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RECEIVED 06 July 2023

ACCEPTED 21 August 2023

PUBLISHED 01 September 2023

CITATION

Patil S, Tang G and Belzig W (2023),
Spectral properties of a mixed singlet-
triplet Ising superconductor.
Front. Electron. Mater. 3:1254302.
doi: 10.3389/femat.2023.1254302

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Spectral properties of a mixed singlet-triplet Ising superconductor

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Conventional two-dimensional superconductivity is destroyed when the critical in-plane magnetic field exceeds the so-called Pauli limit. Some monolayer transition-metal dichalcogenides lack inversion symmetry and the strong spin-orbit coupling leads to a valley-dependent Zeeman-like spin splitting. The resulting spin-valley locking lifts the valley degeneracy and results in a strong enhancement of the in-plane critical magnetic field. In these systems, it was predicted that the density of states in an in-plane field exhibits distinct mirage gaps at finite energies of about the spin-orbit coupling strength, which arise from a coupling of the electron and hole bands at energy larger than the superconducting gap. In this study, we investigate the impact of a triplet pairing channel on the spectral properties, primarily the mirage gap and the superconducting gap, in the clean limit. Notably, in the presence of the triplet pairing channel, the mirage-gap width is reduced for the low magnetic fields. Furthermore, when the temperature is lower than the triplet critical temperature, the mirage gaps survive even in the strong-field limit due to the finite singlet and triplet order parameters. Our work provides insights into controlling and understanding the properties of spin-triplet Cooper pairs.

KEYWORDS

Ising superconductors, spin-orbit coupling, mirage gaps, spin triplet pairing, unconventional superconductivity

1 Introduction

Superconductivity in the presence of magnetism has been a topic of great interest within the scientific community for several decades, and is responsible for many exotic properties. Usually, an external magnetic field destroys superconductivity by aligning the electron spins in the same direction. This is typical in conventional superconductors where Cooper pairs are formed by two electrons with opposite spins. The upper critical field is limited by the Pauli paramagnetic effect [Chandrasekhar \(1962\)](#); [Clogston \(1962\)](#). However, in some superconductors, the Pauli limit can be surpassed by forming Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states [Matsuda and Shimahara \(2007\)](#) or by creating spin-triplet Cooper pairs so that the parallel-aligned spin configuration in Cooper pairs is not affected by Pauli paramagnetism [Aoki et al. \(2001\)](#); [Huy et al. \(2007\)](#); [Aoki and Flouquet \(2012\)](#). The spin-triplet Cooper pairings are important for spintronics applications [Ohnishi et al. \(2020\)](#) as they can generate and control spin currents. They are also proposed as a possible route to realize topological superconductivity which could be used to build robust quantum computers [Frolov et al. \(2020\)](#). Therefore, understanding the properties of spin-triplet Cooper pairs is of great interest.

The transition-metal dichalcogenides serve as a platform for both exploring spin-triplet pairing physics and surpassing the Pauli limit in high-field superconductivity. It has been predicted that equal-spin triplet pairs can form in a superconducting few-layer 2H-NbSe₂ when an in-plane magnetic field is applied [Möckli and Khodas \(2020\)](#). Unlike conventional superconductors, monolayer transition metal dichalcogenides, such as NbSe₂, lack in-plane crystal inversion symmetry [Frigeri et al. \(2004\)](#); [Smidman et al. \(2017\)](#); [Wickramaratne et al. \(2020\)](#); [Ramires \(2022\)](#). This results in a spin-orbit interaction that generates an effective out-of-plane magnetic field, causing the electron spins to point out of the plane [Xiao et al. \(2012\)](#); [Zhu et al. \(2011\)](#). Therefore, it is termed as Ising spin-orbit coupling (ISOC) [Zhou et al. \(2016\)](#); [Saito et al. \(2016\)](#); [Lu et al. \(2015\)](#), and the corresponding Ising superconductivity was experimentally found in numerous transition-metal dichalcogenides [Lu et al. \(2015\)](#); [Saito et al. \(2016\)](#); [Xi et al. \(2016\)](#); [Xing et al. \(2017\)](#); [Dvir et al. \(2018\)](#); [Costanzo et al. \(2018\)](#); [Lu et al. \(2018\)](#); [de la Barrera et al. \(2018\)](#); [Sohn et al. \(2018\)](#); [Li et al. \(2021\)](#); [Cho et al. \(2022\)](#); [Hamill et al. \(2021\)](#); [Idzuchi et al. \(2021\)](#); [Ai et al. \(2021\)](#); [Kang et al. \(2021\)](#); [Kuzmanović et al. \(2022\)](#). ISOC is dependent on momentum and has opposite signs at the *K* and *K'* points of the hexagonal Brillouin zone. It prevents the spin directions from being realigned by an externally applied in-plane magnetic field, thus overcoming the Pauli limit to demonstrate high in-plane critical fields [Ilić et al. \(2017\)](#); [Kuzmanović et al. \(2022\)](#).

