \frac{V_{i_x}}{N}\left(\sum_{k_y>0}\langle c_{i_x,k_y,\uparrow}c_{i_x,-k_y,\downarrow}\rangle + \sum_{k_y<0}\langle c_{i_x,k_y,\uparrow}c_{i_x,-k_y,\downarrow}\rangle + \langle c_{i_x,0,\uparrow}c_{i_x,0,\downarrow}\rangle\right) \\
&= \frac{V_{i_x}}{N}\left(\sum_{k_y>0,n} u_{i_x,n,k_y}x^*_{i_x,n,k_y}\langle\gamma_{n,k_y}\gamma^\dagger_{n,k_y}\rangle\right. \\
&\left. + \sum_{k_y>0} w^*_{i_x,n,k_y}v_{i_x,n,k_y}\langle\gamma_{n,-k_y}\gamma^\dagger_{n,-k_y}\rangle + u_{i_x,n,0}x^*_{i_x,n,0}\langle\gamma_{n,0}\gamma^\dagger_{n,0}\rangle\right)
\end{aligned}$$

In the second step, the sum over $k_y < 0$ was replaced by the sum over $k_y > 0$ by changing the sign of k_y in the whole expression including the operators. The $k_y = 0$ term is treated the same way as in the Hamiltonian and the relations $u_{i_x,2N_x+n,0} = w^*_{i_x,n,0}$ and $x_{i_x,2N_x+n,0} = v^*_{i_x,n,0}$ are used to arrive at the final expression

$$\begin{aligned}
\Delta_{i_x} = \frac{V_{i_x}}{N}\left(\sum_{k_y>0,n}\left[w^*_{i_x,n,k_y}v_{i_x,n,k_y} - u_{i_x,n,k_y}x^*_{i_x,n,k_y}\right]f(E_{n,k_y}) + u_{i_x,n,k_y}x^*_{i_x,n,k_y}\right. \\
\left. + \sum_{E_n\geq 0}\left[w^*_{i_x,n,0}v_{i_x,n,0} - u_{i_x,n,0}x^*_{i_x,n,0}\right]f(E_{n,0}) + u_{i_x,n,0}x^*_{i_x,n,0}\right)
\end{aligned} \tag{3.14}$$

where $\langle\gamma_{n,-k_y}\gamma^\dagger_{n,-k_y}\rangle = f(E_{n,k_y})$ is used and $f(x)$ is again the Fermi-Dirac distribution.
This calculation is done for the singlet-pairing as well as for the triplet-pairing gap. For the latter the explicit form is

$$\begin{aligned}
\Delta_{t,i_x} &= \frac{V_{i_x,j_x}}{N}\sum_{k_y,\sigma}\langle c_{i_x,k_y,\sigma}c_{j_x,-k_y,\sigma}\rangle \\
&= \frac{V_{i_x,j_x}}{N}\left(\sum_{k_y>0,n}\left[w^*_{i_x,n,k_y}u_{j_x,n,k_y} - v_{i_x,n,k_y}x^*_{j_x,n,k_y}\right]f(E_{n,k_y}) + v_{i_x,n,k_y}x^*_{j_x,n,k_y}\right. \\
&\left. + \sum_{E_n\geq 0}\left[w^*_{i_x,n,0}u_{j_x,n,0} - v_{i_x,n,0}x^*_{j_x,n,0}\right]f(E_{n,0}) + v_{i_x,n,0}x^*_{j_x,n,0}\right) \\
&+ \frac{V_{i_x,j_x}}{N}\left(\sum_{k_y>0,n}\left[x^*_{i_x,n,k_y}v_{j_x,n,k_y} - u_{i_x,n,k_y}w^*_{j_x,n,k_y}\right]f(E_{n,k_y}) + u_{i_x,n,k_y}w^*_{j_x,n,k_y}\right. \\
&\left. + \sum_{E_n\geq 0}\left[x^*_{i_x,n,0}v_{j_x,n,0} - u_{i_x,n,0}w^*_{j_x,n,0}\right]f(E_{n,0}) + u_{i_x,n,0}w^*_{j_x,n,0}\right)
\end{aligned} \tag{3.15}$$

The total gap is obtained based on Eq. **??**.
Do I really use the self-consistency equation or do I just set the values? For which reasons?

3.3.2 Local Density of States

Since spin-impurities are introduced into the non-centrosymmetric superconductor and they are expected to interact and interfere with its behavior due to the local RKKY-interaction, it makes sense to study the local density of states (LDOS). It allows to understand study the local symmetry characteristics and their dependencies.
The starting point to derive the LDOS is the local charge in spin-basis, which can be expressed with the LDOS $D_i(E)$ and the occupation probability $f(E)$, which is the Fermi-Dirac distribution. That can be rewritten with the coefficients of the eigenbasis

$$\begin{aligned}\rho_i &= \int_{-\infty}^{\infty} D_i(E) f(E) dE = \sum_{\sigma} \langle c_{i,\sigma}^{\dagger} c_{i,\sigma} \rangle \\ &= \sum_n \left[\left(|u_{i,n}|^2 + |v_{i,n}|^2 \right) (1 - f(E_n)) + \left(|w_{i,n}|^2 + |x_{i,n}|^2 \right) f(E_n) \right]\end{aligned}$$

For a superconducting system, low temperatures can be assumed and therefore the Fermi-Dirac distribution can be approximated as a step-function. That changes the upper limit of the integral $\infty \to 0$ and replaces the $f(E) \to 1$, which in turn allows the formulate the charge density as

$$\begin{aligned}\rho_i &= \sum_n \left[\left(|u_{i,n}|^2 + |v_{i,n}|^2 \right) \Theta(E_n) + \left(|w_{i,n}|^2 + |x_{i,n}|^2 \right) \Theta(-E_n) \right] \\ &= \int_{-\infty}^{0} D_i(E) dE\end{aligned}$$

where $\Theta(E)$ is the Heaveside step function. The LDOS can therefore be obtained by calculating

$$D_i(E) = \sum_n \left[\left(|u_{i,n}|^2 + |v_{i,n}|^2 \right) \delta(E + E_n) + \left(|w_{i,n}|^2 + |x_{i,n}|^2 \right) \delta(E - E_n) \right] \tag{3.16}$$

In the implementation, the Dirac-delta function $\delta(E)$ is approximated by a Gaussian distribution with standard derivation of 0.05.

3.3.3 Orientation of Impurity Spins

The orientation of the impurity spins is discussed analytically in Section **??** and leads to a combination of Heisenberg, Ising and Dzyaloshinskii-Moriya terms.
For a numerical approach the symmetries of the possible impurity spin-1/2 orientations are exploited, which makes it possible to parameterize the spin-orientations and calculate their respective free energies.
What are the symmetries of the spin configurations?
Consequently, Which orientations do I have to consider?
For each of this configurations the Hamiltonian is diagonalized and the free energy of the system is calculated based on

$$F = \sum_{n,k>0} \left[-\frac{E_{n,k}}{2} - \frac{1}{\beta} \ln\left(1 + e^{-\beta E_{n,k}}\right) \right] - \sum_{E_n \geq 0} \frac{E_{n,k=0}}{2} - \sum_{E_{n,k=0} \geq 0} \frac{1}{\beta} \ln\left(1 + e^{-\beta E_{n,k=0}}\right) \tag{3.17}$$

Start with normal metal and look at its RKKY, then normal metal with SOC and RKKY, then SC with RKKY (follow Atousa on that one), finally SC with SOC and RKKY as perturbation.

4 Normal Metal with RKKY interaction

A normal metal can be described by a tight-binding model for fermions, which has the Hamiltonian

$$H_{nm} = H_{kin} + H_{pot} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$$

with the annihilation [creation] operators $c_i^{[\dagger]}$ for fermions with spin σ at lattice site i, and the hopping amplitude t. Only nearest neighbor-hopping is included as indicated by $\langle i,j\rangle$. The lattice can be chosen freely and such that comparisons to possible experimental data become more easy. The potential energy of the system is proportional to the chemical potential μ.
The Hamiltonian can be diagonalized by transforming the fermion operators from real space to k-space via a Fourier-transformation of the form

$$c_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r_i}} c_{k,\sigma} \tag{4.1}$$

and its complex conjugate. For brevity, the vector $\mathbf{k} \in \mathbb{R}^3$ Do I really have 3D here or is it only 2D? going to be written as k only.
By defining the energy $\epsilon_k = -t \sum_{\langle i,j\rangle} \exp\{(-i\mathbf{k}\delta_{ij})\}$, the Hamiltonian can be expressed as

$$H_{nm} = \sum_{k,\sigma,\sigma'} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma'} \tag{4.2}$$

The RKKY interaction as defined in Eq. (**??**) can also be Fourier transformed and then added to H_{nm}. That yields the expression

$$H^{RKKY}_{nm} = \sum_{k,\sigma,\sigma'} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma'} + \sum_{k,k',\sigma,\sigma'} \sum_i \frac{J}{N} e^{i(k-k')r_i} (\mathbf{S}_i \cdot \vec{\sigma}_{\sigma,\sigma'}) c^\dagger_{k,\sigma} c_{k',\sigma'}$$

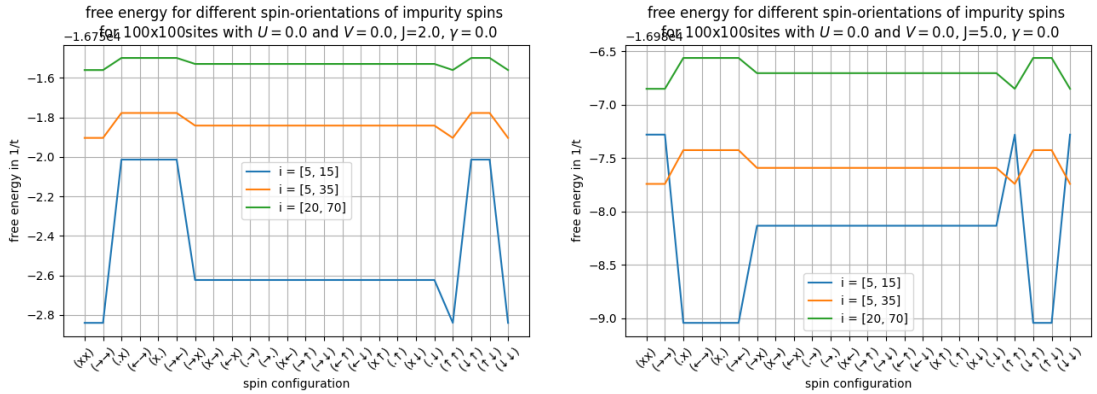
where r_i denotes the position of the impurity spin $\mathbf{S}_i$. The added term containing the RKKY-interaction can be treated as a perturbation to the normal metal, which allows to use the SWT to obtain the effective interaction.
After calculating the necessary commutators and taking the expectation value of the effective Hamiltonian, the spin structure can be identified as

$$\langle H^{RKKY}_{nm} \rangle = \langle H_{nm} \rangle - \sum_{i,j,k,k'} \left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i - r_j)}\, 2\, \mathbf{S}_i \mathbf{S}_j \, (f(E_k) - f(E_{k'})) \tag{4.3}$$

where $f(E_{k,\sigma}) = \langle c^\dagger_{k,\sigma} c_{k,\sigma} \rangle$ denotes the Fermi-Dirac distribution and $\langle H_{nm} \rangle$ is the expectation value for the unperturbed system. This spin structure is of Heisenberg form and, consequently, the preferred orientation of the impurity spins is parallel without any preference regarding the axis, meaning that the system is isotropic in spin.
The numerical solution presented in Fig. **??** displays exactly that behavior. The free energy of the system is the same for parallel orientation of the impurity spins, independent of distance and axis of alignment. Nevertheless, the differences in free energy for different spin orientations decrease with increasing distance. That can be explained by the fact, that the electrons can not travel entirely free within the metal and therefore loose information about the spin while moving from one to the other impurity spin.
In Fig. **??**, parallel spin alignment is visibly favored for longer distances between the impurity spins, but it changes to anti-parallel spin alignment for the shortest distance. The explanation lies in the spin splitting of the metal's bands due to the RKKY interaction takes the form $J\vec{\sigma}\cdot\mathbf{S}$. With increasing interaction strength J, the splitting becomes stronger and pushes the bands away from

the Fermi-energy level as illustrated in Fig. **??**. The two emerging separated bands correspond each to one spin orientation and they are filled up to the Fermi-energy.
These changes in LDOS happen only at the sites of impurity spins, but the LDOS of sites in between impurities are influenced by the changes, because of the interaction between impurity spins. As soon as the overlap of the two bands vanishes and the LDOS at impurity sites shows a gap, the LDOS of sites in between will also show a gap, if the impurity spins are aligned parallel. That can easily understood by looking at Fig. **??**, which shows the LDOS of the two impurity sites as well as one site in between. When the impurity spins are aligned anti-parallel, there are zero energy states at the sites between impurities.
These changes in LDOS in the entire system influences the free energy in such way that an AFM impurity spin orientation is preferred for short distances. For long distances, on the other hand, the influences on the LDOS on sites between impurities is too short ranged to have an effect on the free energy, since they neutralize over distance due to the imperfect conductance of electrons. Therefore the RKKY interaction strength is kept within $J \in [0, 3.5t]$ to avoid such effects.

