Characteristics of the Cooper pairing in two-dimensional noncentrosymmetric electron systems

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A study is made of how the absence of spatial reflection symmetry in the plane of motion affects the superconducting state of two-dimensional electrons. In the absence of an inversion center the spectrum of Cooper pairs can have two energy gaps and the order parameter contains not only a singlet part, but also an admixture of a triplet state, whereas the zero-temperature spin susceptibility is finite. It is shown that a magnetic field induces a condensate phase in an amount proportional to $[\mathbf{H}\times\mathbf{c}]\mathbf{r}$, where $\mathbf{c}$ is one of the inequivalent normals to the two-dimensional layer and $\mathbf{r}$ is the position vector.

1. INTRODUCTION

Some materials exhibiting superconductivity have a stratified electron structure. If in addition such a material consists of several components, then many other atoms and ions may be located between the atomic planes of motion of superconducting electrons. Ions surrounding such a conducting layer are not generally distributed symmetrically relative to the plane of the layer. We shall assume that the tunnel coupling betwen the conducting layers is negligible and discuss just one layer. The loss of symmetry of the immediate environment results in inequivalence of two normals to the layer, i.e., it breaks the "up–down" symmetry giving rise to a spin–orbit term in the electron Hamiltonian

$$\mathscr{H}_{so}=\alpha[\mathbf{pc}]\boldsymbol{\sigma}, \tag{1}$$

where $\mathbf{c}$ is a unit vector along one of the equivalent normals and $\boldsymbol{\sigma}$ are the Pauli matrices. This term has been discussed earlier in the specific case of electron layers in semiconductor heterojunctions.[1,2] One of them lifts the spin degeneracy: two spins of an electron with a given momentum $\mathbf{p}$ acquire different energies because of $\mathscr{H}_{so}$. We shall consider some characteristic features of the superconducting state due to this circumstance. First of all, the presence of $\mathscr{H}_{so}$ implies the absence of spatial parity, which spoils the classification of the superconducting order parameter in terms of the total spin of a Cooper pair, and which should result in singlet–triplet mixing. One can expect also a finite spin susceptibility of the superfluid condensate. Moreover, in the absence of an inversion center the symmetry of a system subjected to an external magnetic field $\mathbf{H}$ does not forbid the appearance of an additional invariant $\mathbf{Q}[\mathbf{c}\times\mathbf{H}]$, where $\mathbf{Q}$ is the momentum of the center of gravity of a pair, in the spectrum of Cooper pairs.

2. BASIC EQUATIONS

For simplicity, we shall assume that the spectrum of the particles in the absence of $\mathscr{H}_{so}$ and of the interparticle interaction is isotropic: $\varepsilon_0(p)=p^2/2m$. When $\mathscr{H}_{so}$ is included, the energy surface of the normal state has two branches

$$\varepsilon_{(\pm)}(p)=\varepsilon_0(p)\pm\alpha p \tag{2}$$

and the Fermi surface represents two circles of radii $p_{(\pm)}\approx p_0\mp\alpha m, p_0=(2m\mu)^{1/2}$. The spin quantization axis for the $\varepsilon_{(+)}$ branch is directed along the $\mathbf{p}\times\mathbf{c}$ so that a pair of particles with opposite momenta has also oppositely directed spins. However, in the case of states in the $\varepsilon_{(-)}$ branch the spin quantization directions are opposite. Therefore, all the states of the $\varepsilon_{(+)}$ branch have positive helicity, opposite to the helicity of the $\varepsilon_{(-)}$ branch states.

In the interparticle interaction

$$\mathscr{H}_{int}=\frac{1}{2V}\sum_{\mathbf{p},\mathbf{q},\mathbf{Q}}\overset{+}{a}_{\mathbf{p}+\mathbf{Q}/2,\alpha}\overset{+}{a}_{-\mathbf{p}+\mathbf{Q}/2,\beta}V^{\alpha\beta|\gamma\delta}(\mathbf{Q};\mathbf{p},\mathbf{q})\,a_{-\mathbf{q}+\mathbf{Q}/2,\delta}a_{\mathbf{q}+\mathbf{Q}/2,\gamma}, \tag{3}$$

which is considered using a weak-coupling theory, we retain only the isotropic part

$$V_s^{\alpha\beta|\gamma\delta}(\mathbf{p},\mathbf{q})=V_s(p,q)g_{\alpha\beta}(-g)_{\gamma\delta} \tag{4}$$

