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Non-centrosymmetric Perturbation on Superconductivity

Semester Thesis

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Abstract

We perform a perturbative calculation to investigate the effect of the Dzyaloshinsky-Moriya interaction on a two-dimensional conventional *s*-wave superconductor. The introduced interaction breaks the space inversion symmetry, making the system non-centrosymmetric. By analyzing the resulting Cooper-pair wavefunction, we identify both even-parity and odd-parity components alongside the original *s*-wave pairing, which all belong to the A_1 representation of C_{4v} , the point group of the underlying lattice. Surprisingly, the pairing structure remains unaffected at half-filling due to an additional sublattice symmetry, which restricts the electrons to either form intra-sublattice pairing or inter-sublattice pairing in real space. The pairings induced by the Dzyaloshinsky-Moriya interaction turn out to be incompatible with the conventional *s*-wave pairing under this symmetry, which are therefore absent at half-filling.

1 Introduction

Superconductivity, a macroscopic quantum phenomenon characterized by zero resistance below some critical temperature T_c , has gathered a significant amount of attention since its discovery over a century ago. The first theoretical breakthrough of superconductivity came from the celebrated Bardeen-Cooper-Schrieffer (BCS) theory [1], which provided a microscopic theory for the phenomenon and described it as a consequence of the condensation of pairing electrons (Cooper pairs) due to the phonon-mediated attractive interactions between the electrons. In the BCS theory, the Cooper pair has zero relative angular momentum and is a spin singlet. The pairing structure is referred to as the conventional s -wave pairing. Since then, different pairings with higher relative angular momentum have been discovered in different materials, ranging from the superfluid phase of ^3He [2, 3], the heavy fermion compounds [4, 5, 6], to the high- T_c cuprates [7, 8, 9]. In the condensed-matter jargon, any superconductor that has pairing structure different from the conventional s -wave pairing is called the unconventional superconductor.

Symmetry is a powerful tool in classifying these unconventional pairing structures [10, 11, 12]. In a nutshell, because the normal-to-superconducting transition is a second-order symmetry-breaking phase transition, the order parameter of the superconducting phase furnishes an irreducible representation of the broken symmetry, according to Landau's phenomenological theory of the second-order phase transition [13]. Compared to the conventional pairing, the unconventional pairing breaks additional symmetries such as the point group symmetry besides the $U(1)$ symmetry. In that case, the order parameter in turn also belongs to an irreducible representation of the point group symmetry. Among all symmetries, the space inversion symmetry is a particularly important symmetry for superconductivity [14], as it connects electrons with opposite momentums, which are the degenerated states needed to form a Cooper pair. For centrosymmetric systems, an immediate consequence from the symmetry perspective is that the even and odd parity representations of the point group symmetry cannot be mixed in the superconducting phase. In addition, because electrons are fermionic, the constraint implies that the Cooper pair is either spin singlet (for even-parity pairing) or spin triplet (for odd-parity pairing) in centrosymmetric systems.

In the past decades, novel superconductors that break the inversion symmetry have been discovered in materials such as CePt₃Si [15], UIr [16], and LaBiPt [17]. Such non-centrosymmetric systems allow antisymmetric spin-orbit couplings. A typical example is the Rashba spin-orbit coupling, which has the form $\mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma}$ with $\mathbf{g}(\mathbf{k}) = \alpha(\hat{x}\sin(k_ya) - \hat{y}\sin(k_xa))$. The coupling splits the Fermi surface and suppresses all triplet pairings but the one with the gap $\mathbf{d}(\mathbf{k})$ vector parallel to $\mathbf{g}(\mathbf{k})$ [18], consistent with Anderson's theorem in general. Furthermore, sys-

tems without the inversion center allow an antisymmetric exchange interaction, known as the Dzyaloshinskii–Moriya interaction. In the following, we examine how this interaction affects the pairing structure by doing a perturbative calculation on a toy model (see Sec. 2). We show that a parity-mixing occurs between the spin singlet and triplet states, in contrast to centrosymmetric superconductors. Furthermore, we find that the conventional s -wave pairing is unaffected by the perturbation at half-filling, which can be understood from the additional sublattice symmetry that arises at this special filling. We also derive a general restriction on the pairing structures for systems with a sublattice symmetry.

2 Microscopic model

We start with a one-band model on a two-dimensional (2D) square lattice, defined as follows:

$$H = H_0 + H_I = \underbrace{\sum_{\mathbf{k}s} \epsilon_{\mathbf{k}} c_{\mathbf{k},s}^\dagger c_{\mathbf{k},s}^{\phantom\dagger} - g \sum_j n_{j\uparrow} n_{j\downarrow}}_{H_0} + \underbrace{\sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)}_{H_I}, \quad (1)$$

where the kinetic energy is $\epsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)] - \mu$ and the coupling g characterizes the on-site attraction. They constitute the unperturbed Hamiltonian H_0 . The Dzyaloshinsky-Moriya interaction H_I is treated as a perturbation with $\mathbf{D}_{ij} = D(\hat{z} \times (\mathbf{r}_i - \mathbf{r}_j))$ ($\langle ij \rangle$ denotes summing over nearest-neighbors).