Can I see the periodic behaviour of RKKY in these plots, too?



(a) Spin structure for normal metal with RKKY $J = 2$ (b) Spin structure for normal metal with RKKY $J = 5$

Figure 1: The free energy for different impurity spin orientations in a normal metal with RKKY interaction. The Heisenberg form of the RKKY interaction is clearly visible, as well as the dependence on the distance between the impurity spins. (a) has a weaker RKKY interaction than (b), which changes the preferred alignment from parallel to anti-parallel.

5 Normal Metal with SOC and RKKY

A local spin-orbit coupling (SOC) with coupling strength γ is introduced to the normal metal now. The SOC strength is assumed to be the same in the entire system, which is reasonable since only the bulk properties are of interest here.Do I have something about this in the theory section already? Write down the SOC term for the Hamiltonian anyways Employing the Fourier transformation of the fermion operators again, leads to the diagonalized Hamiltonian of the system, which is

$$H_{SOC} = \sum_{k,\sigma,\sigma'} [(\epsilon_k - \mu)\delta_{\sigma\sigma'} + \gamma\, \mathbf{n}\, (\mathbf{d}_k \times \vec{\sigma}_{\sigma,\sigma'})] c^\dagger_{k,\sigma} c_{k,\sigma'} \tag{5.1}$$

The Hamiltonian is therefore diagonal in momentum k, but not in spin σ. Since the SOC couples spin and momentum, this is to be expected and leads to the definition of the helicity λ, which expressed exactly this dependency. As a second step, the fermion operators are therefore transformed from spin-space to helicity-space [**samokhin2008gap**, **mukherjee˙soumya˙p˙superconductivity˙2014**] by the transformation

$$b_{k,\lambda} = \frac{Z_{k,\lambda}}{\sqrt{2|\gamma_k|}} \left(\sqrt{(|\gamma_k| + \lambda\gamma_{k,z})} c_{k,\uparrow} + \lambda \sqrt{(|\gamma_k| - \lambda\gamma_{k,z})} c_{k,\downarrow} \right) \tag{5.2}$$

where $\lambda = \pm 1$ is the helicity index, $\gamma(k) = \gamma_k$ and $Z_{k,\lambda} = 1$ for $\lambda = 1$ and $Z_{k,\lambda} = \exp(i\Phi_k)$ for $\lambda = -1$ with

$$\exp(i\Phi_k) = \frac{(\gamma_x + i\gamma_y)}{\sqrt{|\gamma|^2 - \gamma_z^2}} \tag{5.3}$$

being the phase induced by the SOC. This transformation is unitary and therefore preserves the fermionic anti-commutation relations of the c-operators.
Inserting this into the Hamiltonian in Eq.(**??**) leads to the diagonalized expression for the non-centrosymmetric material

$$H_{SOC} = \sum_{k,\lambda} \left((\epsilon_k - \mu) + \lambda|\gamma| \right) b^\dagger_{k,\lambda} b_{k,\lambda} = \sum_{k,\lambda} \xi_{k,\lambda} b^\dagger_{k,\lambda} b_{k,\lambda} \tag{5.4}$$

Therefore the energy spectrum of the spin-orbit coupled electron system in helicity basis is

$$\xi_{k,\lambda} = (\epsilon_k - \mu) + \lambda|\gamma(k)| \tag{5.5}$$

which describes the lift of the spin-degeneracy. Although each helicity-basis operator $b_{k,\lambda}$ contains both $c_{k,\uparrow}$ and $c_{k,\downarrow}$, they are weighted differently. That leads to different energies associated with the different spin-orientations.
By employing the SWT again, the spin structure of two impurity spins interacting via RKKY-interaction is found to be

$$\langle H^{RKKY}_{SOC} \rangle = \langle H_{SOC} \rangle + \sum_{i,j,k,k'} \mathbf{J}^{SOC}_{i,j,k,k'} \mathbf{S}_i \mathbf{S}_j + D^{SOC}_{i,j,k,k'} (S_{i,z} S_{j,x} - S_{i,x} S_{j,z}) \tag{5.6}$$

where the coefficients $\mathbf{J}$ and D are defined as

$$\begin{aligned} \mathbf{J}^{SOC} &= \frac{1}{2} \left(\frac{J}{N} \right) e^{i(k-k')(r_i - r_j)} \begin{pmatrix} K^{k,k'}_{+,+} + K^{k,k'}_{-,-} + K^{k,k'}_{+,-} + K^{k,k'}_{-,+} \\ K^{k,k'}_{+,+} + K^{k,k'}_{-,-} - K^{k,k'}_{+,-} - K^{k,k'}_{-,+} \\ -2(K^{k,k'}_{+,-} + K^{k,k'}_{-,+}) \end{pmatrix} \\ D^{SOC} &= \frac{1}{2} \left(\frac{J}{N} \right) e^{i(k-k')(r_i - r_j)} \left((K^{k,k'}_{+,-} - K^{k,k'}_{-,+}) \left(\frac{\gamma_{k,x} + i\gamma_{k,y}}{|\gamma_k|} - \frac{\gamma_{k',x} - i\gamma_{k',y}}{|\gamma'_k|} \right) \right) \end{aligned} \tag{5.7}$$

with $K^{k,k'}_{\lambda,\lambda'} = \frac{f(E_{k,\lambda}) - f(E_{k',\lambda'})}{\xi_{k',\lambda'} - \xi_{k,\lambda}}$
Adapt notation to the rest of the thesis's notation. Make it fit at this new position. Make it a smooth transition. The following paragraph is an interpretation of the result above
The RKKY interaction and its spin configuration has been investigated in normal metals with SOC [**gong2015dzyaloshinskii**, **imamura2004twisted**, **valizadeh˙mohammad˙m˙magnetic˙2017**].
In a 2-dimensional electron gas (2DEG), spin orbit coupling results in a twisted RKKY-interaction as shown by Imamura et al. [**imamura2004twisted**]. This is shown by looking at a 2DEG with Rashba-SOC and comparing the results for the spin-structure obtained with the Green's function formalism to the inner product of the untwisted spin space of the first spin and the twisted spin space of the second spin. Namely, the spin space of the second impurity spin is twisted as

$$\begin{aligned} S^x_2(\theta_{12}) &= \cos\theta_{12} S^x_2 + \sin\theta_{12} S^z_2 \\ S^y_2 &= S^y_2 \\ S^z_2 &= \cos\theta_{12} S^z_2 - \sin\theta_{12} S^x_2 \end{aligned}$$

where the angle $\theta = 2m\alpha|\mathbf{R}_1 - \mathbf{R}_2|$ with the SOC strength α.
The inner product with the untwisted spin space of the first impurity spin is consequently

$$\mathbf{S}_1 \cdot \mathbf{S}_2(\theta_{12}) = \cos\theta_{12} \mathbf{S}_1 \mathbf{S}_2 + \sin\theta_{12} \left(\mathbf{S}_1 \times \mathbf{S}_2 \right)_y + (1 - \cos\theta_{12}) \mathbf{S}^y_1 \mathbf{S}^y_2 \tag{5.8}$$

This corresponds to a Heisenberg-like interaction with strength $\cos\theta_{12}$, an Ising-like interaction of strength $(1 - \cos\theta_{12})$ and the y-component of a Dzyaloshinskii-Moriya interaction term with strength $\sin\theta_{12}$.
Therefore, a sign- dependency for the spin-configuration in x- and z-direction is expected, while the y-direction should be symmetric for both spin directions. The angle dependence also suggests that for no SOC the Heisenberg- like interaction is going to be the only remaining term in the

spin-structure.
Gong et al. [**gong2015dzyaloshinskii**] confirm this result, but use the Schrieffer-Wolff transformation to obtain the effective RKKY interaction in presence of SOC in a 2D optical square lattice. The Mott insulator regime is chosen since it allows to focus only on the spin degrees of freedom in this system and an external Zeeman field is added. With Rashba-type SOC, they find the effective Hamiltonian

$$H_{eff} = \sum_{\langle i,j \rangle} \sum_{\alpha=x,y,z} J_\alpha S_i^\alpha S_j^\alpha + \sum_i \mathbf{B} \cdot \mathbf{S}_i + \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) + \mathbf{S}_i \cdot \Gamma \cdot \mathbf{S}_j$$

This way of writing the spin structure says nearly nothing about the actual structure, since it allows for all possible combinations of spins
Since the spin-structure in a superconductor without SOC is of Heisenberg and Ising structure, it is similar to a normal metal without SOC. Therefore it is to be expected to find a spin-structure of the same type as Imamura et al. and Gong et al. found.
Additionally, the general spin structure for a 2DEG with SOC and RKKY was calculated with the Green's functions approach by Mohammad [**valizadeh˙mohammad˙m˙magnetic˙2017**]. The notation used in that thesis leads to a spin structure with the three terms identified earlier and reads

$$H_{eff} = J\,\mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}\,(\mathbf{S}_i \times \mathbf{S}_j) + \mathbf{S}_i \cdot \overleftrightarrow{\Gamma} \cdot \mathbf{S}_j \tag{5.9}$$

