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Superconducting Instability Temperature of a Non-Centrosymmetric System

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We discuss a direct effect of the energy band splitting due to the antisymmetric spin–orbit coupling on the superconducting phase transition. Employing the square lattice tight-binding model we show a significant contribution of the spin-split energy band to the pair-breaking effect in the weak- and intermediate-coupling non-centrosymmetric superconductors. We establish a general tendency of the spin–orbit coupling to suppress the critical temperature of the spin singlet and triplet states. For the weak-coupling systems we report a possible development of sharp maxima of the critical temperature for the band fillings which support the spin–orbit coupling induced Fermi surface singularities of the density of states. We note that the initial suppression of the most stable triplet state becomes comparable to the suppression of other triplet states in the intermediate-coupling regime of superconductivity.

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1. Introduction

Discovery of superconductivity in $CePt_3Si$ [1], a compound with no inversion center, began extensive studies of superconductivity in the presence of the antisymmetric spin–orbit coupling (ASOC) [2]. A theoretical calculation of the ASOC effect on the superconducting instability temperature, T_c, based on a conjecture of a negligible induced variation of the density of states at the Fermi level, indicates an approximately unaltered T_c of an s-wave superconductor [3]. Application of this method to triplet states allows for a formulation of the T_c suppression in a form resembling the impurity pair-breaking effect which shows a constant and ASOC independent critical temperature of the p-wave state defined by the order parameter $\boldsymbol{d}(\boldsymbol{k})$ parallel to the spin–orbit coupling vector $\boldsymbol{\gamma}(\boldsymbol{k})$ and a strong suppression of other states [3]. We reexamine the issue of the superconducting instability temperature of a non-centrosymmetric system taking the ASOC induced evolution of the energy band into account. Within the tight-binding model, which captures basic features of the spin-split band structure — the increased band width and a redistribution of spectral weights in the density of states, we establish a general ASOC tendency to suppress the critical temperature of the spin singlet and triplet states. For the weak-coupling systems and for the band fillings which support the ASOC induced Fermi surface singularities of the density of states we report a possible development of sharp T_c peaks. In the limit of the intermediate-coupling superconductivity we communicate a comparable suppression of the $\boldsymbol{d}(\boldsymbol{k}) \parallel \boldsymbol{\gamma}(\boldsymbol{k})$ and $\boldsymbol{d}(\boldsymbol{k}) \nparallel \boldsymbol{\gamma}(\boldsymbol{k})$ triplet states. Units $\hbar = k_B = 1$ are used throughout the paper.

2. Antisymmetric spin–orbit coupling

Broken inversion symmetry leads to the relativistic effect of the antisymmetric spin–orbit coupling which is determined by the parity breaking coupling vector $\boldsymbol{\gamma}(\boldsymbol{k}) = -\boldsymbol{\gamma}(-\boldsymbol{k})$ and results in the spin-split energy band $\varepsilon^{\pm}_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} \pm |\boldsymbol{\gamma}(\boldsymbol{k})|$. The ASOC effect on the energy band $\varepsilon_{\boldsymbol{k}}$ is determined by the Hamiltonian

$$\hat{H}_0 = \sum_{\boldsymbol{k},\alpha} (\varepsilon_{\boldsymbol{k}} - \mu)\, \hat{a}^{\dagger}_{\boldsymbol{k}\alpha} \hat{a}_{\boldsymbol{k}\alpha} + \sum_{\alpha,\beta} \sum_{\boldsymbol{k}} \boldsymbol{\gamma}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}_{\alpha\beta} \hat{a}^{\dagger}_{\boldsymbol{k}\alpha} \hat{a}_{\boldsymbol{k}\beta}, \tag{2.1}$$

where μ is the chemical potential, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the 1/2 spin operator, and $\hat{a}^{\dagger}_{\boldsymbol{k}\alpha}$ and $\hat{a}_{\boldsymbol{k}\alpha}$ represent the particle creation and annihilation operators, respectively. We consider the simplest model that captures basic features of the spin-split energy band, that is the square lattice nearest neighbor tight-binding system, $\varepsilon_{\boldsymbol{k}} = -2t\,(\cos(k_x) + \cos(k_y))$, and the lowest order Rashba-type spin–orbit coupling [4] given for a tetragonal symmetry by $\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_0\,(-\hat{\boldsymbol{x}} \sin(k_y) + \hat{\boldsymbol{y}} \sin(k_x))$. The ASOC induced evolution of the density of states is characterized by the split and broadened spectral weights whose main features include a single van Hove singularity which is split and shifted away from the band center symmetrically for the particle and hole branches as well as a development of the edge singularities which dominate the density of states for strong spin–orbit coupling (Fig. 1).