The unperturbed Hamiltonian H_0 is symmetric under space inversion transformation $P : P c_{\mathbf{r}_i}^{(\dagger)} P^{-1} = c_{-\mathbf{r}_i}^{(\dagger)}$ since $\epsilon_{\mathbf{k}} = \epsilon_{-\mathbf{k}}$. The pairing structure for H_0 can be derived from a simple mean-field approach. By condensing the pairing operator $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ and $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$, and diagonalizing the resulting mean-field Hamiltonian, we arrive at

$$H_0 = \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} + E_{\mathbf{k}} \gamma_{\mathbf{k}2}^\dagger \gamma_{\mathbf{k}2} \right\}, \quad (2)$$

where additional constants are ignored, the excitation energy $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$, and the Bogoliubov particle $(\gamma_{\mathbf{k}}, \gamma_{\mathbf{k}}^\dagger)$ is defined as

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{-\mathbf{k}2}^\dagger \end{pmatrix} \quad (3)$$

with coefficients

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) \quad \text{and} \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right). \quad (4)$$

The gap Δ satisfies the following self-consistent equation at $T = 0$:

$$\Delta = \frac{g}{2\Omega} \sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \quad (5)$$

In particular, the gap function Δ is a constant, corresponding to the conventional s -wave pairing. The ground state $|g_0\rangle$ of Eq. (2) is the state that gets annihilated by all γ operators: $\gamma_{\mathbf{k},\sigma}|g_0\rangle = 0, \forall \mathbf{k}, \sigma$.

The Dzyaloshinsky-Moriya perturbation breaks the inversion symmetry, as it changes sign under P :

$$P \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) P^{-1} = \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_{-i} \times \mathbf{S}_{-j}) = \sum_{\langle i'j' \rangle} -\mathbf{D}_{i'j'} \cdot (\mathbf{S}_{i'} \times \mathbf{S}_{j'}). \quad (6)$$

Moreover, similar to the case of spin-orbit coupling, the point-group transformations of \mathbf{k} and the spin transformations can no longer be treated independently due to the Dzyaloshinsky-Moriya interaction. Specifically, H_I is only invariant under the joint transformation $g : g\mathbf{S}_{r_i}g^{-1} = R^+(g)\mathbf{S}_{R^-(g^{-1})\mathbf{r}_i}$ with R^\pm the representation of $O(3)$ in three-dimensional space with positive or negative inversion operation:

$$\begin{aligned} \sum_{\langle ij \rangle} g\mathbf{D}_{ij} \cdot (\mathbf{S}_{r_i} \times \mathbf{S}_{r_j}) g^{-1} &= \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (R^+(g)\mathbf{S}_{R^-(g^{-1})\mathbf{r}_i} \times R^+(g)\mathbf{S}_{R^-(g^{-1})\mathbf{r}_j}) \\ &= \sum_{\langle ij \rangle} D(R^-(g)\hat{\mathbf{z}} \times (R^-(g)\mathbf{r}_i - R^-(g)\mathbf{r}_j)) \cdot R^+(g)(\mathbf{S}_{r_i} \times \mathbf{S}_{r_j}) \\ &= \sum_{\langle ij \rangle} D[R^-(g)(\hat{\mathbf{z}} \times (\mathbf{r}_i - \mathbf{r}_j))] \cdot [R^+(g)(\mathbf{S}_{r_i} \times \mathbf{S}_{r_j})] \\ &= \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_{r_i} \times \mathbf{S}_{r_j}), \quad \forall g \in \Gamma. \end{aligned} \quad (7)$$

Here Γ is the point group C_{4v} , which is a subgroup of $O(3)$. In the last equality, we used that both representations R^\pm restricted to C_{4v} lead to the same representation since $P \notin C_{4v}$. In the following, we study how this interaction alters the conventional pairing of H_0 .

3 Perturbative treatment

The inversion-symmetry-breaking term written in terms of the bare electron in momentum space reads

$$H_I = \frac{iD}{\Omega} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} \sum_{s_1 s_2 s_3 s_4} \left\{ -\sin[q_y a] \left(\frac{\sigma_{s_1 s_2}^y}{2} \frac{\sigma_{s_3, s_4}^z}{2} - \frac{\sigma_{s_1 s_2}^z}{2} \frac{\sigma_{s_3, s_4}^y}{2} \right) + \sin[q_x a] \left(\frac{\sigma_{s_1 s_2}^z}{2} \frac{\sigma_{s_3, s_4}^x}{2} - \frac{\sigma_{s_1 s_2}^x}{2} \frac{\sigma_{s_3, s_4}^z}{2} \right) \right\} c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2}. \quad (8)$$

In the following, we will take the lattice spacing $a = 1$ for convenience. Analo-

