Paramagnetic limit of superconductivity in a crystal without an inversion center

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The theory of paramagnetic limit of superconductivity in metals without an inversion center is developed. There is, in general, the paramagnetic suppression of a superconducting state. The effect is strongly dependent on field orientation with respect to crystal axes. The reason for this is that the degeneracy of electronic states with opposite momenta **k** and −**k** forming of Cooper pairs is lifted by magnetic fields, but for some field directions this lifting can be small or even absent.

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Quite recently unconventional superconductors without inversion symmetry $CePt_3Si$ (Ref. 1) and UIr (Ref. 2) have been discovered. The former reveals superconductivity in an antiferromagnetic state,[3] while the second is a ferromagnetic superconductor. The microscopic theory of superconductivity in metals without inversion had been developed by Edel'stein[4] some long ago. The different aspects of the theory of superconductivity in such type materials had been discussed at about the same time[5–7] and have been advanced further in more recent publications.[8–15] Finally, the general symmetry approach to the superconductivity in the materials with space parity violation has been developed.[16,17]

Particular attention has been attracted to the question about paramagnetic limit in such type materials. This problem has been treated in two-dimensional (2D) metal with Rashba's Hamiltonian[11,13] and quite recently in three-dimensional (3D) metal[18] by means of calculation of susceptibility in a superconducting state. In other words, it was done in the limit of a negligibly small magnetic field at finite value of the order parameter. Being useful for establishing the Knight shift, the susceptibility is not directly related to the paramagnetic limit determination. The latter has to be properly calculated in the limit of the negligibly small order parameter at finite magnetic field. That was undertaken in the paper by Frigeri *et al.*[15]

It occured that zero-temperature upper critical field in polycrystalline $CePt_3Si$ is about 5 T;[1] meanwhile the simple estimation of paramagnetic limiting field $H_p = \pi T_c / \gamma\sqrt{2}\mu_B$ through the value of critical temperature $T_c = 0.75$ K gives $H_p \approx 1$ T. This observation is incompatible with spin-singlet pairing and rather signals the spin-triplet superconductivity. The situation is even worse in UIr, where superconductivity coexists with ferromagnetism. The big internal field in ferromagnetic metal moves apart the Fermi surfaces of the bands filled by electrons with opposite spins, making the singlet pairing impossible. On the other hand, it is known[4] that the simple division on spin-singlet and spin-triplet pairing states does not work in the crystals without inversion.

Hence, the problem of the paramagnetic limit in superconductors without inversion deserves a special investigation and it was undertaken in the paper by Frigeri *et al.*[15] From our point of view, this paper contains the inconsistency: After the proper description of spinor electronic states in normal metal without inversion, the authors introduce the superconducting pairing interaction in, as usual, BCS theory for the crystals with inversion. So, they impose the pairing interaction between the states which do not exist in normal state. This point of view may be acquitted in the crystal with negligibly small spin-orbital coupling having no influence on the pairing interaction, as it has been considered in the original paper.[4] However, in general, the assumption, that pairing takes place between the states which are not modified by the absence of the inversion center, is equivalent to the assumption that typical for the metal without inversion an odd on electronic momentum spin-orbital coupling is smaller than superconducting critical temperature T_c. This point of inconsistency is absent in the papers,[16,17] where the general symmetry approach to the problem of superconductivity in the crystal without inversion has been developed. There was shown in particular[16] that the band splitting due to the lack of inversion in $CePt_3Si$ cannot at all be considered as small. Hence, from our point of view the problem of paramagnetic limit raised in (Ref. 15) must be reconsidered, and we do it in the present paper.

It is shown that the paramagnetic suppression of a superconducting state in a crystal without an inversion centrum certainly exists, and the effect is strongly dependent on field orientation with respect to crystal axes. Whereas in general the paramagnetic limiting field is roughly the same as in a singlet superconductor, for some field directions H_p is very large or even infinite. These are those directions where the magnetic-field lifting of the degeneracy of electronic states with opposite momenta **k** and −**k** forming the Cooper pairs is absent.