Ising superconductors subjected to an in-plane magnetic field display unique features in their density of states, notably the emergence of additional half-gaps at finite energies of about the ISOC strength [Tang et al. \(2021\)](#). These newly discovered gaps, called mirage gaps, represent a mirroring of the main superconducting gap and are signatures of the equal-spin triplet finite-energy pairing correlations. Their width is determined by the interplay of the in-plane magnetic field and ISOC. In the previous work, the mirage gaps have only been studied in the context of the singlet pairing channel [Tang et al. \(2021\)](#). However, a recent experiment found that the superconducting gap in a few-layer NbSe₂ under an in-plane magnetic field was larger than predictions based solely on the singlet-pairing channel [Kuzmanović et al. \(2022\)](#). This discrepancy was attributed to the existence of a triplet-pairing channel, in which an equal-spin triplet order parameter couples with a singlet one to enhance the critical magnetic field [Ilic et al. \(2023\)](#).

In this work, we investigate the mirage gaps of an Ising superconductor that consists of both singlet and triplet pairing channels [Kuzmanović et al. \(2022\)](#); [Ilic et al. \(2023\)](#). For a fixed temperature, the maximal mirage-gap width by varying the magnetic field decreases with increasing the critical temperature of the triplet pairing channel T_{ct} . When the magnetic field is extremely high and the temperature is lower than T_{ct} , the mirage-gap width remains finite due to the nonvanishing spin-singlet and spin-triplet order parameters. This contrasts with the case without considering the triplet-pairing channel where the mirage gaps always disappear at the critical field for the singlet order parameter [Tang et al. \(2021\)](#).

2 Model and formalism

An Ising superconductor with both a singlet order parameter Δ_s and an equal-spin triplet order parameter Δ_t can be described by a Bogoliubov–de Gennes Hamiltonian near the *K* (*K'*) valley by neglecting the contribution from Γ point [Kuzmanović et al. \(2022\)](#). By applying an in-plane magnetic field \mathbf{B} , the effective Hamiltonian can be written in the Nambu basis $(c_{k,\uparrow}, c_{k,\downarrow}, c_{-k,\uparrow}^\dagger, c_{-k,\downarrow}^\dagger)$ as

$$H_{BdG} = \begin{bmatrix} H_0(\mathbf{k}) & \Delta i\sigma_y \\ -\Delta i\sigma_y & -H_0^*(-\mathbf{k}) \end{bmatrix}, \quad (1)$$

where $H_0(\mathbf{k})$ is given by

$$H_0(\mathbf{k} = \mathbf{p} + s\mathbf{K}) = \xi_p \sigma_0 + s\beta_{so} \sigma_z - \mathbf{B} \cdot \boldsymbol{\sigma}. \quad (2)$$