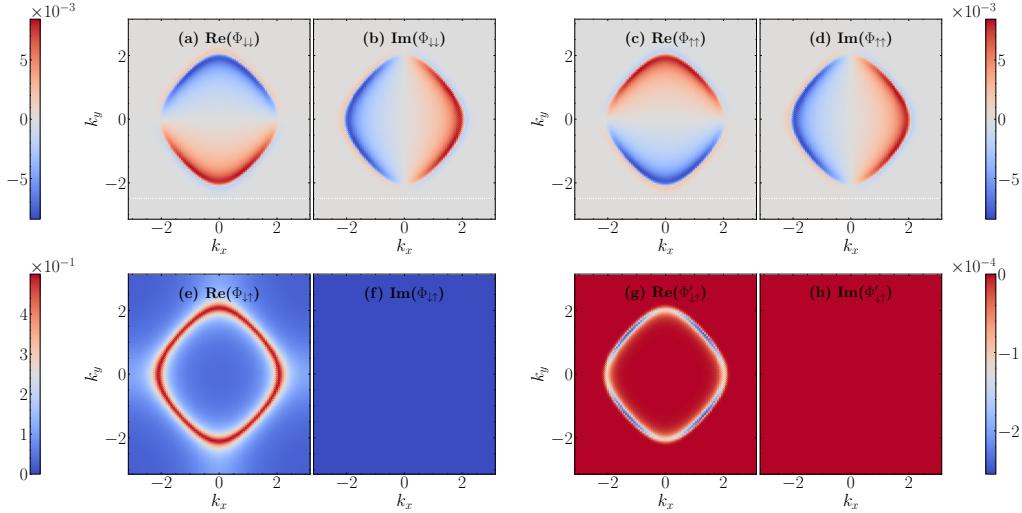


Figure 1: Order parameters $\Phi_{s_1 s_2}$ at chemical potential $\mu = -1$. Other parameters are fixed as $(t, g, D) = (1, 2, 0.5)$. The quantity $\Phi'_{\downarrow\uparrow} = \Phi_{\downarrow\uparrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$ characterizes the new singlet pairing structure due to the perturbation.

gous to the mean-field treatment, we approximate the quartic term by a sum of quadratic terms:

$$\begin{aligned} c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} &= \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger \rangle_0 c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} + c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger \langle c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 \\ &\quad - \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \rangle_0 c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} - c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \langle c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 \\ &\quad + \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} + c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \langle c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \rangle_0. \end{aligned} \quad (9)$$

To treat H_I perturbatively, we evaluate the expectation values using the unperturbed ground state $|g_0\rangle$, i.e., $\langle \cdot \rangle_0 = \langle g_0 | \cdot | g_0 \rangle$, instead of determining the

expectation values through self-consistent equations. After some algebra work, we obtain the resulting Bogoliubov-de-Gennes (BdG) Hamiltonian

$$H_{\text{BdG}} = \sum_{\mathbf{k}} \frac{1}{2} \begin{pmatrix} \gamma_{\mathbf{k}1}^\dagger & \gamma_{\mathbf{k}2}^\dagger & \gamma_{-\mathbf{k}1} & \gamma_{-\mathbf{k}2} \end{pmatrix} \begin{pmatrix} E_{\mathbf{k}} & A_{\mathbf{k}} & B_{\mathbf{k}} & 0 \\ A_{\mathbf{k}}^* & E_{\mathbf{k}} & 0 & -B_{\mathbf{k}}^* \\ B_{\mathbf{k}}^* & 0 & -E_{\mathbf{k}} & -A_{\mathbf{k}}^* \\ 0 & -B_{\mathbf{k}} & -A_{\mathbf{k}} & -E_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{\mathbf{k}2} \\ \gamma_{-\mathbf{k}1}^\dagger \\ \gamma_{-\mathbf{k}2}^\dagger \end{pmatrix}, \quad (10)$$

where

$$A_{\mathbf{k}} = \frac{D}{\Omega} \sum_{\mathbf{k}'} \left(\sin(k'_y - k_y) + i \sin(k'_x - k_x) \right) u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}, \quad (11)$$

$$B_{\mathbf{k}} = -\frac{D}{\Omega} \sum_{\mathbf{k}'} \left(\sin(k'_y - k_y) + i \sin(k'_x - k_x) \right) v_{\mathbf{k}}^2 u_{\mathbf{k}'} v_{\mathbf{k}'}. \quad (12)$$

The BdG Hamiltonian (10) is diagonalized by introducing the new particle $(\alpha_{\mathbf{k}\lambda}, \alpha_{\mathbf{k}\lambda}^\dagger)$:

$$\begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{\mathbf{k}2} \\ \gamma_{-\mathbf{k}1}^\dagger \\ \gamma_{-\mathbf{k}2}^\dagger \end{pmatrix} = S_{\mathbf{k}} \begin{pmatrix} \alpha_{\mathbf{k}1} \\ \alpha_{\mathbf{k}2} \\ \alpha_{-\mathbf{k}1}^\dagger \\ \alpha_{-\mathbf{k}2}^\dagger \end{pmatrix} \quad (13)$$

with $S_{\mathbf{k}}$ a unitary 4×4 matrix. The diagonalized Hamiltonian is

$$H_{\text{BdG}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}1} \alpha_{\mathbf{k}1}^\dagger \alpha_{\mathbf{k}1} + \omega_{\mathbf{k}2} \alpha_{\mathbf{k}2}^\dagger \alpha_{\mathbf{k}2}, \quad (14)$$

where

$$\omega_{\mathbf{k},1} = \sqrt{|A_{\mathbf{k}}|^2 + |B_{\mathbf{k}}|^2 + E_{\mathbf{k}}^2 - \sqrt{(A_{\mathbf{k}}^* B_{\mathbf{k}} + A_{\mathbf{k}} B_{\mathbf{k}}^*)^2 + 4|A_{\mathbf{k}}|^2 E_{\mathbf{k}}^2}}, \quad (15)$$

$$\omega_{\mathbf{k},2} = \sqrt{|A_{\mathbf{k}}|^2 + |B_{\mathbf{k}}|^2 + E_{\mathbf{k}}^2 + \sqrt{(A_{\mathbf{k}}^* B_{\mathbf{k}} + A_{\mathbf{k}} B_{\mathbf{k}}^*)^2 + 4|A_{\mathbf{k}}|^2 E_{\mathbf{k}}^2}}. \quad (16)$$

The new ground state $|g\rangle$ is defined as the state that gets annihilated by all $\alpha_{\mathbf{k}\lambda}$.