3. Superconducting instability temperature

We consider the s-wave and p-wave superconductors defined by a scalar Δ_0 and a vector $\boldsymbol{d}(\boldsymbol{k})$ order parameters, respectively. A solution of the linearized Gor'kov equations [5] for each of these states yields the linearized anomalous Green functions of the singlet s-wave and the triplet p-wave states. The superconducting instability temperature, T_c, of the BCS non-centrosymmetric

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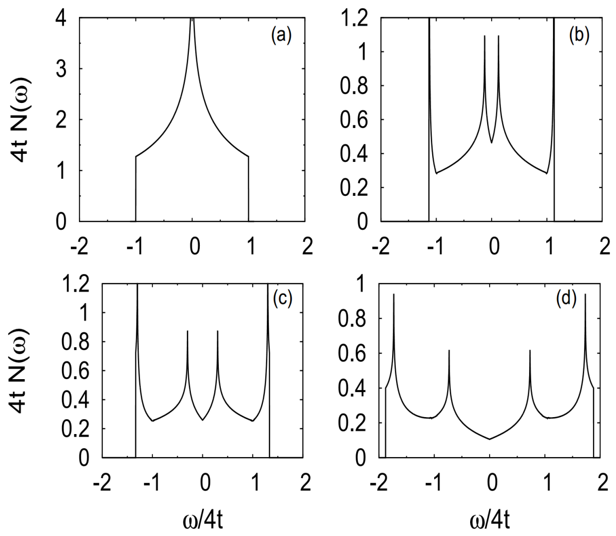

Fig. 1. Dimensionless density of states (normalized to 2) of a tight-binding square lattice system for the spin–orbit coupling rate γ_0/t: (a) 0, (b) 1.5, (c) 2.5, (d) 4.5.

s-wave and p-wave superconductors is determined then by the linearized gap equation which involves a corresponding linearized anomalous Green function and the pair potentials: $V_s(\boldsymbol{k},\boldsymbol{k}') = -V_0 < 0$ for the s-wave, and $V_t(\boldsymbol{k},\boldsymbol{k}') = -3V_1 \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{d}(\boldsymbol{k}')$ for the p-wave state, where $V_1 > 0$. We assume that V_0 and V_1 are unaltered by the spin–orbit coupling. The above method leads to the T_c equation for the s-wave superconductor

$$\Delta_0 = \sum_{\lambda=\pm} \sum_{\boldsymbol{k}'} V_0 \frac{\Delta_0}{4\xi^\lambda_{\boldsymbol{k}'}} \tanh\left(\frac{\xi^\lambda_{\boldsymbol{k}'}}{2T_c}\right), \tag{3.1}$$

which is influenced by the ASOC only through the spin-split quasiparticle excitation energy, $\xi^\pm_{\boldsymbol{k}} = \varepsilon^\pm_{\boldsymbol{k}} - \mu$. In the case of the triplet superconductivity, the effect of the broken inversion symmetry is not limited solely to the normal state properties, like for the singlet superconductivity, but is also present in the superconducting state by the virtue of the term $\boldsymbol{\gamma}(\boldsymbol{k}) \cdot \boldsymbol{d}(\boldsymbol{k})$ which represents the coupling of the order parameter and the ASOC vector, and lifts the degeneracy of the superconducting states corresponding to different irreducible representations of a given symmetry point group. Defining the ASOC unit vector $\hat{\boldsymbol{\gamma}}(\boldsymbol{k}) = \boldsymbol{\gamma}(\boldsymbol{k})/|\boldsymbol{\gamma}(\boldsymbol{k})|$ we can write the linearized gap equation for a triplet superconductor