Here, $s = +1$ corresponds to the valley *K* and $s = -1$ to *K'*. The deviation of the momentum from *K* or *K'* is denoted by \mathbf{p} . The Pauli matrices σ_x , σ_y , and σ_z act on the spin space and σ_0 is the corresponding unit matrix. The dispersion measured from the chemical potential is $\xi_p = p^2/2m - \mu$. The ISOC strength is denoted by β_{so} . The Zeeman term arising from the in-plane magnetic field in the *x*-direction is $B_x \sigma_x$ which absorbs the factor of $g\mu_B/2$ containing the Landé *g* factor and the Bohr magneton μ_B . Note that the ISOC forces the spins to align out of the plane, whereas the in-plane magnetic field aims to align the spins within the plane. The superconducting order parameter can be written as [Kuzmanović et al. \(2022\)](#); [Ilic et al. \(2023\)](#).

$$\Delta = \Delta_s + is\Delta_t \sigma_y. \quad (3)$$

The eigenvalues of the Bogoliubov-de Gennes Hamiltonian are given by

$$\epsilon_{1(2)} = \sqrt{\xi_p^2 + \rho^2 + \Delta_s^2 + \Delta_t^2 \pm 2\sqrt{\rho^2 \xi_p^2 + P^2}} \quad (4)$$

with $\rho = \sqrt{\beta_{so}^2 + B_x^2}$ and $P = B_x \Delta_s - \beta_{so} \Delta_t$. The position ϵ_0 and the width δ of a mirage gap are obtained from the eigenvalues of the Hamiltonian, being given by $\epsilon_0 = \pm(\epsilon_1 + \epsilon_2)/2$ and $\delta = \epsilon_1 - \epsilon_2$, respectively. At $\xi_p = 0$ and in the limit of $\beta_{so} \gg \Delta_s, \Delta_t$, we have $\epsilon_0 \approx \rho$ and

$$\delta \approx 2P/\rho. \quad (5)$$

The approximation indicates that the mirage-gap width is influenced by the interplay of the singlet and triplet order parameters.

Since the superconducting gap and the ISOC are much smaller compared to the Fermi energy, it allows us to use the formalism of quasiclassical Green's function [Eilenberger \(1968\)](#); [Larkin and Ovchinnikov \(1969\)](#); [Belzig et al. \(1999\)](#); [Kopnin \(2001\)](#); [Eschrig \(2015\)](#). The structure of the Green's functions can be written as

$$\hat{g}(\hat{\mathbf{k}}, \epsilon) = \begin{bmatrix} g_0 \sigma_0 + \mathbf{g} \cdot \boldsymbol{\sigma} & (f_0 \sigma_0 + \mathbf{f} \cdot \boldsymbol{\sigma}) i\sigma_y \\ (\bar{f}_0 \sigma_0 + \bar{\mathbf{f}} \cdot \boldsymbol{\sigma}^*) i\sigma_y & \bar{g}_0 \sigma_0 + \bar{\mathbf{g}} \cdot \boldsymbol{\sigma}^* \end{bmatrix}. \quad (6)$$

The bar operation in the above expression is defined as $\hat{q}(\hat{\mathbf{k}}, \epsilon) = \hat{q}(-\hat{\mathbf{k}}, -\epsilon^*)^*$ with $q \in \{g_0, f_0, \mathbf{g}, \mathbf{f}\}$. For a homogeneous system in the clean limit, the Eilenberger equation can be written as