In order to study the pairing structure of the ground state $|g\rangle$, we define the order parameter

$$\Phi_{s_1 s_2} = \langle g | c_{-\mathbf{k}s_1} c_{\mathbf{k}s_2} | g \rangle. \quad (17)$$

Note that we use the bare electron operators inside the bracket. Figures. 1, 2, 3 show the order parameter $\Phi_{s_1 s_2}$ for three different choices of the chemical potential μ while fixing $t = 1, g = 2, D = 0.5$. From Fig. 1(a-d) and Fig. 2(a-d), we observe that odd-parity pairing emerges on top the original even-parity

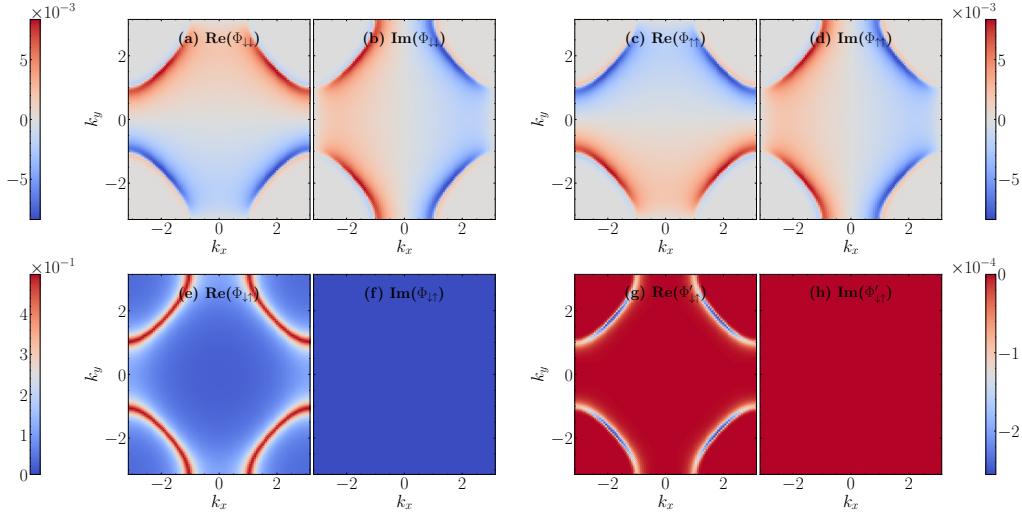


Figure 2: Order parameters $\Phi_{s_1 s_2}$ at chemical potential $\mu = 1$. Other parameters are fixed as $(t, g, D) = (1, 2, 0.5)$. The quantity $\Phi'_{\downarrow\downarrow} = \Phi_{\downarrow\downarrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$ characterizes the new singlet pairing structure due to the perturbation.

pairing. Furthermore, we can get the perturbation effect on the original s-wave singlet pairing by subtracting $\langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$ from $\Phi_{\downarrow\downarrow}$, and we denote the new quantity as $\Phi'_{\downarrow\downarrow}$, as shown in Fig. 1(g-h) and Fig. 2(g-h). The pattern of $\Phi'_{\downarrow\downarrow}$ implies the additional extended s-wave pairing of the form $\cos(k_x) + \cos(k_y)$.

Surprisingly, the non-centrosymmetric perturbation does not alter the pairing structure at half-filling ($\mu = 0$) in our calculations, as shown in Fig. 3. Specifically, at $\mu = 0$,

$$A_{\mathbf{k}} = -\frac{u_{\mathbf{k}} v_{\mathbf{k}} D}{2} \int \frac{d^2 k'}{(2\pi)^2} \frac{\Delta [\cos(k'_y) \sin(k_y) + i \cos(k'_x) \sin(k_x)]}{\sqrt{4t^2(\cos(k'_x) + \cos(k'_y))^2 + \Delta^2}} = 0, \\ B_{\mathbf{k}} = \frac{v_{\mathbf{k}}^2 D}{2} \int \frac{d^2 k'}{(2\pi)^2} \frac{\Delta [\cos(k'_y) \sin(k_y) + i \cos(k'_x) \sin(k_x)]}{\sqrt{4t^2(\cos(k'_x) + \cos(k'_y))^2 + \Delta^2}} = 0. \quad (18)$$

Therefore, in our perturbation scheme, H_I doesn't couple to H_0 at half-filling.

4 Sublattice symmetry at half-filling

We provide a symmetry argument for understanding the absence of the odd-parity pairing component at $\mu = 0$, which relies on the additional sublattice