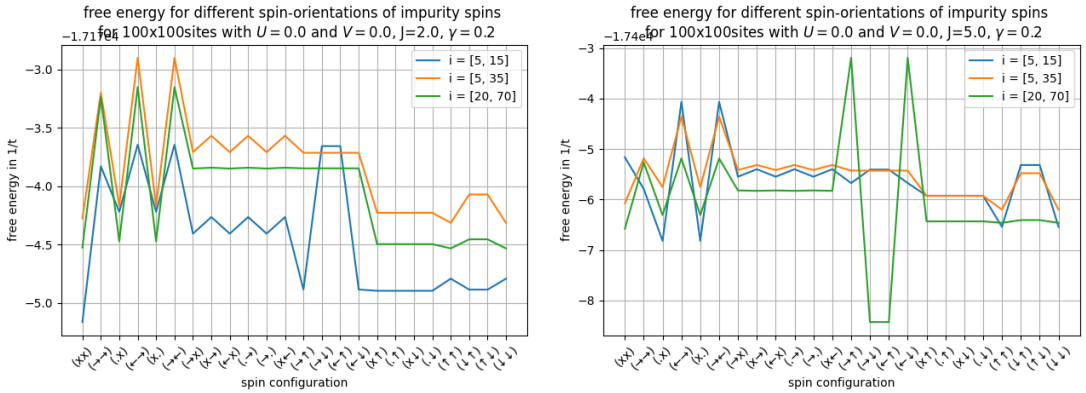
This notation of the spin structure is not unique, since Mohammad chooses a specific representation for the Green's functions and assigns very specific combinations of them to the coefficients, which is not given naturally from the problem (see Eq.3.7, 3.9, 3.10)
There is no magnetic field and therefore no Zeeman splitting term present in this approach. Consequently, this notation is going to be used in this work to denote the different spin terms of a non-centrosymmetric superconductor with RKKY interaction. Add Mohammad to explanation, add Frigeri for explanation of preferred orientation of spin because of SOC Since parts of this spin structure stem solely from SOC, the preferred spin direction can be explained with the direction of the SOC as done by Frigeri et al. [**frigeri2004superconductivity**]. In their work, the SOC is defined as $H_{RKKY}^{\text{Frigeri}} = \alpha \sum_{k,s,s'} \mathbf{g_k} \sigma_{s,s'} c_{k,s}^\dagger c_{k,s'}$, where σ is the Pauli matrix vector, s, s' are spin indices and $\mathbf{g}_k = -\mathbf{g}_{-k}$ is the SOC vector. This term is embedded into a superconductor that consequently exhibits singlet and triplet pairing. The coupling depends on the difference of DOS on the two separated Fermi surfaces and therefore is of order $\alpha/\epsilon_F << 1$, where ϵ_F is the Fermi energy of the higher Fermi surface. That allows to decouple the singlet and triplet gap equations and to find the transition temperature T_c for singlet and triplet pairing separately. For the singlet pairing the transition temperature is found to be given by

$$\ln\left(\frac{T_c}{T_{cs}}\right) = O\left(\frac{\alpha^2}{\epsilon_F^2}\right)$$

which means that the transition temperature essentially is the same with and without SOC.
For the triplet pairing the transition temperature is given by

$$\ln\left(\frac{T_c}{T_{ct}}\right) = 2\langle\left(|\mathbf{d}(\mathbf{k})|^2 - |\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k})|^2\right) f(\rho_k)\rangle_k + O\left(\frac{\alpha^2}{\epsilon_F^2}\right) \tag{5.10}$$

where $\mathbf{d}(\mathbf{k})$ is the normalized triplet gap function and the function $f(\rho)$ is dependent on the SOC, but not relevant for the further argumentation and therefore not specified here. The highest possible transition temperature is according to Eq. (**??**) reached at $T_c = T_{ct}$, which is the case for $\mathbf{d}(\mathbf{k}) || \mathbf{g_k}$. This suggests a preferred spin alignment parallel to the SOC and that there might be triplet states, which are unaffected by the lack of inversion symmetry.



(a) LDOS for SOC with RKKY $J = 2$

(b) LDOS for SOC with RKKY $J = 5$

Figure 2: The free energy for different impurity spin orientations in a normal metal with SOC and RKKY interaction. The Heisenberg form of the RKKY interaction is clearly visible, as well as the dependence on the distance between the impurity spins.(a) has a weaker RKKY interaction than (b), which changes the preferred alignment from parallel to anti-parallel.

6 Superconductor with RKKY

Atousa's PhD thesis covers nearly everything A superconductor can be described as a normal metal with an additional attractive interaction term between two fermions. The Hamiltonian consequently takes the from

$$H_{SC} = H_{nm} + \sum_i V c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow}$$

where $V < 0$ Is it really < 0? denotes the strength of the attractive potential, which is a BCS on-site attractive interaction.
As the first step to diagonalize this Hamiltonian, the attractive interaction term is transformed into k-space and a mean-field treatment is performed as introduced in Sec. **??**. H_{SC} reads afterwards

$$H_{SC} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \sum_{k,\sigma} \left[\Delta c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} + \Delta^* c_{-k,\downarrow} c_{k,\uparrow} \right] - \frac{|\Delta|^2}{V}$$

The attractive interaction leads to an s-wave superconductor with $\Delta \in \mathrm{R}$. How do I know that? Important, so I can later distinguish the p-wave case.
Secondly, a BdG transformation as described in Sec. **??** is applied which defines new fermion operators as

$$\begin{aligned} c_{k,\sigma} &= \eta_k \, \gamma_{k,\sigma} + \sigma \, \nu_k \, \gamma^\dagger_{-k,-\sigma} \\ c^\dagger_{-k,-\sigma} &= -\sigma \, \nu_k \, \gamma_{k,\sigma} + \eta_k \, \gamma^\dagger_{-k,-\sigma} \end{aligned}$$

where

$$\begin{aligned} \eta_k &= \frac{(\sqrt{(\epsilon_k - \mu)^2 + \Delta^2} + \epsilon_k - \mu)}{\sqrt{(\sqrt{(\epsilon_k - \mu)^2 + \Delta^2} + \epsilon_k - \mu)^2 + \Delta^2}} \\ \nu_k &= \frac{\Delta}{\sqrt{(\sqrt{(\epsilon_k - \mu)^2 + \Delta^2} + \epsilon_k - \mu)^2 + \Delta^2}} \end{aligned}$$

and the notation is adapted from Ghanbari [**ghanbari˙rkky˙nodate**].
Ultimately, the diagonalized H_{SC} takes the form

$$\begin{aligned} H_{SC} &= -\frac{|\Delta|^2}{V} + \sum_k (\epsilon_k - \mu) + \sum_{k,\sigma} \sqrt{(\epsilon_k - \mu)^2 + \Delta^2} \left(\gamma^\dagger_{k,\sigma} \gamma_{k,\sigma} - \frac{1}{2} \right) \\ &= -\frac{|\Delta|^2}{V} + \sum_k (\epsilon_k - \mu) + \sum_{k,\sigma} E^{SC}_k \left(\gamma^\dagger_{k,\sigma} \gamma_{k,\sigma} - \frac{1}{2} \right) \end{aligned}$$

The RKKY interaction is treated perturbatively again and therefore an SWT is applied. The ansatz $S = \sum_{k,k',\alpha,\beta} (A_{k,k',\alpha,\beta} \gamma^\dagger_{k,\alpha} \gamma_{k',\beta} + B_{k,k',\alpha,\beta} \gamma^\dagger_{k,\alpha} \gamma^\dagger_{-k',-\beta} + C_{k,k',\alpha,\beta} \gamma_{-k,-\alpha} \gamma_{k',\beta} + D_{k,k',\alpha,\beta} \gamma_{-k,-\alpha} \gamma^\dagger_{-k',\beta})$ is used in the SWT and yields the four coefficients

$$\begin{aligned} A_{k,k',\alpha,\beta} &= i \sum_i \frac{J}{N} e^{i(k-k')r_i} \left(\mathbf{S}_i \cdot \vec{\sigma}_{\alpha,\beta} \right) \frac{\eta^*_k \eta_{k'}}{E_{k'} - E_k} \\ B_{k,k',\alpha,\beta} &= -\beta i \sum_i \frac{J}{N} e^{i(k-k')r_i} \left(\mathbf{S}_i \cdot \vec{\sigma}_{\alpha,\beta} \right) \frac{\eta^*_k \nu_{k'}}{E_{-k'} + E_k} \\ C_{k,k',\alpha,\beta} &= \alpha i \sum_i \frac{J}{N} e^{i(k-k')r_i} \left(\mathbf{S}_i \cdot \vec{\sigma}_{\alpha,\beta} \right) \frac{\nu^*_k \eta_{k'}}{E_{k'} + E_{-k}} \\ D_{k,k',\alpha,\beta} &= \alpha\beta i \sum_i \frac{J}{N} e^{i(k-k')r_i} \left(\mathbf{S}_i \cdot \vec{\sigma}_{\alpha,\beta} \right) \frac{\nu^*_k \nu_{k'}}{-E_{-k'} + E_{-k}} \end{aligned} \tag{6.1}$$

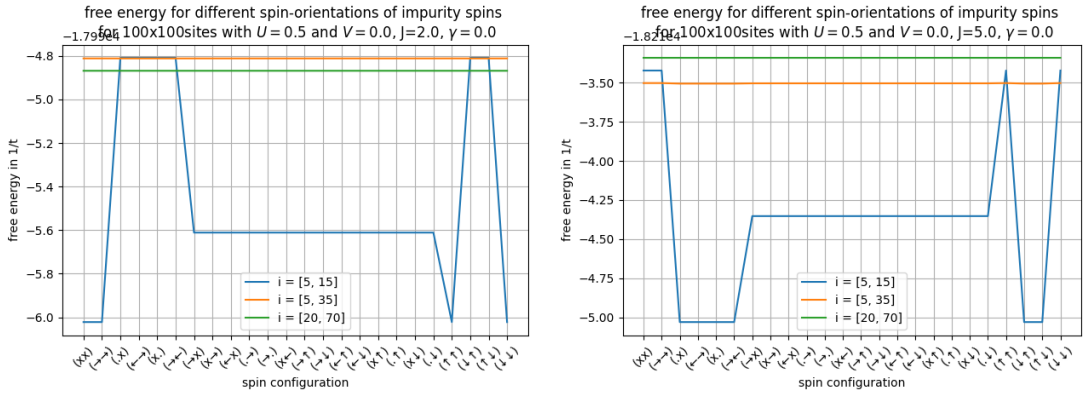
Based on this coefficients, the effective interaction H^{RKKY}_{SC} can be calculated. After some algebra, $\langle H^{RKKY}_{SC} \rangle$ is determined and the spin structure can be written in form of Heisenberg interaction:

$$\langle H^{RKKY}_{SC} \rangle = \langle H_{SC} \rangle + \sum_{i,j,k,k'} J^{SC} \mathbf{S}_i \mathbf{S}_j \tag{6.2}$$

where J^{SC} is defined as

$$\begin{aligned} J^{SC} =& \sum_{k,k'} \left(\frac{J}{N} \right)^2 e^{i(k-k')(r_1 - r_2)} \\ & \times \left[\left(|\eta_k \eta_{k'}|^2 + |\nu_k \nu_{k'}|^2 \right) \frac{f(E_k) - f(E_{k'})}{E_{k'} - E_k} - 2\eta^*_k \eta_{k'} \nu^*_k \nu_{k'} \frac{f(E_{k'}) - f(E_k)}{E_{k'} - E_k} \right] \end{aligned} \tag{6.3}$$

Numerically, the same spin structure is found as can be seen in Fig. **??** The switch between FM and AFM spin orientation for $J > 3.8t$ has the same reasons as in a normal metal. Additionally, in a superconductor the distance between impurities has consequently no influence, since electrons are conduct perfectly.
Therefore the RKKY interaction strength is kept within $J \in [0, 3.5t]$ to avoid such effects for superconducting systems, too.



(a) Spin structure for SC with RKKY $J = 2$ (no SOC) (b) Spin structure for SC with RKKY $J = 5$ (no SOC)

Figure 3: The free energy of a superconductor with RKKY interaction for different orientations of the two impurity spins. (a) has a weaker RKKY interaction than (b), which changes the preferred alignment from parallel to anti-parallel.