$$[\epsilon \sigma_0 \tau_3 - \hat{\Delta} - \hat{v}, \hat{g}] = 0. \quad (7)$$

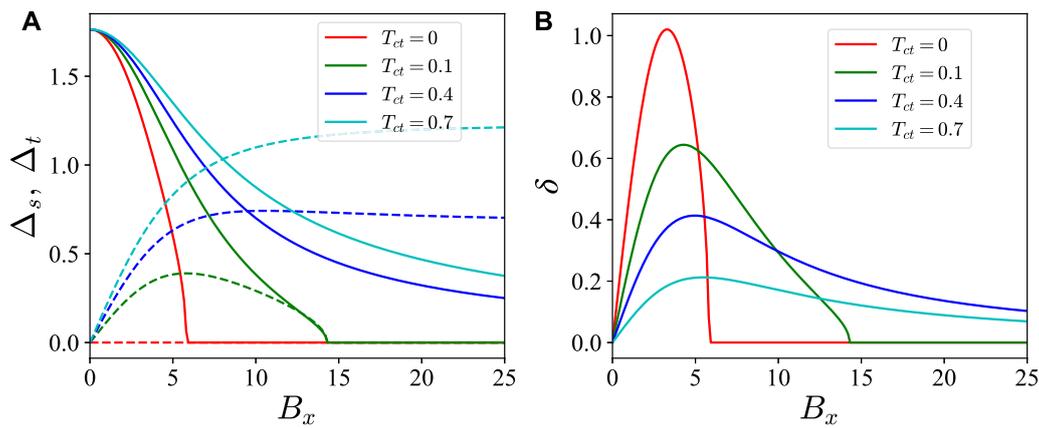


FIGURE 1 (A) Singlet (Δ_s , solid lines) and triplet (Δ_t , dashed lines) order parameters versus in-plane magnetic field B_x under different triplet critical temperatures T_{ct} . (B) The mirage-gap width δ versus B_x under different T_{ct} . The temperature is $T=0.2$. All the quantities are in the units of T_{cs} .

The order parameter term $\hat{\Delta}$ consisting of both the singlet and triplet components can be written as

$$\hat{\Delta} = \begin{bmatrix} 0 & (\Delta_s \sigma_0 + \Delta_t \cdot \sigma) i \sigma_y \\ (\bar{\Delta}_s \sigma_0 + \bar{\Delta}_t \cdot \sigma^*) i \sigma_y & 0 \end{bmatrix}, \quad (8)$$

with $\Delta_t = (0, i\Delta_t, 0)$. The Zeeman and ISOC fields are included in the term \hat{v} as

$$\hat{v} = s\beta_{so}\sigma_z\tau_3 - \begin{bmatrix} \mathbf{B} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \mathbf{B} \cdot \boldsymbol{\sigma}^* \end{bmatrix}. \quad (9)$$

The Pauli matrices τ_1, τ_2 , and τ_3 act on the Nambu space and τ_0 is the corresponding unit matrix. Using the notation $\mathbf{g}_{\pm} = (\mathbf{g} \pm \bar{\mathbf{g}})/2$, we can write the Eilenberger equation as the following set of equations

$$\epsilon f_0 - \nu_+ \cdot \mathbf{f} + \Delta_s g_0 + \Delta_t \cdot \mathbf{g}_+ = 0, \quad (10)$$

$$\epsilon \mathbf{f} - f_0 \nu_+ - i\nu_- \times \mathbf{f} + g_0 \Delta_t + \Delta_s \mathbf{g}_+ + i\mathbf{g}_- \times \Delta_t = 0, \quad (11)$$

$$-\epsilon \bar{f}_0 - \nu_+ \cdot \bar{\mathbf{f}} - \bar{\Delta}_s g_0 + \bar{\Delta}_t \cdot \mathbf{g}_+ = 0, \quad (12)$$

$$-\epsilon \bar{\mathbf{f}} - \bar{f}_0 \nu_+ - i\nu_- \times \bar{\mathbf{f}} - g_0 \bar{\Delta}_t + \bar{\Delta}_s \mathbf{g}_+ + i\mathbf{g}_- \times \bar{\Delta}_t = 0. \quad (13)$$