Let us start from the description of normal state in the crystal without an inversion centrum. For each band its single-electron Hamiltonian has the form

$$H = \varepsilon^0_{\mathbf{k}} + \boldsymbol{\alpha}_{\mathbf{k}}\boldsymbol{\sigma}, \tag{1}$$

where **k** is the wave vector, $\varepsilon^0_{\mathbf{k}} = \varepsilon^0_{-\mathbf{k}}$ is the even function of **k**, $\boldsymbol{\alpha}_{\mathbf{k}} = -\boldsymbol{\alpha}_{-\mathbf{k}}$ is the odd pseudovectorial function of **k**, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector consisting of Pauli matrices. The eigenvalues and eigenfunctions of this Hamiltonian are

$$\varepsilon_{\mathbf{k}\lambda} = \varepsilon^0_{\mathbf{k}} - \lambda|\boldsymbol{\alpha}_{\mathbf{k}}|, \tag{2}$$

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$$\Psi_\lambda(\mathbf{k}) \propto \begin{pmatrix} -\boldsymbol{\alpha}_{\mathbf{k}x} + i\boldsymbol{\alpha}_{\mathbf{k}y} \\ \boldsymbol{\alpha}_{\mathbf{k}z} + \lambda|\boldsymbol{\alpha}_{\mathbf{k}}| \end{pmatrix}. \quad (3)$$

So, we have obtained the band splitting and $\lambda=\pm$ is the band index. As a result, there are two Fermi surfaces determined by the equation

$$\varepsilon_{\mathbf{k}\lambda} = \varepsilon_F, \quad (4)$$

which may of course have the degeneracy points or lines for some directions of $\mathbf{k}$. The symmetry of directions of the dispersion laws $\varepsilon_{\mathbf{k}\lambda}$ has to correspond to the crystal symmetry. Particular attention, however, deserves to be given to the operation of reflection $\mathbf{k}$ to $-\mathbf{k}$ which creates the time-reversed states.

By application of the operator of time inversion $\hat{K} = -i\sigma_y K_0$, where K_0 is the complex-conjugation operator, one can see that the state $\Psi_\lambda(\mathbf{k})$ and the state inversed in time $\hat{K}\Psi_\lambda(\mathbf{k}) \propto \Psi_\lambda(-\mathbf{k})$ are degenerate. In other words, they correspond to the same energy $\varepsilon_{\mathbf{k}\lambda} = \varepsilon_{-\mathbf{k}\lambda}$. So, the Fermi surfaces in a crystal without an inversion center still have mirror symmetry. This is the consequence of time inversion symmetry.

Let us look now at the modifications which appear by the application of an external magnetic field. It is known[19] that the field introduction in the Hamiltonian is made by the Peierls' substitution $\mathbf{k} \to \mathbf{k} + \left(\frac{e}{2\hbar c}\right)\left[\mathbf{H}\frac{\partial}{\partial \mathbf{k}}\right]$. Being interested in paramagnetic influence on superconductivity and considering only the field values $\mu_B H \ll \varepsilon_F$, one can neglect the term with magnetic field in the Peierls' substitution and take into account only direct paramagnetic influence of magnetic field

$$H = \varepsilon_{\mathbf{k}}^0 + \boldsymbol{\alpha}_{\mathbf{k}}\boldsymbol{\sigma} - \mu_{\mathbf{k}i} H_i \boldsymbol{\sigma}, \quad (5)$$

where $\mu_{\mathbf{k}i} = \mu_{-\mathbf{k}i}$ is the even tensorial function of $\mathbf{k}$. In the isotropic approximation $\mu_{ij} = \mu_B g \delta_{ij}/2$, where g is gyromagnetic ratio. The eigenvalues of this Hamiltonian are

$$\varepsilon_{\mathbf{k}\lambda} = \varepsilon_{\mathbf{k}}^0 - \lambda|\boldsymbol{\alpha}_{\mathbf{k}} - \mu_{\mathbf{k}i} H_i|. \quad (6)$$

It is obvious from here that the time-reversal symmetry is lost $\varepsilon_{-\mathbf{k}\lambda} \neq \varepsilon_{\mathbf{k}\lambda}$ and the shape of the Fermi surfaces does not obey the mirror symmetry.

If we have the normal one-electron state's classification in a crystal without inversion symmetry it is quite natural to describe the superconductivity directly on the basis of these states. So, the BCS Hamiltonian in the space homogeneous case, which we discuss, looks as follows:

$$H_{BCS} = \sum_{\mathbf{k},\lambda} \xi_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\lambda,\nu} V_{\lambda\nu}(\mathbf{k},\mathbf{k}') a_{-\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k}',\nu}\, a_{-\mathbf{k}',\nu}, \quad (7)$$

where $\lambda, \nu = \pm$ are the band indices for the bands introduced above and