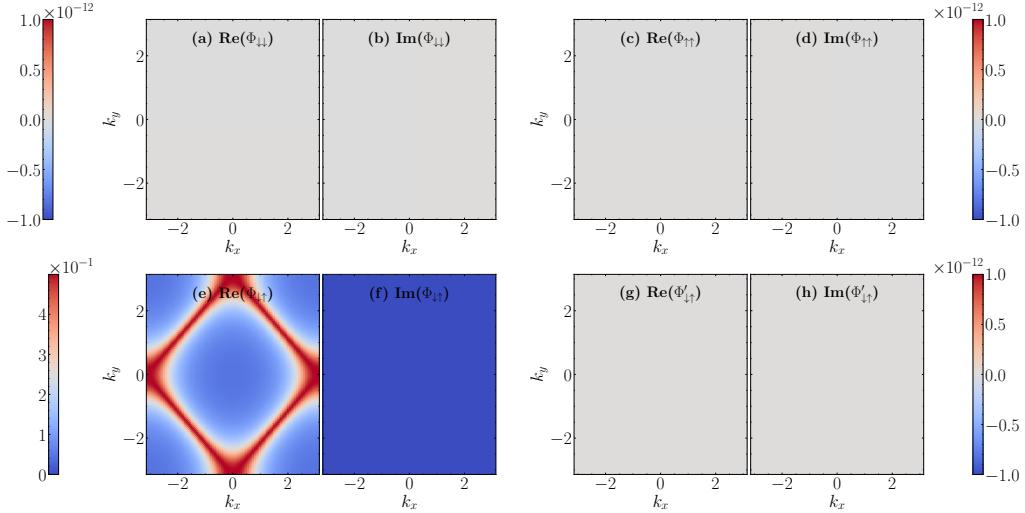


Figure 3: Order parameters $\Phi_{s_1 s_2}$ at chemical potential $\mu = 0$. Other parameters are fixed as $(t, g, D) = (1, 2, 0.5)$. The quantity $\Phi'_{\downarrow\uparrow} = \Phi_{\downarrow\uparrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$ characterizes the new singlet pairing structure due to the perturbation.

symmetry of the system at half-filling. At half-filling ($\mu = 0$), we define the following sublattice transformation K :

$$\begin{aligned} K c_{is} K^{-1} &= c_{is}^\dagger, & i \in A \text{ sublattice}, \\ K c_{is} K^{-1} &= -c_{is}^\dagger, & i \in B \text{ sublattice}, \\ K i K^{-1} &= -i, \end{aligned} \quad (19)$$

where we have divided the 2D square lattice into sublattices A and B , as shown in Fig. 4(a), and the last line of Eq. (19) implies that K is anti-unitarily realized in the many-particle Fock space [19]. The sublattice symmetry K can also be viewed as the product of the time-reversal transformation T and particle-hole transformation \mathcal{C} , i.e., $K = T \cdot \mathcal{C}$ with

$$\begin{aligned} T c_{is} T^{-1} &= (-i\sigma_y)_{ss'} c_{is'}, & \mathcal{C} c_{is} \mathcal{C}^{-1} &= (i\sigma_y)_{ss'} c_{is'}^\dagger, & i \in A \text{ sublattice}, \\ T c_{is} T^{-1} &= (-i\sigma_y)_{ss'} c_{is'}, & \mathcal{C} c_{is} \mathcal{C}^{-1} &= (-i\sigma_y)_{ss'} c_{is'}^\dagger, & i \in B \text{ sublattice}, \\ T i T^{-1} &= -i. & \mathcal{C} i \mathcal{C}^{-1} &= i. \end{aligned} \quad (20)$$

In the following, we will first show that the full-interacting Hamiltonian (1) is invariant under K at half-filling. Then the application of K to the BCS mean-field Hamiltonian is examined, from which we derive the transformation rule for the gap function under K . Based on the irreducible representations of the

sublattice symmetry, we obtain a constraint for the mixing-parity pairing, which explains the absence of the odd-parity state at half-filling. Within this section, we always assume $\mu = 0$.

4.1 Sublattice transformation on the full-interacting Hamiltonian

We examine how the full Hamiltonian (1) transforms under the sublattice transformation K defined above. For the hopping term, we have

$$Kt_{ij}(c_{is}^\dagger c_{js} + c_{js}^\dagger c_{is})K^{-1} = -t_{ij}(c_{is}c_{js}^\dagger + c_{js}c_{is}^\dagger) = t_{ij}(c_{js}^\dagger c_{is} + c_{is}^\dagger c_{js}). \quad (21)$$

Therefore, the kinetic part is invariant under K . For the on-site repulsive interaction, we first derive the transformation for the particle number operator:

$$Kn_{is}K^{-1} = K(c_{is}^\dagger c_{is})K^{-1} = c_{i\bar{s}}c_{i\bar{s}}^\dagger = 1 - n_{i,\bar{s}}, \quad (22)$$

where $\bar{s} = -s$. Therefore, we have

$$Kgn_{i\uparrow}n_{i\downarrow}K^{-1} = g(1 - n_{i\downarrow})(1 - n_{i\uparrow}) = g(1 - (n_{i,\uparrow} + n_{i,\downarrow}) + n_{i\uparrow}n_{i\downarrow}) = gn_{i\uparrow}n_{i\downarrow} \quad (23)$$

where we have used the half-filling condition $n_i = n_{i\uparrow} + n_{i\downarrow} = 1$ in the last step. Again, the on-site interaction is invariant under K . For the Dzyaloshinsky-Moriya interaction, we first derive the transformations for the spin operators:

$$\begin{aligned} K\vec{S}_iK^{-1} &= K(c_{is_1}^\dagger \frac{\vec{\sigma}_{s_1 s_2}}{2} c_{is_2})K^{-1} = c_{is_1} \frac{\vec{\sigma}_{s_1 s_2}^*}{2} c_{is_2}^\dagger \\ &= (\delta_{s_1 s_2} - c_{is_2}^\dagger c_{is_1})(\frac{\vec{\sigma}}{2})_{s_2 s_1} = c_{is_2}^\dagger \frac{\vec{\sigma}_{s_2 s_1}}{2} c_{is_1} = \vec{S}_i, \end{aligned} \quad (24)$$

from which we find that the Dzyaloshinsky-Moriya interaction $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ is invariant under K . In summary, we show that the full-interacting Hamiltonian (1) has a sublattice symmetry at half-filling.