7 Superconductor with SOC and RKKY

The interactions within a non-centrosymmetric superconductor can be expressed by the following Hamiltonian:

$$H_{uSC} = H_{SOC} + H_{int} \tag{7.1}$$

The diagonalization of H_{SOC} is already known and written out in Eq. (**??**), therefore the attractive interaction between electrons H_{int} has to be added and the final Hamiltonian diagonalized. The RKKY interaction is going to be treated as a perturbation to that Hamiltonian.
The attractive interaction term of the non-centrosymmetric superconductor is based on BCS theory and reads in helicity space

$$H_{int} = \sum_{k,k',q} \sum_{\alpha,\alpha',\beta,\beta'} -\frac{1}{2} V_{\alpha,\alpha',\beta,\beta'}(k,k',q) b^\dagger_{k,\alpha} b^\dagger_{-k+q,\beta} b_{-k'+q,\beta'} b_{k',\alpha'}$$

where α, β are helicity-band-indices and $V_{\alpha,\alpha',\beta,\beta'}(k,k',q)$ denotes the interaction strength. The SOC is assumed to be large compared to the size of the gaps, which suppresses interband hopping.
Maybe: Reference numerical study on what this actually means
Therefore, the helicity indices are set to $\alpha = \beta = \lambda$ and $\alpha' = \beta' = \lambda'$.
Since the phase space changes with the value of q and is maximal for $q = 0$, all other contributions are negligibly small for large enough SOC [**samokhin2004cept**, **samokhin2008gap**].
This leads to the following expression of the interaction term

$$H_{int} = \sum_{k,k'} \sum_{\lambda,\lambda'} -\frac{1}{2} V_{\lambda,\lambda'}(k,k') b^\dagger_{k,\lambda} b^\dagger_{-k,\lambda} b_{-k',\lambda'} b_{k',\lambda'} \tag{7.2}$$

which allows for intraband pairing as well as pair-hopping.
Next, a mean-field approximation is done by introducing the average $a_{k,\lambda} = \langle b_{-k,\lambda} b_{k,\lambda} \rangle$. The deviation from this average is assumed to be small in the system, such that the approximation $b_{-k,\lambda} b_{k,\lambda} = a_{k,\lambda} + \delta_{k,\lambda}$ holds, when disregarding terms of order δ^2.
This allows to rewrite the Hamiltonian (**??**) as

$$H_{int} = \sum_{k,k',\lambda,\lambda'} -\frac{1}{2} V_{\lambda,\lambda'}(k,k') \left[a^\dagger_{k,\lambda} b_{-k',\lambda'} b_{k',\lambda'} + a_{\lambda'}(k') b^\dagger_{k,\lambda} b^\dagger_{-k,\lambda} - a^\dagger_\lambda(k) a_{k',\lambda'} \right] \tag{7.3}$$

By defining the order parameter

$$\Delta_{k,\lambda} = \sum_{\lambda',k'} V_{\lambda,\lambda'}(k,k') a_{k',\lambda'} \tag{7.4}$$

which is called gap in the BCS theory, the Hamiltonian (**??**) can be further rewritten into the form

$$H_{int} = -\sum_{k,\lambda} \frac{1}{2} \left[\Delta_{k,\lambda} b^{\dagger}_{k,\lambda} b^{\dagger}_{-k,\lambda} + \Delta^{\dagger}_{k,\lambda} b_{-k,\lambda} b_{k,\lambda} \right] + \Delta_{k,\lambda} a^{\dagger}_{k,\lambda} \tag{7.5}$$

where the last term is constant and is going to be disregarded for now.

7.1 Singlet and Triplet Pairing Interaction

The attractive interaction between electrons in a non-centrosymmetric superconductor does not only lead to spin-singlet pairs but also to spin-triplet pairs [QUELLE]. The Hamiltonian for attractive electron interaction in the helicity basis is introduced in Eq. **??** and treated with a mean field approach it reads

$$H_{int} = -\frac{1}{2} \sum_{k,\lambda} \left(\Delta_{k,\lambda} b^{\dagger}_{k,\lambda} b^{\dagger}_{-k,\lambda} + h.c. \right) \tag{7.6}$$

where the constant term is neglected (compare Eq. **??**).
The Hamiltonian including tight binding model and spin-orbit-coupling is diagonalized by fermionic operators in helicity space and its eigen-energies are symmetric in k. That allows to write the operation of the time-reversal operator $K = i\sigma_y K_0$, where K_0 is the complex conjugation, acting on a state $|k,\lambda\rangle$ as $K|k,\lambda\rangle = t_{k,\lambda}|-k,\lambda\rangle$ [**samokhin2008gap**]. Here, the nontrivial phase factor $t_{k,\lambda}$ is defined and for the eigenbasis in helicity space it reads

$$t_{k,\lambda} = \lambda \frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|} \tag{7.7}$$

and therefore depends on the lattice symmetry as well as the chosen type of SOC. Note that this is exactly the phase factor introduced for the basis transformation between the fermion operators in spin-space and helicity space in Eq. **??**
The phase factor allows to write the interaction potential and the gap as

$$V_{k,k',\lambda,\lambda'} = t_{k,\lambda} t^{*}_{k',\lambda'} \tilde{V}_{k,k',\lambda,\lambda'} \tag{7.8}$$

$$\Delta_{k,\lambda} = t_{k,\lambda} \tilde{\Delta}_{k,\lambda} \tag{7.9}$$

In addition, it is possible to split the gap in the spin-space into positive and negative helicity parts

$$\Delta_{k,\sigma,\sigma'} = \left[\left(\Delta_{s,k} + \mathbf{d}_k \sigma \right) i\sigma_y \right]_{\sigma,\sigma'} \tag{7.10}$$

$$\Delta_{s,k} = \frac{\tilde{\Delta}_{k,+} + \tilde{\Delta}_{k,-}}{2}$$

$$\mathbf{d}_k = \frac{\tilde{\Delta}_{k,+} - \tilde{\Delta}_{k,-}}{2} \gamma_k = \Delta_{t,k} \frac{\gamma_k}{|\gamma_k|}$$

This is a 2x2 matrix expressed in helicity basis variables for the different possible spin-configurations. Furthermore, the definition of $\mathbf{d}_k$ implies that only the orientation parallel to the SOC is allowed. In the case of Rashba-SOC, it is possible to specify the expression for $\mathbf{d}_k$ in terms of the SOC vector γ_k and the triplet-pairing strength Δ_t [**Ikegaya˙2021˙tunableMajorana**], so that the total gap reads in spin-space

$$\Delta_k = \begin{pmatrix} -i\frac{\Delta_{t,k}}{|\gamma_k|}(k_x + ik_y) & \Delta_{s,k} \\ -\Delta_{s,k} & i\frac{\Delta_{t,k}}{|\gamma_k|}(k_y - ik_x) \end{pmatrix} \tag{7.11}$$

For a square lattice, the interaction potential can be expressed as a 2x2 matrix of the structure [**samokhin2008gap**]

$$\tilde{V}_{k,k',\lambda,\lambda'} = \frac{1}{2} V_g \left(\sigma_0 + \sigma_x \right) + \frac{1}{2} \lambda\lambda' V_{u,k,k'} \left(\sigma_0 - \sigma_x \right) \tag{7.12}$$

$$= \begin{bmatrix} \tilde{V}^{d}_{k,k',\lambda,\lambda'} & \tilde{V}^{o}_{k,k',\lambda,\lambda'} \\ \tilde{V}^{o}_{k,k',\lambda,\lambda'} & \tilde{V}^{d}_{k,k',\lambda,\lambda'} \end{bmatrix}$$

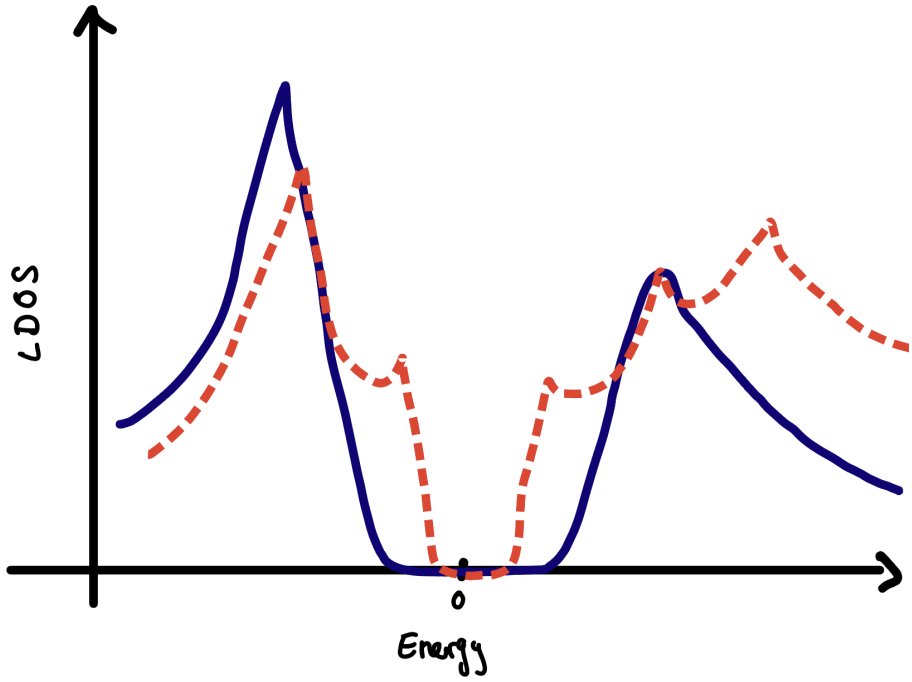


Figure 4: General behavior of singlet-pairing (blue, continuous) and triplet-pairing (red, dashed) superconducting gaps. This should be replaced by one of my python graphs and the characteristics explained with the help of that. I also need another reference to make this point, best one with nice graphs.

where $V_{g[u]}$ represents the even [odd] parts of the interaction in spin-basis. The case of only singlet-pairing corresponds to $V_u = 0$ and $V_g \neq 0$.

Furthermore holds for a square lattice that SOC generally is $\gamma(\mathbf{k}) = \gamma_0 \mathbf{k}$ and an attractive interaction is most likely mediated by phonons, which leads to a k-independent even part V_g. The resulting gap function is isotropic, because phonons lead to local interactions in most cases. The magnitudes of the gaps corresponding to the different helicity bands can generally be different and their difference depends on the strength of the spin-orbit coupling [**samokhin2008gap**]. Their ratio determines the ratio $|\mathbf{d}_k|/|\Delta_{s,k}|$ and suggests that for weak SOC singlet-pairing dominates while triplet-pairing dominates for strong SOC.

What do I expect to be the influence of the triplet pairing on the RKKY?
Since the triplet-pairing mode allows for non-zero spin of Cooper pairs, these Cooper pairs can potentially influence the RKKY interaction. Single electrons and Cooper pairs have different movement behaviors, which can lead to differences in the RKKY interaction caused by the triplet-pairs. They are an effect of SOC, which in itself has already an impact or not???

Taking the triplet-pairing into account alters the shape of the gap expected to be seen in the density of states. For singlet pairing, there is one region close to $E = 0$ where the density of states becomes zero. It is clearly visible for a large enough attractive potential U and the typical shape can be seen in Fig. **??** when looking at the continuous line. The dotted line depicts the gap when influenced by triplet-pairing. There the shape changes to two overlapping gaps, which can be seen by the step-like behavior of the density of states next to the singlet gap.