$$\boldsymbol{d}(\boldsymbol{k}) = \sum_{\lambda=\pm} \sum_{\boldsymbol{k}'} V_t(\boldsymbol{k},\boldsymbol{k}') \frac{1}{4\xi^\lambda_{\boldsymbol{k}'}} \tanh\left(\frac{\xi^\lambda_{\boldsymbol{k}'}}{2T_c}\right) \times \left[\frac{\xi^\lambda_{\boldsymbol{k}'}}{\xi_{\boldsymbol{k}'}} \boldsymbol{d}(\boldsymbol{k}') - \frac{\lambda}{\xi_{\boldsymbol{k}'}} \left(\boldsymbol{d}(\boldsymbol{k}') \cdot \boldsymbol{\gamma}(\boldsymbol{k}')\right) \text{-} \boldsymbol{\gamma}(\boldsymbol{k}')\right] \tag{3.2}$$

The T_c Eqs. (3.1) and (3.2) are accomplished by the relation that determines the chemical potential for a given band filling

$$n = 1 - \frac{1}{2N_0} \sum_{\lambda=\pm} \sum_{\boldsymbol{k}} \tanh\left(\frac{\xi^\lambda_{\boldsymbol{k}}}{2T_c}\right) \tag{3.3}$$

where $2N_0$ represents a total number of states in a band.

4. Results

We discuss the solutions of Eqs. (3.1) and (3.2) for the weak- and intermediate-coupling regimes of superconductivity and present them for the s-wave state in Figs. 2a, b and for the p-wave states in Figs. 2c,d. We consider the band fillings $n = 0.8$ and $n = 1$ which correspond to two possible types of the ASOC induced evolution of the density of states in the vicinity of the Fermi level. Whereas for the band filling $n = 0.8$ the singularity of the density of states crosses the Fermi level for $\gamma_0/t = 2.1$, in the case of $n = 1$ it is being shifted away from the Fermi surface, which is singular for $\gamma_0 = 0$. For both considered density of states structures and for both types of superconductivity we report a general ASOC tendency to suppress the critical temperature, which is a result of a broadened spin-split energy band.

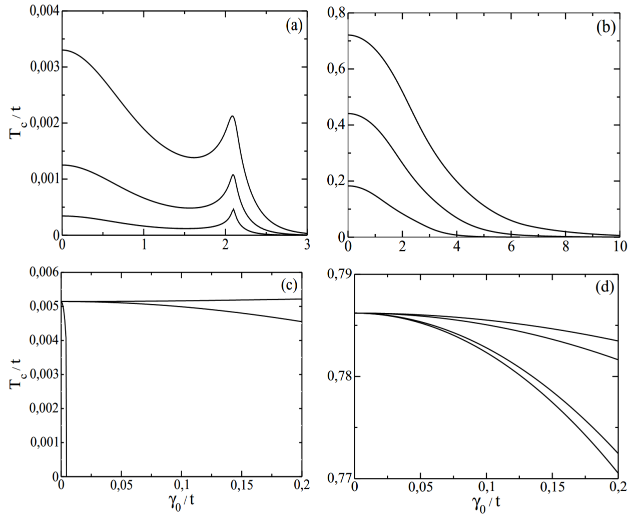

Fig. 2. Critical temperature dependence on the ASOC rate γ_0. T_c of the s-wave state for the band filling $n = 0.8$: (a) weak-coupling pair potential (from bottom to top) $V_0/t = 0.6, 0.7, 0.8$; (b) intermediate-coupling pair potential (from bottom to top) $V_0/t = 2, 3, 4$. T_c of the p-wave states for the half-filled band, the curves from top to bottom correspond to A_2, B_1, B_2, and A_1 state, respectively: (c) weak-coupling pair potential $V_1/t = 0.8$, (d) intermediate-coupling pair potential $V_1/t = 4$.