4.2 Sublattice transformation on the mean-field Hamiltonian

The mean-field Hamiltonian of Eq. (1) can be casted into the following general BCS mean-field Hamiltonian

$$H_{\text{MF}} = \sum_{\mathbf{k}, s} \epsilon_{\mathbf{k}} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} + \sum_{\mathbf{k}} (\Delta_{s_1 s_2}(\mathbf{k}) c_{\mathbf{k}, s_1}^\dagger c_{-\mathbf{k}, s_2}^\dagger + \Delta_{s_1 s_2}^*(\mathbf{k}) c_{-\mathbf{k}, s_2} c_{\mathbf{k}, s_1}), \quad (25)$$

where the gap $\Delta(\mathbf{k}) = -\Delta^T(-\mathbf{k})$ since the electrons are fermionic. For non-centrosymmetric systems, the gap function is parametrized as

$$\Delta(\mathbf{k}) = i\sigma_y \psi(\mathbf{k}) + i(\mathbf{d}(\mathbf{k}) \cdot \vec{\sigma})\sigma_y, \quad (26)$$

with $\psi(\mathbf{k}) = \psi(-\mathbf{k})$ characterizing the singlet pairing and $\mathbf{d}(\mathbf{k}) = -\mathbf{d}(-\mathbf{k})$ characterizing the triplet pairing. Because the kinetic energy in H_{MF} is the same as that of the full Hamiltonian, which is invariant under K , we now focus on how the pairing terms transform under the sublattice transformations.

The momentum state transforms as follows under K :

$$\begin{aligned} K c_{\mathbf{k}s} K^{-1} &= \frac{1}{\sqrt{N}} \left(\sum_{i \in A} K c_{is} e^{-i\mathbf{k} \cdot \mathbf{r}_i} K^{-1} + \sum_{i \in B} K c_{is} e^{-i\mathbf{k} \cdot \mathbf{r}_i} K^{-1} \right) \\ &= \frac{1}{\sqrt{N}} \left(\sum_{i \in A} c_{is}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}_i} - \sum_{i \in B} c_{is}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}_i} \right) = c_{\mathbf{k}+\mathbf{Q},s}^\dagger, \end{aligned} \quad (27)$$

where $\mathbf{Q} = (\pi, \pi)$. Therefore, the pairing term transforms as

$$\begin{aligned} \sum_{\mathbf{k}, s_1, s_2} K \Delta_{s_1 s_2}(\mathbf{k}) c_{\mathbf{k}, s_1}^\dagger c_{-\mathbf{k}, s_2}^\dagger K^{-1} &= \sum_{\mathbf{k}, s_1, s_2} \Delta_{s_1 s_2}^*(\mathbf{k}) c_{\mathbf{k}+\mathbf{Q}, s_1} c_{-\mathbf{k}-\mathbf{Q}, s_2} \\ &= \sum_{\mathbf{k}, s_1, s_2} -\Delta_{s_1 s_2}^*(\mathbf{k} - \mathbf{Q}) c_{-\mathbf{k}, s_2} c_{\mathbf{k}, s_1}. \end{aligned} \quad (28)$$

By rewriting $K H_{\text{MF}} K^{-1}$ in a similar form to Eq. (25), we get the action of K on the gap function $\Delta(\mathbf{k})$,

$$\begin{aligned} K : \Delta(\mathbf{k}) &\rightarrow -\Delta(\mathbf{k} - \mathbf{Q}) \\ \implies \psi(\mathbf{k}) &\rightarrow -\psi(\mathbf{k} - \mathbf{Q}), \quad \mathbf{d}(\mathbf{k}) \rightarrow -\mathbf{d}(\mathbf{k} - \mathbf{Q}). \end{aligned} \quad (29)$$

In particular, the transformation K acts linearly (not anti-linearly) on the gap function. We note that the mean-field Hamiltonian may or may not break the sublattice symmetry, depending on the specific form of the gap function $\psi(\mathbf{k})$ and $\mathbf{d}(\mathbf{k})$. Nevertheless, since the sublattice symmetry transformations form a \mathbb{Z}_2 group ($K^2 = 1$), the gap function is either in the trivial representation of \mathbb{Z}_2 (when the sublattice symmetry is preserved) or the non-trivial representation of \mathbb{Z}_2 (when the sublattice symmetry is spontaneously broken), as detailed in the following subsection.

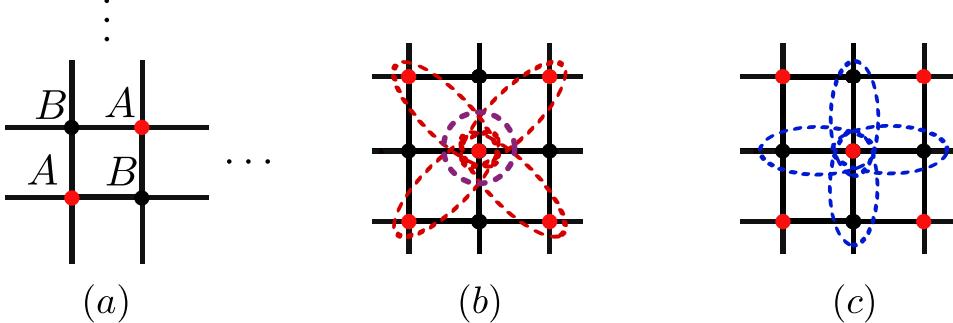


Figure 4: (a) The 2D square lattice is divided into A (red) and B (black) sublattices. (b) Intra-sublattice pairing for the sign representation $\Delta(\mathbf{k} - \mathbf{Q}) = \Delta(\mathbf{k})$, as indicated by purple and red dashed lines. (c) Inter-sublattice pairing for the trivial representation $\Delta(\mathbf{k} - \mathbf{Q}) = -\Delta(\mathbf{k})$, as indicated by blue dashed lines.