7.2 Diagonalization

Combining all individual terms of the Hamiltonian, the system can be described by

$$\begin{aligned} H_0 &= H_{kin} + H_{pot} + H_{SOC} + H_{int} \\ &= \sum_{k,\lambda} \frac{1}{2} \phi_k^\dagger \begin{bmatrix} \xi_{k,\lambda} & -\Delta_{k,\lambda} \\ -\Delta_{k,\lambda}^\dagger & -\xi_{-k,\lambda} \end{bmatrix} \phi_k + \sum_k \xi_k \end{aligned} \tag{7.13}$$

with the basis vectors $\phi_k^\dagger = (b_{k,\lambda}^\dagger, b_{-k,\lambda}^\dagger)$ and ϕ_k its complex conjugate.
This matrix can easily be diagonalized and has eigenvalues

$$E_{k,\lambda}^{\pm} = \pm\sqrt{\xi_{k,\lambda}^2 + |\Delta_{k,\lambda}|^2} \tag{7.14}$$

which have been simplified by using that time reversal symmetry is preserved $\epsilon_k = \epsilon_{-k}$.
The components of the eigenvectors are

$$\eta_{k,\lambda} = \frac{E_{k,\lambda}^+ + \xi_{k,\lambda}}{\sqrt{(E_{k,\lambda} + \xi_{k,\lambda})^2 + |\Delta_{k,\lambda}|^2}} \tag{7.15}$$

$$\nu_{k,\lambda} = \frac{\Delta_{k,\lambda}}{\sqrt{(E_{k,\lambda} + \xi_{k,\lambda})^2 + |\Delta_{k,\lambda}|^2}} \tag{7.16}$$

and the eigenvectors read $\mathrm{v}_1^\dagger = (\eta_{k,\lambda}, \nu_{k,\lambda})$ and $\mathrm{v}_2^\dagger = (\nu_{k,\lambda}^\dagger, \eta_{k,\lambda})$ [**ghanbari˙rkky˙nodate**].
The diagonalized Hamiltonian can therefore expressed in the form of a Fermi-gas

$$H_0 = \sum_{k,\lambda} \left[E_{k,\lambda}^+ (d_{k,\lambda}^\dagger d_{k,\lambda} - d_{-k,\lambda}^\dagger d_{-k,\lambda}) \right] + \frac{|\Delta|^2}{V} + \sum_k \xi_k - \sum_k E_k \tag{7.17}$$

where $d^{[\dagger]}$ is the annihilation [creation] operator for the quasi-particles that diagonalize the total Hamiltonian. They are defined via the transformation from the helicity basis with matrix $P_{k,\lambda}$, which contains the eigenvectors as columns.

$$\begin{pmatrix} d_{k,\lambda} \\ d_{-k,\lambda}^\dagger \end{pmatrix} = \begin{bmatrix} \eta_{k,\lambda} b_{k,\lambda} + \nu_{k,\lambda}^\dagger b_{-k,\lambda}^\dagger \\ \nu_{k,\lambda} b_{k,\lambda} + \eta_{k,\lambda} b_{-k,\lambda}^\dagger \end{bmatrix} \tag{7.18}$$

The anti-commutation-relations of the d-operators are fermionic again, since $P_{k,\lambda}$ is unitary.

7.3 Free Energy and Gap Equation

The Hamiltonian in Eq. (**??**) has the form of a Fermi-gas, so the partition function can be calculated based on

$$Z = \prod_{k,\lambda} \left(1 + e^{-\beta E_{k,\lambda}}\right) \left(1 + e^{\beta E_{k,\lambda}}\right) e^{-\beta \Delta_{k,\lambda} a_{k,\lambda}^\dagger + \sum_k \xi_k - \sum_k E_k} \tag{7.19}$$

where $\beta = 1/k_B T$, when it is not an index, and $E_{k,\lambda} = E_{k,\lambda}^+$ [**sudbo˙asle˙superconductivity˙2004**].
From that the free energy can be calculated as $F = -\frac{1}{\beta} \ln(Z)$ with $ln()$ being the natural logarithm.
The gap function is the functional derivative of the free energy with respect to the order parameter

i.e. gap $\Delta_{k,\lambda}$:

$$\frac{\partial F}{\partial \Delta_{k,\lambda}} \tag{7.20}$$
$$= -\frac{1}{\beta}\frac{\partial}{\partial \Delta_{k,\lambda}} \sum_{k,\lambda} \left[\ln\left(1+e^{-\beta E_{k,\lambda}}\right) + \ln\left(1+e^{\beta E_{k,\lambda}}\right) + \ln\left(e^{-\beta \Delta_{k,\lambda} a^\dagger_{k,\lambda} + \sum_k \xi_k - \sum_k E_k}\right)\right]$$
$$= \frac{\partial E_{k,\lambda}}{\partial \Delta_{k,\lambda}}\left(\frac{e^{-\beta E_{k,\lambda}}}{1+e^{-\beta E_{k,\lambda}}} - \frac{e^{\beta E_{k,\lambda}}}{1+e^{\beta E_{k,\lambda}}}\right) + \frac{\partial}{\partial \Delta_{k,\lambda}}\left(\Delta_{k,\lambda} a^\dagger_{k,\lambda} + \sum_k \xi_k - \sum_k E_k\right)$$
$$= \frac{\partial E_{k,\lambda}}{\partial \Delta_{k,\lambda}} \tanh\left(\frac{\beta E_{k,\lambda}}{2}\right) + \frac{\partial}{\partial \Delta_{k,\lambda}}\left(\Delta_{k,\lambda} a^\dagger_{k,\lambda} + \sum_k \xi_k - \sum_k E_k\right)$$
$$= \frac{\Delta^\dagger_{k,\lambda}}{2E_{k,\lambda}} \tanh\left(\frac{\beta E_{k,\lambda}}{2}\right) - a^\dagger_{k,\lambda} \tag{7.21}$$

Changing the derivative and identifying the tanh lead to the final expression in Eq. (**??**).
Setting this to zero allows to find the extrema of the free energy. Since the free energy is always bound from below, there is at least one minimum to find. In order to make sure that the found extremum is that minimum, one has to reinsert the following expression of the gap equation into the free energy:

$$0 = -\sum_{k,\lambda} V_{k,k',\lambda,\lambda'}\left[\frac{\Delta^\dagger_{k,\lambda}}{4E_{k,\lambda}} \tanh\left(\frac{\beta E_{k,\lambda}}{2}\right) - a^\dagger_{k,\lambda}\right]$$
$$\Leftrightarrow \Delta^\dagger_{k,\lambda} = -\sum_{k,\lambda} V_{k',k',\lambda,\lambda'} \frac{\Delta^\dagger_{k,\lambda}}{4E_{k,\lambda}} \tanh\left(\frac{\beta E_{k,\lambda}}{2}\right) \tag{7.22}$$

The complex conjugate of the gap equation can be acquired the same way as this one, but the derivative of the free energy is taken with respect to $\Delta^\dagger_{k,\lambda}$.

7.3.1 Andreev Reflection

Add explanation of Andreev states and explanation for when they are present by Eschrig.
Explanation of Anreev is missing completely!
It as something to do with electron (hole) approaching a material, where there is a gap while there is no gap in energy in the current system, which leads to the electron (hole) to be reflected as a hole (electron), while a Cooper pair is formed in the material that has the energy gap. [**ghanbari˙rkky˙nodate**]
In a superconducting system that allows for triplet pairing, the surface states are strongly influenced by the relative magnitude of the singlet and triplet gap order parameter Δ_s and Δ_t, respectively. To see that, the surface or boundary conditions in wave function formalism are defined by setting the wave function to zero at the boundary. Based on that the bound state condition can be expressed in dependence of singlet and triplet gap as well as the energy of the system and a proportionality constant $\xi \leq 1$ [**eschrig2010theoretical**]. This bound state condition reads

$$\sqrt{(\Delta_1^2 - E^2)(\Delta_2^2 - E^2)} = \frac{1-\xi}{1+\xi}(E^2 + \gamma\Delta_1\Delta_2)$$
$$\xi = 1 \quad \text{for} \quad \Theta_c < |\Theta_2| \leq \pi/2$$
$$\xi = \frac{\sin^2(\frac{1}{2}[\Theta_1 + \Theta_2])}{\cos^2(\frac{1}{2}[\Theta_1 - \Theta_2])} \quad \text{for} \quad |\Theta_2| \leq \Theta_c$$

with $\xi \leq 1$, $\cos\Theta_1 = k_{1x}/k_1$ and $\cos\Theta_2 = k_{2x}/k_2$. And the critical angle $\Theta_C = \arcsin(k_1/k_2)$. Therefore, the proportionality constant depends on the relative magnitude of singlet and triplet gap. The bound state condition reveals that only for $|\Theta_2| \leq \Theta_c$ and $\gamma = 1$ zero-energy states are possible. Consequently, they do only appear when the triplet gap is larger than the singlet gap $\Delta_s < \Delta_t$. This has to be more detailed, since it is going to be a check for my program.

7.4 RKKY as Perturbation

The fermionic, itinerant spins in the non-centrosymmetric superconductor described above are able to interact locally with impurities spins, which leads to the RKKY interaction between the impurity spins. This interaction is introduced in Sec. **??** and is of second order in perturbation theory. Therefore the local spin-interaction term

$$H_{RKKY} = \sum_{\sigma,\sigma',k,k'} \sum_i \frac{J}{N} e^{i(k-k')r_i} (\mathbf{S}_i \cdot \vec{\sigma}_{\sigma,\sigma'}) c^\dagger_{k,\sigma} c_{k',\sigma'}$$

is treated as a perturbation to the system and firstly is transformed into helicity basis by means of Eq. (**??**):

$$H_{RKKY} = \sum_{k,k',i,\lambda,\lambda'} T^\gamma_{i,k,k',\lambda,\lambda'} b^\dagger_{k,\lambda} b_{k',\lambda'}$$

where $T_{\gamma,k,k',i,\lambda,\lambda'}$ contains all pre-factors. The exact expression for T can be found in App. **??**. After another transformation using Equation (**??**), the RKKY-interaction reads in the eigenbasis of the unperturbed Hamiltonian:

$$H_{RKKY} = \sum_{i,k,k',\lambda,\lambda'} T^\gamma_{i,k,k',\lambda,\lambda'} \tag{7.23}$$
$$\left(\eta^\dagger_{k,\lambda}\eta_{k',\lambda'} d^\dagger_{k,\lambda} d_{k',\lambda'} + \nu_{k,\lambda}\nu^\dagger_{k',\lambda'} d_{-k,\lambda} d^\dagger_{-k',\lambda'} - \nu_{k,\lambda}\eta_{k',\lambda'} d_{-k,\lambda} d_{k',\lambda'} - \eta^\dagger_{k,\lambda}\nu^\dagger_{k',\lambda'} d^\dagger_{k,\lambda} d^\dagger_{-k',\lambda'}\right)$$

The interaction between impurity spins and superconductor aka. itinerant spins is approximated to be into one direction only. The changes within the superconductor because of the impurities is neglected and only the influence of the superconducting environment onto the configuration of the impurity spins is investigated. This simplification can be justified by the low density of impurity spins in the superconducting system.

8 Effective Interaction

In order to obtain the Hamiltonian describing the effective interaction of the system including the perturbation, a Schrieffer-Wolff-transformation is applied. Following the procedure as explained in Sec. **??**, the commutator $[S, H_0]$ is computed using the ansatz:

$$S = \sum_{\substack{i,k,k' \\ \lambda,\lambda'}} \left(A^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} d^\dagger_{k,\lambda} d_{k',\lambda'} + B^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} d_{-k,\lambda} d^\dagger_{-k',\lambda'} + C^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} d_{-k,\lambda} d_{k',\lambda'} + D^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} d^\dagger_{k,\lambda} d^\dagger_{-k',\lambda'} \right) \tag{8.1}$$

Afterwards, the requirement $H_{RKKY} + i[S, H_0] = 0$ is applied to it. The calculation can be found in Appendix **??** and leads to the following coefficients:

$$\begin{aligned}
A^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} &= i \sum_i T^\gamma_{i,k,k',\lambda,\lambda'} \frac{\eta^\dagger_{k,\lambda}\eta_{k',\lambda'}}{E_{k,\lambda} - E_{k',\lambda'}} \\
B^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} &= -i \sum_i T^\gamma_{i,k,k',\lambda,\lambda'} \frac{\nu_{k,\lambda}\nu^\dagger_{k',\lambda'}}{E_{-k,\lambda} - E_{-k',\lambda'}} \\
C^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} &= -i \sum_i T^\gamma_{i,k,k',\lambda,\lambda'} \frac{\nu_{k,\lambda}\eta_{k',\lambda'}}{E_{-k,\lambda} + E_{k',\lambda'}} \\
D^\gamma_{\substack{i,k,k' \\ \lambda,\lambda'}} &= i \sum_i T^\gamma_{i,k,k',\lambda,\lambda'} \frac{\eta^\dagger_{k,\lambda}\nu^\dagger_{k',\lambda'}}{E_{k,\lambda} + E_{-k',\lambda'}}
\end{aligned} \tag{8.2}$$

Based on that, the commutator $[S, H_{RKKY}]$ is calculated as shown in Appendix **??** and the effective Hamiltonian is formulated.