and the first angular harmonic

$$V_p^{\alpha\beta|\gamma\rho}(\mathbf{p},\mathbf{q})=V_p(p,q)\,(\sigma^i g)_{\alpha\beta}(\hat{\mathbf{p}}\hat{\mathbf{q}})\,(-g\sigma^i)_{\gamma\rho}, \tag{5}$$

where $\hat{g}=i\sigma_2$. Below the critical temperature in the range $T<T_c$ the Gor'kov equations for the Green's functions have the standard form

$$\check{G}=\check{G}_0+\check{G}_0\check{M}\check{G},$$

$$\check{G}_0^{-1}=\begin{pmatrix} i\varepsilon-H_0(\mathbf{p}) & 0\\ 0 & i\varepsilon+H_0{}^t(-\mathbf{p})\end{pmatrix},\quad \check{M}=\begin{pmatrix}0 & \hat{\Delta}(\mathbf{p})\\ \hat{\Delta}^+(\mathbf{p}) & 0\end{pmatrix},$$

$$\check{G}=\begin{pmatrix}\check{G}(i\varepsilon,\mathbf{p}) & \check{F}(i\varepsilon,\mathbf{p})\\ \check{F}^+(-i\varepsilon,\mathbf{p}) & -\check{G}^t(-i\varepsilon,-\mathbf{p})\end{pmatrix}, \tag{6}$$

where

$$\hat{H}_0(\mathbf{p})=\frac{p^2}{2m}+\alpha[\mathbf{pc}]\sigma,$$

$$\Delta_{\alpha\beta}(\mathbf{p})=-T\sum_{\varepsilon}\int\frac{d^2k}{(2\pi)^2}V^{\alpha\beta|\gamma\rho}(\mathbf{p},\mathbf{k})F_{\rho\gamma}(i\varepsilon,-\mathbf{k}), \tag{7}$$

and the sign of t denotes transposition; the definitions of all the Green's functions are the same as in Ref. 3. It follows from Eqs. (6) and (7) that the Green's function of the noninteracting particles is

$$\hat{G}_0(i\varepsilon,\mathbf{p})=\hat{\Pi}^{(+)}(\mathbf{p})G^0_{(+)}(i\varepsilon,p)+\hat{\Pi}^{(-)}(\mathbf{p})G^0_{(-)}(i\varepsilon,p)$$

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$$G^{0}_{(\pm)}(i\varepsilon,p)=[i\varepsilon-\xi_{(\pm)}(p)]^{-1},\quad \xi_{(\pm)}(p)=\varepsilon_{(\pm)}(p)-\mu,$$
$$\Pi^{(\pm)}_{\alpha\beta}(\mathbf{p})=(\delta_{\alpha\beta}\pm[\hat{\mathbf{p}}\mathbf{c}]\sigma_{\alpha\beta})/2. \tag{8}$$

The operators $\hat{\Pi}^{(\pm)}$ represent projections onto states with a definite helicity.

In the mass operator $\hat{M}$ we retain only the off-diagonal terms in the particle–hole channels. The first-order contributions to the diagonal elements are (Fig. 1)

$$M^{(1)}_{\alpha\gamma}(\mathbf{p})=T\sum_{\varepsilon}\int\frac{d^2k}{(2\pi)^2}e^{+i\varepsilon 0}\Big[V^{\alpha\beta|\gamma\rho}\Big(\frac{\mathbf{p}-\mathbf{k}}{2},\frac{\mathbf{p}-\mathbf{k}}{2}\Big)$$
$$-V^{\alpha\beta|\rho\gamma}\Big(\frac{\mathbf{p}-\mathbf{k}}{2},\frac{\mathbf{k}-\mathbf{p}}{2}\Big)\Big]\,G_{\rho\beta}{}^{0}(i\varepsilon,\mathbf{k}). \tag{9}$$

Using the identities

$$g_{\alpha\beta}g_{\gamma\rho}=\delta_{\alpha\gamma}\delta_{\beta\rho}-\delta_{\alpha\rho}\delta_{\beta\gamma},$$
$$\sigma_{\alpha\beta}\sigma_{\gamma\rho}=2\delta_{\alpha\rho}\delta_{\beta\gamma}-\delta_{\alpha\beta}\delta_{\gamma\rho},\quad -g\sigma^t g^t=\sigma, \tag{10}$$

we can show that $\hat{M}^{(1)}(\mathbf{p})$ has a matrix structure of the form

$$M^{(1)}_{\alpha\beta}(\mathbf{p})=A(p)\delta_{\alpha\beta}+B(p)[\hat{\mathbf{p}}\mathbf{c}]\sigma_{\alpha\beta}. \tag{11}$$

Comparing Eq. (11) with $H_0(p)$ from Eq. (7), we can see that inclusion of $M^{(1)}$ leads to renormalization of the spectrum and of the chemical potential, but does not affect classification of the particles in accordance with their helicity.