The normalization condition $\hat{g}\hat{g} = \sigma_0\tau_0$ then gives us the following equations

$$g_0^2 + g_+^2 + g_-^2 - f_0 \bar{f}_0 + \mathbf{f} \cdot \bar{\mathbf{f}} = 1, \quad (14)$$

$$\bar{f}_0 f - f_0 \bar{f} = 2g_0 \mathbf{g}_+, \quad (15)$$

$$i\bar{\mathbf{f}} \times \mathbf{f} = 2g_0 \mathbf{g}_-. \quad (16)$$

By combining the Eilenberger equation with $\text{tr}(\hat{g}) = 0$ and the normalization condition $\hat{g}\hat{g} = \sigma_0\tau_0$, we can get the components of the Green's function. Defining $\Sigma = \Delta_s^2 + \Delta_t^2 - \epsilon^2 + \rho^2$ and $\Omega = \sqrt{2(\Sigma - 2\rho^2 + \sqrt{\Sigma^2 - 4P^2})}$, we can express $g_0, g_{+,x}, g_{-,z}, f_0, f_x$ and f_y , respectively, as

$$g_0 = \frac{i\epsilon}{\Omega} \left(\frac{\Sigma}{\sqrt{\Sigma^2 - 4P^2}} + 1 \right), \quad (17)$$

$$g_{+,x} = \frac{1}{\Omega} \left(\frac{B_x \Sigma - 2\Delta_s P}{\sqrt{\Sigma^2 - 4P^2}} + B_x \right), \quad (18)$$

$$g_{-,z} = \frac{s}{\Omega} \left(\frac{\beta_{so} \Sigma + 2\Delta_t P}{\sqrt{\Sigma^2 - 4P^2}} + \beta_{so} \right), \quad (19)$$

$$f_0 = \frac{i}{\Omega} \left(\frac{\Delta_s \Sigma - 2B_x P}{\sqrt{\Sigma^2 - 4P^2}} + \Delta_s \right), \quad (20)$$

$$f_x = \frac{i\epsilon P}{\Omega \sqrt{\Sigma^2 - 4P^2}}, \quad (21)$$

$$f_y = \frac{s}{\Omega} \left(\frac{\Delta_t \Sigma + 2\beta_{so} P}{\sqrt{\Sigma^2 - 4P^2}} + \Delta_t \right). \quad (22)$$

We also find that $g_0 = \bar{g}_0, f_0 = \bar{f}_0, f_x = -\bar{f}_x, f_y = \bar{f}_y$, and $f_z = \bar{f}_z$. The remaining Green's functions $f_z, g_{+,z}, g_{-,x}$ and $g_{-,y}$ are zero. We can use Green's functions f_0 in Eq. 18 and f_y in Eq. 22 to derive the self-consistent equations for the singlet and the triplet order parameters. The cut-off frequencies $\Omega_{s(t)}$ are related to the critical temperatures $T_{cs(t)}$ and the coupling constants $\nu_{s(t)}$ by $\Omega_{s(t)} = 1.764 T_{cs(t)} \sinh(1/\nu_{s(t)})$. Assuming the same cut-off frequency for the singlet and the triplet pairing channels, we obtain $\nu_t = \nu_s/[1 + \nu_s \ln(T_{cs}/T_{ct})]$. The singlet and triplet order parameters are coupled with the relations

$$\Delta_s = 2\pi T |\nu_s| \sum_{\omega_n > 0} \frac{1}{\Omega} \left(\frac{\Delta_s \Sigma - 2B_x P}{\sqrt{\Sigma^2 - 4P^2}} + \Delta_s \right), \quad (23)$$

and

$$\Delta_t = 2\pi T |\nu_t| \sum_{\omega_n > 0} \frac{1}{\Omega} \left(\frac{\Delta_t \Sigma + 2\beta_{so} P}{\sqrt{\Sigma^2 - 4P^2}} + \Delta_t \right). \quad (24)$$

At very high magnetic field and in the limit of $B_x \gg \beta_{so}, \epsilon, \Delta_s, \Delta_t$, one can show that $\Delta_s = 2\pi T |\nu_s| \sum_{\omega_n > 0} \beta_{so} \Delta_t / (B_x \sqrt{\omega_n^2 + \Delta_t^2})$, and $2\pi T |\nu_t| \sum_{\omega_n > 0} \frac{1}{\sqrt{\omega_n^2 + \Delta_t^2}} = 1$. This leads to $\Delta_s = \nu_s \beta_{so} \Delta_t / (\nu_t B_x)$ so that $P = (\nu_s / \nu_t - 1) \beta_{so} \Delta_t$. Therefore, at high magnetic fields, the mirage gaps remain finite as long as the order parameters are finite.