The expectation value of the effective Hamiltonian $H_{eff} = H_0 - i[S, H_{RKKY}]$ is presented in Appendix **??**.
The effective Hamiltonian contains terms of different spin-structures as well as feedback terms between the impurity spins and the superconductor. Since the density of impurity spins in the system is chosen to be very low, the feedback between them and the superconductor is neglected. The different spin-structures originate from the factors A, B, C, D and T, since they contain the product $\mathbf{S}_i \cdot \vec{\sigma}_{\sigma,\sigma'}$ with σ being a spin index again.

8.1 Bound states

In d-wave superconductors, there are bound states at impurities to be expected [**balatsky2006impurity**].
in p-wave superconductors, YSR bound states are to be expected [**kim2015impurity**], original paper from Shiba that talks about classical spins in superconductors [**shiba1968classical**]
spin glass vs. superconductivity investigates the influence of RKKY interaction onto superconducting transition and gap [**galitski2002spin**]

explain.

8.2 Spin Structure

The spin structure of the expectation value of the effective Hamiltonian is determined in order to allow for statements about the preferred spin configuration of the impurity spins. Since all terms contain factors of the type $\Lambda^{\gamma}_{\substack{j,q,q' \\ \beta,\beta'}} T^{\gamma}_{i,k,k',\lambda,\lambda'}$, where $\Lambda = A, B, C, D$, the individual parameter combinations for helicity and momentum are going to determine the effective spin-structure.
While the spin-structure for a simple normal metal with RRKY is of Heisenberg- type, it gets more complicated with more included interactions. For a conventional superconductor without SOC but with spin-splitting due to an external magnetic field, a mixture of Ising and Heisenberg like spin-terms is present [**ghanbari˙rkky˙nodate**]. For a normal metal with SOC of Rashba-type, the spin-structure contains Heisenberg and Dzyaloshinskii–Moriya like spin-interactions as well as interactions of type $\mathbf{S}_i \cdot \overleftrightarrow{\Gamma} \mathbf{S}_i$ [**valizadeh˙mohammad˙m˙magnetic˙2017**]. Therefore it is possible that the spin-structure for a non-centrosymmetric superconductor is a combination of Heisenberg, Ising, Dzyaloshinskii–Moriya and tensor-product like terms.
As the transformation between spin- and helicity-basis in Eq. (**??**) shows does each helicity-basis operator contain a spin-up and a spin-down operator regardless of their helicity. Consequently, all spin-combinations are possible in the first place and are weighted and canceled solely based on the energy terms associated with them as well as the choice of SOC and dependencies of momenta to each other.
Evaluating the expression of the commutator $[S, H_{RKKY}]$ leads to two distinct possible parameter combinations for helicity and momentum:

$$\begin{array}{lllll} (1st) & (k,\lambda)(k',\lambda') & \text{with} & (k',\lambda')(k,\lambda) \\ (2nd) & (k,\lambda)(k',\lambda') & \text{with} & (-k,\lambda)(-k',\lambda') \end{array}$$

In order to determine the effective spin structure of the non-centrosymmetric superconductor with RKKY-interaction, each of terms in $\langle H_{eff} \rangle$ (Eq. (**??**)) has to be evaluated individually. The resulting spin structure contains Heisenberg, DM and Ising terms, which are labeled in accordance with Sec. **??**. The coefficients $\mathbf{J}, \mathbf{D}, \overleftrightarrow{\Gamma}$ for $\langle H_{eff} \rangle$ in the non-centrosymmetric superconductor

with RKKY-interaction are found to be

$$\mathbf{J}_1 = \sum_{i,j,k,k'} \frac{1}{2}\left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i-r_j)} \begin{pmatrix} F^{k,k'}_{+,+} + F^{k,k'}_{-,-} + F^{k,k'}_{+,-} + F^{k,k'}_{-,+} \\ F^{k,k'}_{+,+} + F^{k,k'}_{-,-} - F^{k,k'}_{+,-} - F^{k,k'}_{-,+} \\ -2(F^{k,k'}_{+,-} + F^{k,k'}_{-,+}) \end{pmatrix} \tag{8.3}$$

$$\mathbf{D}_1 = \sum_{i,j,k,k'} \frac{1}{2}\left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i-r_j)} \begin{pmatrix} 0 \\ (F^{k,k'}_{+,-} - F^{k,k'}_{-,+})\left(\frac{\gamma_{k,x}+i\gamma_{k,y}}{|\gamma_k|} - \frac{\gamma_{k',x}-i\gamma_{k',y}}{|\gamma'_k|}\right) \\ 0 \end{pmatrix}$$

$$\overleftrightarrow{\Gamma} = 0$$

for the first parameter set. The energy terms $F^{k,k'}_{\pm,\pm}$ consist of the sum of all prefactor combinations that yield a non-zero contribution to $\langle H_{eff}\rangle$. They take the following form Should I write it out at least once? -¿ that would probably make it easier to understand. Point out that this is the same as Eq. (**??**) in the limit of $\Delta = 0$, which is important for validation. But I can not turn off SOC, since it is too deep entangled with everything and phase factors are overall.
The second parameter set yields

$$\mathbf{J}_2 = \sum_{i,j,k,k'} \frac{1}{4}\left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i-r_j)} \begin{pmatrix} -\left[(F^{k,k'}_{+,+} + F^{k,k'}_{-,-})\Theta_+ + (\tilde{F}^{k,k'}_{+,-} + F^{k,k'}_{-,+})\Theta_-\right] \\ -\left[(F^{k,k'}_{+,+} + F^{k,k'}_{-,-})\Theta_- + (\tilde{F}^{k,k'}_{+,-} + F^{k,k'}_{-,+})\Theta_+\right] \\ 4(F^{k,k'}_{+,-} + F^{k,k'}_{-,+}) \end{pmatrix} \tag{8.4}$$

$$\mathbf{D}_2 = \sum_{i,j,k,k'} \frac{1}{2}\left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i-r_j)} \begin{pmatrix} 0 \\ (F^{k,k'}_{+,-} - F^{k,k'}_{-,+})\left(\frac{\gamma_{k,x}-i\gamma_{k,y}}{|\gamma_k|} - \frac{\gamma_{k',x}+i\gamma_{k',y}}{|\gamma'_k|}\right) \\ 0 \end{pmatrix}$$

$$\Gamma_{xy} = \Gamma_{yx} = \sum_{i,j,k,k'} \frac{1}{4}\left(\frac{J}{N}\right)^2 e^{i(k-k')(r_i-r_j)} \left(F^{k,k'}_{+,+} + F^{k,k'}_{-,-} + F^{k,k'}_{+,-} + F^{k,k'}_{-,+}\right)\left[\left(\frac{\gamma_{k,x}-i\gamma_{k,y}}{|\gamma_k|}\right)^2 - \left(\frac{\gamma_{k',x}+i\gamma_{k',y}}{|\gamma'_k|}\right)^2\right]$$

which leads to less additional terms in the Ising, but more contributions in the Dzyaloshinskii-Moriya term.
Note that $\mathbf{D}_1$ and $\mathbf{D}_2$ are identical up to the phase, which is complex conjugated. $\mathbf{J}_2$ acquires phases, too, which was not the case for $\mathbf{J}_1$.
Moreover, the anisotropy in the Heisenberg term changes its form.
The short hand notation

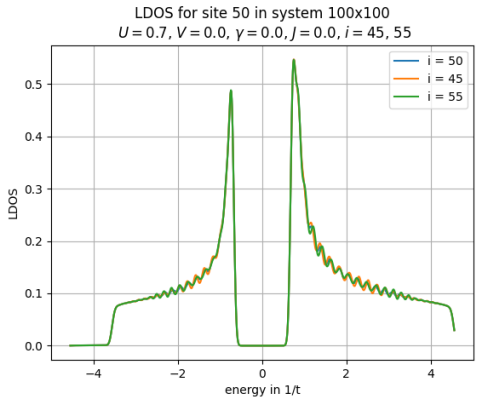
$$\Theta_\pm = \left(\frac{\gamma_{k,x}-i\gamma_{k,y}}{|\gamma_k|}\right)^2 + \left(\frac{\gamma_{k',x}+i\gamma_{k',y}}{|\gamma'_k|}\right)^2 \pm 2\left(\frac{\gamma_{k',x}+i\gamma_{k',y}}{|\gamma_{k'}|}\frac{\gamma_{k,x}-i\gamma_{k,y}}{|\gamma_k|}\right)$$

is used for the phase factors from the SOC.
Give a Einordnung for the complete spin structure, compare with the spin structures of other systems - what is the same and what is new?

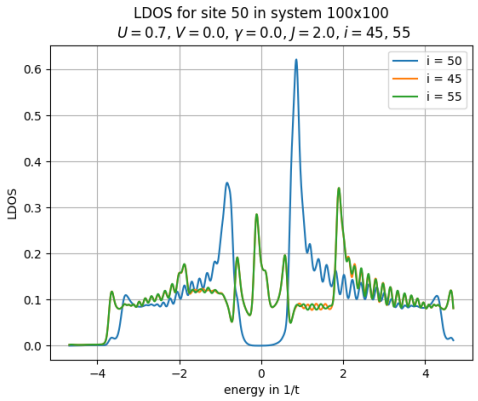
8.2.1 Free energies from the analytical approach

I need to find realistic numbers for my parameters and plug them into my analytical free energy, best would be to create a phase diagram one in dependence of γ and one of Δ_t
gap seems to be around 0.5 meV for $T_c = 3.8K$ in the material α-BiPd (fully gapped, weakly correlated superconductor) [**smidman2017superconductivity**]
for my model, I assumed that the gap magnitudes are identical on both spin-split Fermi surfaces, which implies that the SOC is much smaller than the chemical potential $\rightarrow \gamma << \mu \approx 1$eV

9 Discussion

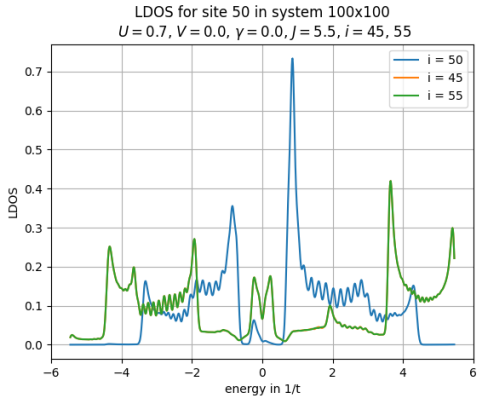


(a) Spinstructure for SC with RKKY $J = 2$ (no SOC)

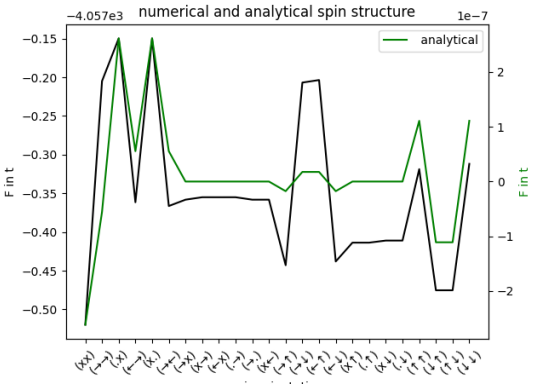


(b) Spinstructure for SC with RKKY $J = 5$ (no SOC)