$$\xi_{\mathbf{k}\lambda} = \varepsilon_{\mathbf{k}\lambda} - \mu \quad (8)$$

are the band energies counted from the chemical potential. Due to the big difference between the Fermi momenta we neglect by the pairing of electronic states from different bands. The structure of theory is now very similar to the theory of ferromagnetic superconductors with triplet pairing.[20] For Gor'kov equations in each band we have

$$(i\omega_n - \xi_{\mathbf{k}\lambda}) G_\lambda(\mathbf{k},\omega_n) + \Delta_{\mathbf{k}\lambda} F_\lambda^\dagger(\mathbf{k},\omega_n) = 1, \quad (9)$$

$$(i\omega_n + \xi_{-\mathbf{k}\lambda}) F_\lambda^\dagger(\mathbf{k},\omega_n) + \Delta_{\mathbf{k}\lambda}^\dagger G_\lambda(\mathbf{k},\omega_n) = 0, \quad (10)$$

where $\omega_n = \pi T(2n+1)$ are Matsubara frequencies. The equations for each band are only coupled through the order parameters given by the self-consistency equations,

$$\Delta_{\mathbf{k}\lambda} = -T\sum_n \sum_{\mathbf{k}'} \sum_\nu V_{\lambda\nu}(\mathbf{k},\mathbf{k}') F_\nu(\mathbf{k}',\omega_n). \quad (11)$$

The superconductor Green's functions are

$$G_\lambda(\mathbf{k},\omega_n) = \frac{i\omega_n + \xi_{-\mathbf{k}\lambda}}{(i\omega_n - \xi_{\mathbf{k}\lambda})(i\omega_n + \xi_{-\mathbf{k}\lambda}) - \Delta_{\mathbf{k}\lambda}\Delta_{\mathbf{k}\lambda}^\dagger}, \quad (12)$$

$$F_\lambda(\mathbf{k},\omega_n) = \frac{-\Delta_{\mathbf{k}\lambda}}{(i\omega_n - \xi_{\mathbf{k}\lambda})(i\omega_n + \xi_{-\mathbf{k}\lambda}) - \Delta_{\mathbf{k}\lambda}\Delta_{\mathbf{k}\lambda}^\dagger}. \quad (13)$$

The energies of elementary excitations are given by

$$E_{\mathbf{k}\lambda} = \frac{\xi_{\mathbf{k}\lambda} - \xi_{-\mathbf{k}\lambda}}{2} \pm \sqrt{\left(\frac{\xi_{\mathbf{k}\lambda} + \xi_{-\mathbf{k}\lambda}}{2}\right)^2 + \Delta_{\mathbf{k}\lambda}\Delta_{\mathbf{k}\lambda}^\dagger}. \quad (14)$$

For simplicity, let us assume that we have pairing only in one band: $\lambda = +$. The treatment of the general case is similar but more lengthy. There was shown in Ref. 17 that in the case of crystals without inversion: (i) $\Delta_{\mathbf{k}} = t(\mathbf{k})\Sigma_i \eta_i \varphi_i(\mathbf{k})$, where $t(\mathbf{k}) = -t(-\mathbf{k})$ is an odd phase factor; (ii) a potential of the pairing interaction is represented as an expansion over $t(\mathbf{k})\varphi_i(\hat{\mathbf{k}})$, where $\varphi_i(\hat{\mathbf{k}})$ are the even basis functions of an irreducible representation of the crystal point symmetry group. For tetragonal crystal $CePt_3Si$ this group is C_{4v}, and for monoclinic crystal UIr it is C_2. If we limited ourselves by considering only one-dimensional representations when we have $V_{++}(\mathbf{k},\mathbf{k}') = Vt(\mathbf{k})t^*(\mathbf{k}')\varphi(\hat{\mathbf{k}})\varphi^*(\hat{\mathbf{k}}')$, then the equation for critical temperature that is the linear version of (11) has in this case the form

$$1 = -VT\sum_n \sum_{\mathbf{k}} \frac{\varphi^*(\hat{\mathbf{k}})\varphi(\mathbf{k})}{(i\omega_n - \xi_{\mathbf{k}})(-i\omega_n - \xi_{-\mathbf{k}})}. \quad (15)$$

It is clear from here and from Eqs. (6) and (8) that the coherence between the normal-metal states and states with Green's functions $G^0(\mathbf{k},\omega_n)$ and $G^0(-\mathbf{k},-\omega_n)$ is broken by magnetic field. The oppositely directed momenta $\mathbf{k}$ and $-\mathbf{k}$ on the Fermi surface have a different length. Hence, the magnetic field will suppress superconductivity, which means that the critical temperature will be a decreasing function of magnetic field. It is also clear that it will be an anisotropic function of the field orientation with respect to crystallographic directions.