4.3 Classification of the gap function under sublattice symmetry

Let's first consider the simple case where the Dzyaloshinsky-Moriya interaction is ignored, i.e., the conventional s -wave pairing with $\psi(\mathbf{k}) = \text{const.}$ and $\mathbf{d}(\mathbf{k}) = 0$. In this case, the mean-field Hamiltonian H_{MF} is not invariant under K , while the full-interacting Hamiltonian (without the spin-spin coupling) is invariant. This implies that the half-filling conventional s -wave pairing breaks the $U(1)$ and sublattice symmetry simultaneously. Hence, we can further classify the order parameter $\Delta(\mathbf{k})$ according to the irreducible representations of the sublattice transformations [12, 13], i.e., a \mathbb{Z}_2 group. For the conventional pairing, the order parameter belongs to the sign representation of \mathbb{Z}_2 , in which the non-trivial element $K \in \mathbb{Z}_2$ maps $\psi(\mathbf{k})$ to $-\psi(\mathbf{k})$.

With the Dzyaloshinsky-Moriya interaction, a mixing of the even-parity and the odd-parity states is allowed since the symmetry group changes from D_{4h} to C_{4v} . The mean-field Hamiltonian H_{MF} may or may not break the sublattice symmetry, depending on which representation of C_{4v} the order parameter $\Delta(\mathbf{k})$ lives in. Nevertheless, the representation should furnish an irreducible representation of \mathbb{Z}_2 . More concretely, the gap should satisfy either

$$\begin{aligned} K : \Delta(\mathbf{k}) &\rightarrow -\Delta(\mathbf{k} - \mathbf{Q}) = \Delta(\mathbf{k}) && (\text{trivial repr. of } \mathbb{Z}_2) \\ \implies \psi(\mathbf{k}) &\rightarrow -\psi(\mathbf{k} - \mathbf{Q}) = \psi(\mathbf{k}), \quad \mathbf{d}(\mathbf{k}) \rightarrow -\mathbf{d}(\mathbf{k} - \mathbf{Q}) = \mathbf{d}(\mathbf{k}), \end{aligned} \quad (30)$$

or

$$\begin{aligned} K : \Delta(\mathbf{k}) &\rightarrow -\Delta(\mathbf{k} - \mathbf{Q}) = -\Delta(\mathbf{k}) && (\text{sign repr. of } \mathbb{Z}_2) \\ \implies \psi(\mathbf{k}) &\rightarrow -\psi(\mathbf{k} - \mathbf{Q}) = -\psi(\mathbf{k}), \quad \mathbf{d}(\mathbf{k}) \rightarrow -\mathbf{d}(\mathbf{k} - \mathbf{Q}) = -\mathbf{d}(\mathbf{k}). \end{aligned} \quad (31)$$

In our model, the order parameter for the unperturbed Hamiltonian H_0 has the form $\psi(\mathbf{k}) = \text{const.}$ and $\mathbf{d}(\mathbf{k}) = 0$, which furnishes a sign representation for the sublattice transformation. When the perturbation is weak, we expect that the gap function $\Delta(\mathbf{k})$ remains in the sign representation by continuity. Therefore, we obtain that $\psi(\mathbf{k})$ and $\mathbf{d}(\mathbf{k})$ should satisfy $\psi(\mathbf{k}) = \psi(\mathbf{k} - \mathbf{Q})$ and $\mathbf{d}(\mathbf{k} - \mathbf{Q}) = \mathbf{d}(\mathbf{k})$, respectively. On the other hand, the Dzyaloshinsky-Moriya perturbation can be rewritten as

$$H_I \approx \frac{1}{2} \sum_{\mathbf{kk}'} \sum_{s_1 s_2 s'_1 s'_2} \sum_{\nu} \frac{D}{4} \left([\phi_s(\mathbf{k}) g_s^{\nu}(\mathbf{k}') - \phi_d(\mathbf{k}) g_d^{\nu}(\mathbf{k}')] (i\sigma^y)_{s_1 s_2} (i\sigma^{\nu} \sigma^y)_{s'_2 s'_1}^{\dagger} + [\phi_s(\mathbf{k}') g_s^{\nu}(\mathbf{k}) - \phi_d(\mathbf{k}') g_d^{\nu}(\mathbf{k})] (i\sigma^{\nu} \sigma^y)_{s_1 s_2} (i\sigma^y)_{s'_2 s'_1}^{\dagger} \right) c_{\mathbf{k}s_1}^{\dagger} c_{-\mathbf{k}s_2}^{\dagger} c_{-\mathbf{k}'s'_2} c_{\mathbf{k}'s'_1}, \quad (32)$$

where we restrict to zero-momentum Cooper-pair scatterings. The basis functions $(\phi_s(\mathbf{k}), \mathbf{g}_s(\mathbf{k}))$ and $(\phi_d(\mathbf{k}), \mathbf{g}_d(\mathbf{k}))$ live in the A_1 and B_1 irreducible representations of C_{4v} , respectively:

$$A_1 \text{ irrep of } C_{4v} : \phi_s(\mathbf{k}) = \cos(k_x) + \cos(k_y), \quad \mathbf{g}_s(\mathbf{k}) = \sin(k_y) \hat{\mathbf{x}} - \sin(k_x) \hat{\mathbf{y}}; \quad (33)$$

$$B_1 \text{ irrep of } C_{4v} : \phi_d(\mathbf{k}) = \cos(k_x) - \cos(k_y), \quad \mathbf{g}_d(\mathbf{k}) = \sin(k_y) \hat{\mathbf{x}} + \sin(k_x) \hat{\mathbf{y}}. \quad (34)$$