3 Numerical results

In the numerical calculation, the ISOC strength is set as $\beta_{so} = 7T_{cs}$. In Figure 1A, we plot the singlet (Δ_s) and triplet (Δ_t) order parameters

versus the in-plane magnetic field B_x by varying the triplet critical temperature T_{ct} at a fixed temperature T . The behavior of the order parameters in the cases of $T > T_{ct}$ and $T < T_{ct}$ will be discussed separately in the following. For the case where $T > T_{ct}$, with increasing magnetic field, the singlet order parameter Δ_s decreases and finally vanishes at the critical field. This is attributed to the pair-breaking effect of the magnetic field which tries to align the spins of the spin-singlet Cooper pairs in its direction. On the other hand, the in-plane magnetic field induces the equal-spin triplet pairings which are coupled to the singlet pairings. The triplet order parameter Δ_t first increases with increasing the in-plane magnetic field since the field attempts to align the spins in the plane which is favorable for the formation of triplet pairs. It then decreases due to its coupling with Δ_s as seen from the self-consistent gap equations. Finally, both Δ_s and Δ_t vanish at the same critical magnetic field for $T > T_{ct}$. For the case where $T < T_{ct}$, at small magnetic fields, Δ_s decreases, and Δ_t begins to increase in a similar manner to the case where $T > T_{ct}$. The behavior of both order parameters differ from that of $T > T_{ct}$ case at high magnetic fields. Both Δ_s and Δ_t reach saturated values instead of vanishing at a critical field. This is because the triplet order parameter is preserved by the in-plane field as the field favors the formation of triplet pairs. Consequently, Δ_s does not vanish due to its coupling with Δ_t .

Figure 1B shows the mirage-gap width δ for different triplet critical temperatures T_{ct} . The maximal mirage-gap width by varying the magnetic field decreases with increasing T_{ct} . The mirage gaps vanish at the critical in-plane field when $T > T_{ct}$. This is due to the dependence of mirage-gap width on the order parameters which vanish at the critical field. On the other hand, the mirage gaps are finite even at extremely high in-plane fields in the scenarios where $T < T_{ct}$. This is because the order parameters remain finite in the high field limit at $T < T_{ct}$.

4 Conclusion

To conclude, we have studied the effect of a triplet pairing channel on the spectral properties of an Ising superconductor. The presence of a triplet order parameter reduces the maximal mirage-gap width by varying the in-plane magnetic field. Notably, at a temperature lower than T_{ct} , both the order parameters and the mirage gap are finite even at very high fields. In contrast, for the case where the temperature is higher than T_{ct} , both the order parameters and the mirage gaps vanish at the critical field. From an experimental standpoint, it is important to note that the intervalley scattering influences both the order parameters, effectively eliminating equal-spin triplet pairing under moderate intervalley disorder Ilic et al. (2023). Our work provides a better understanding about the spin-triplet pairings in Ising superconductors.

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Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

Author contributions

SP: Formal Analysis, Investigation, Methodology, Validation, Writing—original draft, Writing—review and editing. GT: Conceptualization, Formal Analysis, Investigation, Project administration, Writing—original draft, Writing—review and editing. WB: Conceptualization, Formal Analysis, Funding acquisition, Methodology, Supervision, Validation, Writing—review and editing.

Funding

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)—Project-ID 443404566—SPP 2244.

Acknowledgments

We acknowledge useful discussions with M. Aprili, C. Bruder, A. Di Bernardo, and D. Nikolić.

Conflict of interest

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