Figure 5: bands are splitting

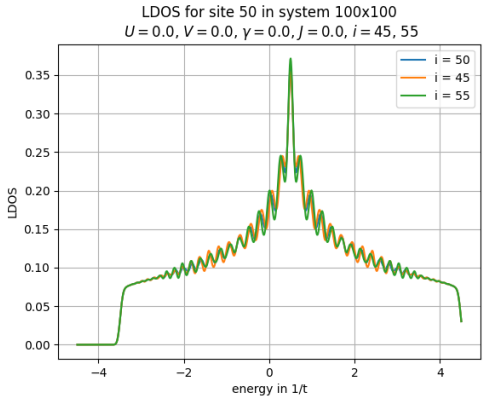


(a) Spinstructure for SC with RKKY $J = 2$, with SOC

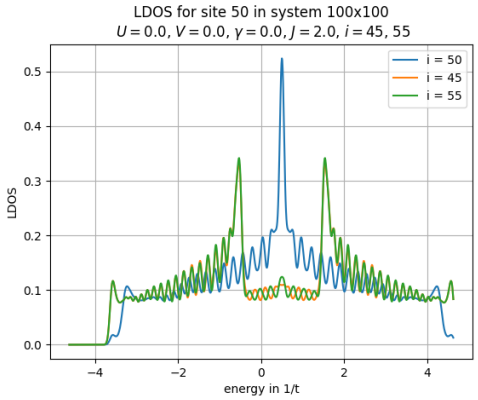


(b) 40x40, mu=0.5, U=0.5, V=1.2, gamma=0.15, J=2, i=15,25;
t=1, U=0.1, V=0.4, gamma=0.2, J=0.3, mu=0.5, N=10, i=3,6

Figure 6: bands do not overlap any longer; analytical vs. numerical result

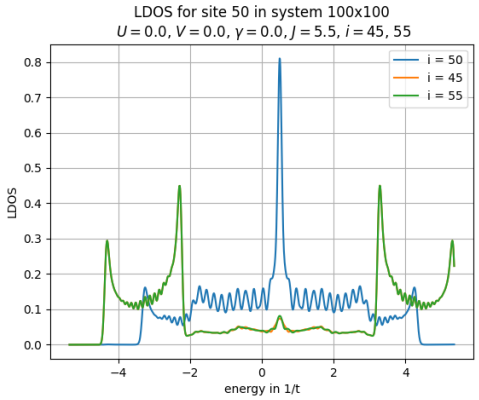


(a) Spinstructure for SC with RKKY $J = 2$ (no SOC)



(b) Spinstructure for SC with RKKY $J = 5$ (no SOC)

Figure 7: bands are splitting



(a) Spinstructure for SC with RKKY $J = 2$, with SOC

Figure 8: bands do not overlap any longer; analytical vs. numerical result

A Basis Transformation Coefficient

arrows ($\uparrow, \downarrow$) correspond to spin (up, down), while + and − correspond to positive and negative helicity, respectively

$$
\begin{aligned}
H_{RKKY} = \sum_{\substack{i,k,k' \\ \lambda,\lambda'}} \frac{J}{N} \frac{e^{i(k-k')r_i}}{2\sqrt{|\gamma(k)||\gamma(k')|}} \qquad (A.1)\\
\times [\ & \delta_{\lambda,\lambda'} \left(S_z^i \sqrt{|\gamma_k| + \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| + \lambda\gamma_{k',z}} - S_z^i \sqrt{|\gamma_k| - \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| - \lambda\gamma_{k',z}} \right. \\
& + \frac{\gamma_{k',x} + i\gamma_{k',y}}{\sqrt{\gamma_{k',x}^2 + \gamma_{k',y}^2}} (S_x^i - iS_y^i) \lambda \sqrt{|\gamma_k| + \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| - \lambda\gamma_{k',z}} \\
& \left. + \frac{\gamma_{k,x} - i\gamma_{k,y}}{\sqrt{\gamma_{k,x}^2 + \gamma_{k,y}^2}} (S_x^i + iS_y^i) \lambda \sqrt{|\gamma_k| - \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| + \lambda\gamma_{k',z}} \right) \\
+\ & \delta_{-\lambda,\lambda'} \left(S_z^i \sqrt{|\gamma_k| + \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| - \lambda\gamma_{k',z}} + S_z^i \sqrt{|\gamma_k| - \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| + \lambda\gamma_{k',z}} \right. \\
& - \frac{\gamma_{k',x} + i\gamma_{k',y}}{\sqrt{\gamma_{k',x}^2 + \gamma_{k',y}^2}} (S_x^i - iS_y^i) \lambda \sqrt{|\gamma_k| + \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| + \lambda\gamma_{k',z}} \\
& \left. + \frac{\gamma_{k,x} - i\gamma_{k,y}}{\sqrt{\gamma_{k,x}^2 + \gamma_{k,y}^2}} (S_x^i + iS_y^i) \lambda \sqrt{|\gamma_k| - \lambda\gamma_{k,z}} \sqrt{|\gamma_{k'}| - \lambda\gamma_{k',z}} \right) b_{k,\lambda}^\dagger b_{k',\lambda'}
\end{aligned}
$$

for Rashba-type SOC the expression simplifies to

$$
\begin{aligned}
H_{RKKY} = \sum_{\substack{i,k,k' \\ \lambda,\lambda'}} \frac{J}{N} \frac{e^{i(k-k')r_i}}{2\lambda} \times \Bigg[& \delta_{\lambda,\lambda'} \left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{\sqrt{\gamma_{k',x}^2 + \gamma_{k',y}^2}} (S_x^i - iS_y^i) + \frac{\gamma_{k,x} - i\gamma_{k,y}}{\sqrt{\gamma_{k,x}^2 + \gamma_{k,y}^2}} (S_x^i + iS_y^i) \right) \\
& + \delta_{-\lambda,\lambda'} \left(2\lambda S_z^i - \frac{\gamma_{k',x} + i\gamma_{k',y}}{\sqrt{\gamma_{k',x}^2 + \gamma_{k',y}^2}} (S_x^i - iS_y^i) + \frac{\gamma_{k,x} - i\gamma_{k,y}}{\sqrt{\gamma_{k,x}^2 + \gamma_{k,y}^2}} (S_x^i + iS_y^i) \right) \Bigg] b_{k,\lambda}^\dagger b_{k',\lambda'}
\end{aligned}
$$

B Commutators

B.1 $[S, H_0]$

With using the anti-commutation relations of the $d^{[\dagger]}$-operators, this commutator reads:

$$\begin{aligned}
&\sum_{\substack{k,k'\\ \lambda,\lambda'}}\sum_{q,\beta}\Big[A^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d^{\dagger}_{k,\lambda} d_{k',\lambda'} + B^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d_{-k,\lambda} d^{\dagger}_{-k',\lambda'} \\
&\qquad + C^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d_{-k,\lambda} d_{k',\lambda'} + D^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d^{\dagger}_{k,\lambda} d^{\dagger}_{-k',\lambda'}\,,\, E_{q,\beta} d^{\dagger}_{q,\beta} d_{q,\beta}\Big] \qquad \text{(B.1)}\\
= -&\sum_{\substack{k,k'\\ \lambda,\lambda'}}\sum_{q,\beta}\Bigg(A^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} E_{q,\beta}\left(d^{\dagger}_{q,\beta} d_{k',\lambda'}\{d_{q,\beta}\,,\, d^{\dagger}_{k,\lambda}\} - d^{\dagger}_{k,\lambda} d_{q,\beta}\{d^{\dagger}_{q,\beta}\,,\, d_{k',\lambda'}\}\right)\\
&\qquad + B^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} E_{q,\beta}\left(-d^{\dagger}_{q,\beta} d_{-k,\lambda}\{d_{q,\beta}\,,\, d^{\dagger}_{-k',\lambda'}\} + d^{\dagger}_{-k',\lambda'} d_{q,\beta}\{d^{\dagger}_{q,\beta}\,,\, d_{-k,\lambda}\}\right)\\
&\qquad + C^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} E_{q,\beta}\left(d_{k',\lambda'} d_{q,\beta}\{d^{\dagger}_{q,\beta}\,,\, d_{-k,\lambda}\} - d_{-k,\lambda} d_{q,\beta}\{d^{\dagger}_{q,\beta}\,,\, d_{k',\lambda'}\}\right)\\
&\qquad + D^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} E_{q,\beta}\left(d^{\dagger}_{q,\beta} d^{\dagger}_{-k',\lambda'}\{d_{q,\beta}\,,\, d^{\dagger}_{k,\lambda}\} - d^{\dagger}_{q,\beta} d^{\dagger}_{k,\lambda}\{d_{q,\beta}\,,\, d^{\dagger}_{-k',\lambda'}\}\right)\Bigg)\\
= -&\sum_{\substack{k,k'\\ \lambda,\lambda'}}\Bigg(A^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d^{\dagger}_{k,\lambda} d_{k',\lambda'}(E_{k,\lambda} - E_{k'\lambda'}) + B^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d_{-k,\lambda} d^{\dagger}_{-k',\lambda'}(E_{-k',\lambda'} - E_{-k,\lambda})\\
&\qquad - C^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d_{-k,\lambda} d_{k',\lambda'}(E_{-k,\lambda} + E_{k'\lambda'}) + D^{\gamma}_{\substack{i,k,k'\\ \lambda,\lambda'}} d^{\dagger}_{k,\lambda} d^{\dagger}_{-k',\lambda'}(E_{k,\lambda} + E_{-k',\lambda'})\Bigg) \qquad \text{(B.2)}
\end{aligned}$$

B.2 $[S, H_{RKKY}]$

With disregarding all terms that contain either $d_{k,\lambda} d_{k',\lambda'}$ or $d^{\dagger}_{k,\lambda} d^{\dagger}_{k',\lambda'}$, sinee they are not going to contribute to the expectation value and are therefore of no interest in this case, this commutator reads:

$$
\begin{aligned}
&[\sum_{\substack{q,q'\\ \beta,\beta'}} A^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} d^{\dagger}_{q,\beta} d_{q',\beta'} + B^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} d_{-q,\beta} d^{\dagger}_{-q',\beta'} + C^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} d_{-q,\beta} d_{q',\beta'} + D^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} d^{\dagger}_{q,\beta} d^{\dagger}_{-q',\beta'} \,, \\
&\quad \sum_{\substack{i,k,k'\\ \lambda,\lambda'}} T^{\gamma}_{i,k,k',\lambda,\lambda'} \left(\eta^{\dagger}_{k,\lambda} \eta_{k',\lambda'} d^{\dagger}_{k,\lambda} d_{k',\lambda'} + \nu_{k,\lambda} \nu^{\dagger}_{k',\lambda'} d^{\dagger}_{k,\lambda} d_{-k',\lambda'} + \nu_{k,\lambda} \eta_{k',\lambda'} d^{\dagger}_{-k,\lambda} d_{k',\lambda'} + \eta^{\dagger}_{k,\lambda} \nu^{\dagger}_{k',\lambda'} d^{\dagger}_{k,\lambda} d_{-k',\lambda'} \right)] \\
&= \sum_{\substack{q,q',k,k'\\ \beta,\beta',\lambda,\lambda'}} -A^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} \Big(T^{\gamma}_{i,k,q,\lambda,\beta} \eta^{\dagger}_{k,\lambda} \eta_{q,\beta} d^{\dagger}_{k,\lambda} d_{q',\beta'} - T^{\gamma}_{i,q',k',\beta',\lambda'} \eta^{\dagger}_{q',\beta'} \eta_{k',\lambda'} d^{\dagger}_{q,\beta} d_{k',\lambda'} \\
&\qquad\qquad -T^{\gamma}_{i,k,-q',\lambda,\beta'} \nu_{k,\lambda} \nu^{\dagger}_{-q',\beta'} d_{-k,\lambda} d^{\dagger}_{q,\beta} + T^{\gamma}_{i,-q,k',\beta,\lambda'} \nu_{-q,\beta} \nu^{\dagger}_{k,\lambda} d_{q',\beta'} d^{\dagger}_{-k',\lambda'} \Big) \\
&\qquad -B^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} \Big(-T^{\gamma}_{i,k,-q',\lambda,\beta'} \eta^{\dagger}_{k,\lambda} \eta_{-q',\beta'} d^{\dagger}_{k,\lambda} d_{-q,\beta} + T^{\gamma}_{i,-q,k',\beta,\lambda'} \eta^{\dagger}_{-q,\beta} \eta_{k',\lambda'} d^{\dagger}_{-q',\beta'} d_{k',\lambda'} \\
&\qquad\qquad +T^{\gamma}_{i,k,q,\lambda,\beta} \nu_{k,\lambda} \nu^{\dagger}_{q,\beta} d_{-k,\lambda} d^{\dagger}_{-q',\beta'} - T^{\gamma}_{i,q',k',\beta',\lambda'} \nu_{q',\beta'} \nu^{\dagger}_{k',\lambda'} d_{-q,\beta} d^{\dagger}_{-k',\lambda'} \Big) \\
&\qquad -C^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} \Big(T^{\gamma}_{i,k,q,\lambda,\beta} \eta^{\dagger}_{k,\lambda} \nu^{\dagger}_{q,\beta} d^{\dagger}_{k,\lambda} d_{q',\beta'} - T^{\gamma}_{i,k,-q',\lambda,\beta'} \eta^{\dagger}_{k,\lambda} \nu^{\dagger}_{-q',\beta'} d^{\dagger}_{k,\lambda} d_{-q,\beta} \\
&\qquad\qquad +T^{\gamma}_{i,-q,k',\beta,\lambda'} \eta^{\dagger}_{-q,\beta} \nu^{\dagger}_{k',\lambda'} d_{q',\beta'} d^{\dagger}_{-k',\lambda'} - T^{\gamma}_{i,q',k',\beta',\lambda'} \eta^{\dagger}_{q',\beta'} \nu^{\dagger}_{k',\lambda'} d_{-q,\beta} d^{\dagger}_{-k',\lambda'} \Big) \\
&\qquad -D^{\gamma}_{\substack{j,q,q'\\ \beta,\beta'}} \Big(T^{\gamma}_{i,k,q,\lambda,\beta} \nu_{k,\lambda} \eta_{q,\beta} d_{-k,\lambda} d^{\dagger}_{-q',\beta'} - T^{\gamma}_{i,k,-q',\lambda,\beta'} \nu_{k,\lambda} \eta_{-q',\beta'} d_{-k,\lambda} d^{\dagger}_{q,\beta} \\
&\qquad\qquad +T^{\gamma}_{i,-q,k',\beta,\lambda'} \nu_{-q,\beta} \eta_{k',\lambda'} d^{\dagger}_{-q',\beta'} d_{k',\lambda'} - T^{\gamma}_{i,q',k',\beta',\lambda'} \nu_{q',\beta'} \eta_{k',\lambda'} d^{\dagger}_{q,\beta} d_{k',\lambda'} \Big)
\end{aligned}
$$