Because the unperturbed gap function $\psi(\mathbf{k}) = \text{const.}$ belongs to the A_1 representation of C_{4v} , the possible pairing channels induced by the Dzyaloshinsky-Moriya perturbation are $\psi^{(\text{ind})}(\mathbf{k}) \propto \cos(k_x) + \cos(k_y)$ and $\mathbf{d}^{(\text{ind})}(\mathbf{k}) \propto \sin k_y \hat{\mathbf{x}} - \sin k_x \hat{\mathbf{y}}$, which are incompatible with the constraint $\psi(\mathbf{k}) = \psi(\mathbf{k} - \mathbf{Q})$ and $\mathbf{d}(\mathbf{k} - \mathbf{Q}) = \mathbf{d}(\mathbf{k})$. Consequently, at half-filling there is no induced parity-mixing pairing.

More generally, the sublattice symmetry at half-filling restricts the electrons to either form intra-sublattice pairing or inter-sublattice pairing in real space. To show this, we introduce the pairing wavefunction in real space

$$\Phi_{ss'}(\mathbf{r}_i - \mathbf{r}_j) = \langle c_{is} c_{js'} \rangle = \frac{1}{\Omega} \sum_{\mathbf{k}} \langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)}. \quad (35)$$

Since $\langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle$ has the same symmetry as the gap $\Delta(\mathbf{k})$, the two representations of \mathbb{Z}_2 lead to two different pairing patterns:

$$\begin{aligned} \Delta(\mathbf{k}) = \Delta(\mathbf{k} - \mathbf{Q}) \implies \Phi_{ss'}(\mathbf{r}_i - \mathbf{r}_j) &= \frac{1}{\Omega} \sum_{\mathbf{k}} \langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \\ &= \frac{1}{\Omega} \sum_{\mathbf{k}} \langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle e^{i(\mathbf{k} - \mathbf{Q}) \cdot (\mathbf{r}_i - \mathbf{r}_j)} = 0, \quad \text{for } i \in A, j \in B, \end{aligned} \quad (36)$$

corresponding to the intra-sublattice pairing, and

$$\begin{aligned}\Delta(\mathbf{k}) = -\Delta(\mathbf{k} - \mathbf{Q}) \implies \Phi_{ss'}(\mathbf{r}_i - \mathbf{r}_j) &= \frac{1}{\Omega} \sum_{\mathbf{k}} \langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \\ &= -\frac{1}{\Omega} \sum_{\mathbf{k}} \langle c_{\mathbf{k}s} c_{-\mathbf{k}s'} \rangle e^{i(\mathbf{k}-\mathbf{Q})\cdot(\mathbf{r}_i - \mathbf{r}_j)} = 0, \quad \text{for } i, j \in A \text{ or } i, j \in B,\end{aligned}\tag{37}$$

corresponding to the inter-sublattice pairing, as illustrated in Fig. 4(b-c). Combined with the irreducible representations of the point group, the possible forms of the pairing wavefunction at half-filling is quite limited.

5 Conclusion

In this work, we explore the perturbative effect of the Dzyaloshinsky-Moriya interaction H_I on a conventional s -wave superconductor with on-site interactions, situated on a 2D square lattice. The additional interaction H_I breaks the inversion symmetry of the system and reduces the symmetry group from D_{4h} to C_{4v} . Physically, it explicitly introduces a coupling between the even-parity pairing channel and the odd-parity pairing channel.

Using a perturbative approach, we find that, for generic chemical potential $\mu \neq 0$, the Cooper pair wavefunction has both the even-parity component $\psi(\mathbf{k}) \propto \cos(k_x) + \cos(k_y)$ and the odd-parity component $\mathbf{d}(\mathbf{k}) \propto \sin(k_y)\hat{\mathbf{x}} - \sin(k_x)\hat{\mathbf{y}}$, in addition to the original conventional s -wave pairing $\psi(\mathbf{k}) = \text{const.}$ The result is consistent with the group-theoretical perspective, as both the induced pairings and original pairing fall into the A_1 representation of C_{4v} .

Besides, we observe that the pairing structure is unaffected by the perturbation at $\mu = 0$, which can be explained by the presence of an extra sublattice symmetry at half-filling. We demonstrate that the full-interacting Hamiltonian at half-filling is symmetric under the sublattice transformation K , defined in Eq. (19). In the superconducting phase, the system may or may not break this additional symmetry spontaneously, in conjunction with $U(1)$ and the point group C_{4v} . Consequently, this allows us to further classify the order parameter Δ in the irreducible representation of \mathbb{Z}_2 . We find that the induced pairing channels by H_I are incompatible with the conventional pairing channel under the sublattice symmetry, clarifying the absence of parity-mixing pairing. In real space, the sublattice symmetry K can be understood as requiring the electrons to form either intra-sublattice pairing or inter-sublattice pairing.

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