For tetragonal crystal $CePt_3Si$ one can take as the simplest form of gyromagnetic tensor $\mu_{ij}=\mu_B[g_\perp(\hat{x}_i\hat{x}_j+\hat{y}_i\hat{y}_j)+g_\parallel\hat{z}_i\hat{z}_j]/2$ and the pseudovector function $\boldsymbol{\alpha}_{\mathbf{k}}=\alpha(\hat{z}\times\mathbf{k})+\beta\hat{z}k_xk_yk_z(k_x^2-k_y^2)$. The latter is chosen following the discussion in the paper by Samokhin.[18] Then for the normal metal-energy of excitations we have

$$\xi_k=\varepsilon_{\mathbf{k}}^0-\sqrt{\left(\boldsymbol{\alpha}k_y+\frac{g_\perp}{2}\mu_BH_x\right)^2+\left(\boldsymbol{\alpha}k_x-\frac{g_\perp}{2}\mu_BH_y\right)^2+\left(\beta k_xk_yk_z(k_x^2-k_y^2)-\frac{g_\parallel}{2}\mu_BH_z\right)^2}. \quad (16)$$

As a result of simple calculations near T_c we obtain

$$T_c(\mathbf{H})=T_c\left\{1-\frac{7\zeta(3)\mu_B{}^2}{32\pi^2T_c{}^2}\left(ag_\perp^2(H_x^2+H_y^2)+bg_\parallel^2H_z^2\right)+\ldots\right\}, \quad (17)$$

that looks like similar to usual superconductivity with singlet pairing. Here a and b are coefficients of the order of unity. Their exact values depend on the particular form of $\varphi(\hat{\mathbf{k}})$ functions in pairing interaction as well on the particular form of $\boldsymbol{\alpha}_{\mathbf{k}}$.

On the other hand, let as assume that due to some particular reason coefficient β is small. Then for the field direction $\mathbf{H}=H\hat{z}$ for $\mu_Bg_\parallel H\gg\beta k_F^5$ we have for the excitation energy

$$\xi_{\mathbf{k}}=\xi^0{}_{\mathbf{k}}-\sqrt{(\alpha k_y)^2+(\alpha k_x)^2+\left(\frac{g_\parallel}{2}\mu_BH_z\right)^2}, \quad (18)$$

that is now the even function of the wave vector $\xi_{\mathbf{k}}=\xi_{-\mathbf{k}}$, and the equation for the critical temperature is

$$1=-VT\sum_n\int d\xi\,N_{\xi=0}(\hat{\mathbf{k}})\frac{dS_{\hat{\mathbf{k}}}}{S_F}\frac{\varphi^*(\hat{\mathbf{k}})\varphi(\mathbf{k})}{(i\omega_n-\xi)(-i\omega_n-\xi)}. \quad (19)$$

Here we can first integrate over the energy variable ξ and then over the Fermi suface. After the first integration the magnetic-field dependence disappears from the equation and we obtain the standard BCS formula $T_c=(2\gamma/\pi)\epsilon\exp(-1/g)$ for critical temperature determination. So, the suppression of critical temperature by magnetic field is saturated at finite value, which differs from its value at $H=0$ due to field variation of the density of states and pairing interaction at $\xi=0$.

These results can be, in principle, valid for any direction of magnetic field if paramagnetic interaction exceeds a spin-orbital splitting $|\boldsymbol{\mu}_iH_i|>|\boldsymbol{\alpha}|$. Of course, the superconductivity in the region of the large fields still exists if g is positive on the Fermi surface $\xi=0$. Thus, at large fields the situation is similar to what we have in the superconductors with triplet pairing.

We have demonstrated that the paramagnetic suppression of a superconducting state in a crystal without an inversion centrum certainly exists, and the effect depends on field orientation with respect to crystal axes. The paramagnetic suppression of superconductivity takes place due to magnetic-field lifting of the degeneracy of electronic states with opposite momenta $\mathbf{k}$ and $-\mathbf{k}$ forming the Cooper pairs. For some directions of fields the degeneracy is recreated. That is why the paramagnetic limit of superconductivity in the crystals without inversion can be, in principle, absent.

The similar conclusions have been obtained in the paper by Frigeri *et al.*[15] on the assumption of negligibly small band splitting. So, our main result is the development of proper theoretical treatment of the paramagnetic limitations of superconductivity in noncentrosymmetric metals with large band splitting.

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