C Expectationvalue of H_{eff}

It is used that $\langle H_0\rangle = E_0$ is the expectation-value in the groundstate of the unperturbed system and $f(x)$ is the Fermi-Dirac distribution. λ, λ' are helicity indices and k, k' are momenta. In addition, i, j are the positions of the impurity spins, which are introduced with the RKKY-interaction.

$$\langle H_{eff}\rangle = \langle H_0\rangle - i\langle[S, H_{RKKY}]\rangle \tag{C.1}$$

$$\begin{aligned}
&= E_0 - i\sum_{\substack{i,k,k'\\ \lambda,\lambda'}}\sum_{\substack{j,q,q'\\ \beta,\beta'}}\langle\Big[A_{i,k,k',\lambda,\lambda'}d^\dagger_{k,\lambda}d_{k',\lambda'} + B_{i,k,k',\lambda,\lambda'}d_{-k,\lambda}d^\dagger_{-k',-\lambda'} + C_{i,k,k',\lambda,\lambda'}d_{-k,\lambda}d^\dagger_{k',\lambda'} + D_{i,k,k',\lambda,\lambda'}d^\dagger_{k,\lambda}d^\dagger_{-k',\lambda'},\\
&\qquad a_{j,q,q',\beta,\beta'}d^\dagger_{q,\beta}d_{q',\beta'} + b_{j,q,q',\beta,\beta'}d_{-q,\beta}d^\dagger_{-q',\beta'} + c_{j,q,q',\beta,\beta'}d_{-q,\beta}d_{q',\beta'} + d_{j,q,q',\beta,\beta'}d^\dagger_{q,\beta}d^\dagger_{-q',\beta'}\Big]\rangle\\
&= E_0 - \sum_{\substack{i,j,k,k'\\ \lambda,\lambda'}}\Bigg(\frac{|\eta_{k,\lambda}|^2|\eta_{k',\lambda'}|^2}{E_{k',\lambda'}-E_{k,\lambda}}T_{i,k,k',\lambda,\lambda'}T_{j,k',k,\lambda',\lambda}(f(E_{k,\lambda})-f(E_{k',\lambda'}))\\
&\qquad + \frac{\eta^\dagger_{k,\lambda}\nu_{-k,\lambda}\eta_{k',\lambda'}\nu^\dagger_{-k',\lambda'}}{E_{k',\lambda'}-E_{k,\lambda}}T_{i,k,k',\lambda,\lambda'}T_{j,-k,-k',\lambda,\lambda'}(f(E_{k',\lambda'})-f(E_{k,\lambda}))\Bigg)\\
&\quad + \Bigg(\frac{\nu_{k,\lambda}\nu^\dagger_{k',\lambda'}\eta^\dagger_{-k,\lambda}\eta_{-k',\lambda'}}{E_{-k,\lambda}-E_{-k',\lambda'}}T_{i,k,k',\lambda,\lambda'}T_{j,-k,-k',\lambda,\lambda'}(f(E_{-k,\lambda})-f(E_{-k',\lambda}))\\
&\qquad + \frac{|\nu_{k,\lambda}|^2|\nu_{k',\lambda'}|^2}{E_{-k,\lambda}-E_{-k',\lambda'}}T_{i,k,k',\lambda,\lambda'}T_{j,k',k,\lambda',\lambda}(f(E_{-k',\lambda'})-f(E_{-k,\lambda}))\Bigg)\\
&\quad + \Bigg(-\frac{|\nu_{k,\lambda}|^2|\eta_{k',\lambda'}|^2}{E_{-k,\lambda}+E_{k',\lambda'}}T_{i,k,k',\lambda,\lambda'}T_{j,k',k,\lambda',\lambda}(1-f(E_{-k,\lambda})-f(E_{k',\lambda'}))\\
&\qquad - \frac{\nu_{k,\lambda}\nu^\dagger_{-k',\lambda'}\eta^\dagger_{-k,\lambda}\eta_{k',\lambda'}}{E_{-k,\lambda}+E_{k',\lambda'}}T_{i,k,k',\lambda,\lambda'}T_{j,-k,-k',\lambda,\lambda'}((f(E_{k',\lambda'})-1+f(E_{-k,\lambda}))\Bigg)\\
&\quad + \Bigg(\frac{|\eta_{k,\lambda}|^2|\nu_{k',\lambda'}|^2}{E_{-k',\lambda'}+E_{k,\lambda}}T_{i,k,k',\lambda,\lambda'}T_{j,k',k,\lambda',\lambda}(f(E_{k,\lambda})-1+f(E_{-k',\lambda'}))\\
&\qquad + \frac{\eta^\dagger_{k,\lambda}\nu_{-k,\lambda}\eta_{-k',\lambda'}\nu^\dagger_{k',\lambda'}}{E_{-k',\lambda'}+E_{k,\lambda}}T_{i,k,k',\lambda,\lambda'}T_{j,-k,-k',\lambda,\lambda'}(1-f(E_{-k',\lambda'})-f(E_{k,\lambda}))\Bigg)
\end{aligned}$$

C.1 spin structure

The spin structure can be calculated in two steps.
The first step is to take the product $T_\chi T_\zeta$, where χ, ζ are two different sets of quantum numbers and is done here.
The second step is to take the sum over the helicity indices, which require to take the entire terms into account and can be found in Section **??**.
There are tow combinations of $T_\chi T_\zeta$ are the final products read for Rashba-SOC $\gamma = k_y\sigma_x - k_x\sigma_y$:

$$T_{\substack{i,k,k'\\ \lambda,\lambda'}} T_{\substack{j,k',k\\ \lambda',\lambda}} = \left(\frac{J}{N}\right)^2 \frac{e^{i(k-k')(r_i-r_j)}}{4\lambda\lambda'} \tag{C.2}$$

$$\begin{aligned}
&\times \Bigg[\delta_{\lambda,\lambda'} \Bigg(S_{i,y}S_{j,y}(1 - \frac{\gamma_{k',x}\gamma_{k,x} + \gamma_{k',y}\gamma_{k,y}}{|\gamma_k||\gamma_{k'}|}) + S_{i,x}S_{j,x}(\frac{\gamma_{k',x}\gamma_{k,x} + \gamma_{k',y}\gamma_{k,y}}{|\gamma_k||\gamma_{k'}|} + 1)\Bigg) \\
&+\delta_{\lambda,-\lambda'} \Bigg(2S_{i,z}S_{j,z} + S_{i,x}S_{j,x}(\frac{\gamma_{k',x}\gamma_{k,x} + \gamma_{k',y}\gamma_{k,y}}{|\gamma_k||\gamma_{k'}|} - 1) \\
&-S_{i,y}S_{j,y}(\frac{\gamma_{k',x}\gamma_{k,x} + \gamma_{k',y}\gamma_{k,y}}{|\gamma_k||\gamma_{k'}|} + 1) \\
&+\lambda S_{i,z}S_{j,x}\left[\frac{\gamma_{k',x} - i\gamma_{k',y}}{|\gamma_{k'}|} - \frac{\gamma_{k,x} + i\gamma_{k,y}}{|\gamma_k|}\right] + \lambda S_{i,x}S_{j,z}\left[\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|} - \frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right] \\
&(iS_{i,x}S_{j,y} + iS_{i,y}S_{j,x})\left[\frac{-i(\gamma_{k',x}\gamma_{k,y} + \gamma_{k',y}\gamma_{k,x})}{|\gamma_k||\gamma_{k'}|}\right]\Bigg)\Bigg]
\end{aligned}$$

For the second combination of indices and Rashba-type SOC, the product becomes

$$T_{\substack{i,k,k'\\ \lambda,\lambda'}} T_{\substack{j,-k,-k'\\ \lambda,\lambda'}} = \left(\frac{J}{N}\right)^2 \frac{e^{i(k-k')(r_i-r_j)}}{4\lambda\lambda'} \tag{C.3}$$

$$\begin{aligned}
&\times \Bigg[\delta_{\lambda,\lambda'} \Bigg(-S_{i,x}S_{j,x}(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)^2 + \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)^2 + 2\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)\left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)) \\
&+S_{i,y}S_{j,y}(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)^2 + \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)^2 - 2\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)\left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)) \\
&+i(S_{i,x}S_{j,y} + S_{i,y}S_{j,x})(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)^2 - \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)^2)\Bigg) \\
&+\delta_{\lambda,-\lambda'} (4S_{i,z}S_{j,z} \\
&-(S_{i,x}S_{j,x} + S_{i,y}S_{j,y})(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)^2 + \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)^2 - 2\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)\left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)) \\
&+i(S_{i,x}S_{j,y} + S_{i,y}S_{j,x})(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right)^2 - \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right)^2)\Bigg) \\
&+2\lambda\delta_{\lambda,-\lambda'} \Bigg((S_{i,z}S_{j,x} - S_{i,x}S_{j,z})(\left(\frac{\gamma_{k',x} + i\gamma_{k',y}}{|\gamma_{k'}|}\right) - \left(\frac{\gamma_{k,x} - i\gamma_{k,y}}{|\gamma_k|}\right))\Bigg)\Bigg)
\end{aligned}$$

I used $i \leftrightarrow j$ for the $S_{i,z}S_{j,y}$ terms, so that they vanished in both cases.
I used $k \leftrightarrow k'$ for the $S_{i,z}S_{j,x}$ terms of the first product, so that they got the form of a cross product. For that I had to use the symmetry properties of the energy prefactor.

These products lead to a spin structure that has to be expressed with Heisenberg, DM and Ising terms. (xx,yy,zz, zx-xz, xy+yx)