However, for a singular Fermi surface density of states the monotonic suppression of the weak-coupling states is modified by a significant rise of T_c for the ASOC rate corresponding to the singularity of the density of states at the Fermi level. Such a T_c peak behavior, which is particularly eminent for the s-wave superconductivity, is presented in Fig. 2a for the band filling $n = 0.8$. For the sake of completeness, we remark that a similar but smaller T_c peak is observed for the weak-coupling p-wave states. When the critical temperature is not entirely determined by the Fermi surface density of states, which is the case of the intermediate-coupling superconductivity, the T_c is monotonically decreased by an increasing ASOC rate even despite the singular behavior of the Fermi surface density of states (Fig. 2b). This effect of a continuous T_c suppression, presented in Fig. 2b for the s–wave pairing, is common for singlet and triplet intermediate–coupling superconductors. Moreover, in the case of a non singular Fermi surface density of states ($n = 1$) the monotonic T_c suppression is characteristic for the intermediate- as well as the weak-coupling superconducting states.

The lifted degeneracy of the triplet states is illustrated by the initial ASOC induced development of the critical temperature. We present the split of the critical temperature for the tetragonal C_{4v} lattice p-wave states defined by the order parameters $\boldsymbol{d}(\boldsymbol{k})$ [3, 6, 7]: $\hat{\boldsymbol{x}}\sin(k_x) + \hat{\boldsymbol{y}}\sin(k_y)$ (A_1 state), $-\hat{\boldsymbol{x}}\sin(k_y) + \hat{\boldsymbol{y}}\sin(k_x)$ (A_2 state), $-\hat{\boldsymbol{x}}\sin(k_x) + \hat{\boldsymbol{y}}\sin(k_y)$ (B_1 state), $\hat{\boldsymbol{x}}\sin(k_y) + \hat{\boldsymbol{y}}\sin(k_x)$ (B_2 state) in Figs. 2c and d for the half-filled band. We observe a general ASOC pair-breaking effect and a suppression of all spin-split triplet states. However, for the weak-coupling superconductivity a presence of a singularity of the density of states in a close vicinity of the Fermi surface (Fig. 1b) results in a small local enhancement of the critical temperature of the most stable A_2 state (Fig. 2c). We note that this effect follows directly from a particular Fermi surface nodal structure of the triplet A_2 state at half filling and is not displayed by the s-wave superconductivity, which is monotonically depleted for $n = 1$.

In the regime of the intermediate–coupling superconductivity the spin–orbit coupling becomes less detrimental to the states formed by the interband (A_1) and mixed intra- and interband (B_1, B_2) interactions, which are characterized by the order parameter $\boldsymbol{d}(\boldsymbol{k}) \nparallel \boldsymbol{\gamma}(\boldsymbol{k})$. This feature is manifested in Fig. 2d by a comparable suppression of the A_2 and B_1 states, and a significant enhancement of the critical temperature of the A_1 state. For the sake of clarity, we elucidate that we have considered the uniform superconducting states and a possibility of a development of the nonuniform superconductivity in the non–centrosymmetric systems was discussed by Tanaka et al. [8].

5. Conclusion

We have studied the effect of the antisymmetric spin–orbit coupling on the critical temperature of the s-wave and p-wave superconducting states. Although the quantitative discussion has been carried out for the nearest neighbor tight-binding model, we emphasize that the qualitative results follow from two basic features of the spin–orbit coupling — the split of the energy band and a redistribution of the spectral weights — and are representative for any non-centrosymmetric superconducting system. Concluding, we have shown that the enhanced width of the spin–split energy band leads to the suppression of superconductivity in systems with no inversion center whereas the possible ASOC induced van Hove singularities at the Fermi level may give rise to sharp T_c maxima in the case of the weak–coupling pairing. Concerning the intermediate–coupling superconductivity we have established a significant raise of the interband pairing manifested by a comparable initial suppression of the $\boldsymbol{d}(\boldsymbol{k}) \parallel \boldsymbol{\gamma}(\boldsymbol{k})$ and $\boldsymbol{d}(\boldsymbol{k}) \nparallel \boldsymbol{\gamma}(\boldsymbol{k})$ states, as well as a considerable increase of the critical temperature of the interband A_1 state. Recent theoretical studies [9] of the s-wave superfluid fermions paired on the optical lattice in the presence of a non-Abelian parity breaking spin–orbit coupling potential lead to the conclusions corresponding to our singlet state solution.

Acknowledgments

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