The spin–orbit interaction constant α occurs in two dimensionless parameters. One of these parameters $\delta=\alpha m/p_0=\alpha p_0/2\mu$, representing the ratio of the spin–orbit energy to the Fermi value, is treated as being so small that all the powers of δ in excess of the first can be ignored. The second dimensionless parameter $\varkappa=\alpha p_0/T_c$ is regarded as small only to simplify the calculations, so that all the necessary powers of $\varkappa$ are included.

3. STRUCTURE OF THE ORDER PARAMETER

The treatment in Ref. 4 is concerned with the case when the interaction contains only the isotropic part of Eq. (4),

$$V_s(p,\ q)=\lambda_s u(p)u(q)\vartheta_p\vartheta_q, \tag{12}$$

where the presence of the functions $u(p)=1+\beta(p-p_0)/p_0$ allows for the possibility that the interaction force between quasiparticles depends on the magnitudes of their momenta, whereas ϑ_p is a truncation factor which is unity for $v_0(p-p_0)<\omega_D$ and vanishes in all other cases. Then, the order parameter $\Delta_{\alpha\beta}(\mathbf{p})$ has only the singlet component $\Delta_s(p)g_{\alpha\beta}$. We show below that allowance for the anisotropy of Eq. (5) gives rise to an additional triplet term, so that the order parameter becomes

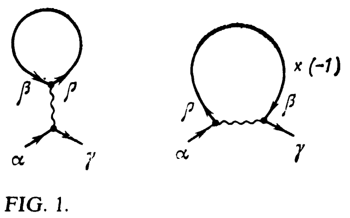

FIG. 1.

$$\Delta_{\alpha\beta}(\mathbf{p})=\Delta_s(p)g_{\alpha\beta}+\Delta_t(p)[\hat{\mathbf{p}}\mathbf{c}]\sigma_{\alpha\gamma}g_{\gamma\beta}, \tag{13}$$

where $\Delta_t/\Delta_s\approx\alpha m/p_0$.

It follows from the system (6) and the relations

$$[\hat{\mathbf{p}}\mathbf{c}]\sigma\hat{\Pi}^{(\pm)}(\mathbf{p})=\pm\hat{\Pi}^{(\pm)}(\mathbf{p}),$$
$$g\hat{\Pi}^{t(\pm)}(-\mathbf{p})g^t=\hat{\Pi}^{(\pm)}(\mathbf{p}), \tag{14}$$

that

$$\hat{F}(i\varepsilon,\mathbf{p})=[\hat{\Pi}^{(+)}(\mathbf{p})F_{(+)}(i\varepsilon,p)+\hat{\Pi}^{(-)}(\mathbf{p})F_{(-)}(i\varepsilon,p)]\hat{g},$$
$$F_{(\pm)}=\Delta_{(\pm)}(p)/[(i\varepsilon)^2-E^2_{(\pm)}(p)],$$
$$\hat{G}(i\varepsilon,\mathbf{p})=\hat{\Pi}^{(+)}(\mathbf{p})G_{(+)}(i\varepsilon,p)+\hat{\Pi}^{(-)}(\mathbf{p})G_{(-)}(i\varepsilon,p), \tag{15}$$
$$G_{(\pm)}(i\varepsilon,p)=[i\varepsilon+\xi_{(\pm)}(p)]/[(i\varepsilon)^2-E^2_{(\pm)}(p)],$$
$$E^2_{(\pm)}(p)=\xi^2_{(\pm)}(p)+|\Delta_{(\pm)}(p)|^2,\quad \Delta_{(\pm)}=\Delta_s\pm\Delta_t.$$

These expressions describe fully the spinor structure of the solutions of the Gor'kov equations. We can find the functions $\Delta_s(p)$ and $\Delta_t(p)$ by substituting Eqs. (13) and (15) into the self-consistency equation, which yields two scalar equations

$$\Delta_s(p)=-T\sum_{\varepsilon}\int\frac{k\,dk}{2\pi}V_s(p,k)[F_{(+)}(i\varepsilon,k)+F_{(-)}(i\varepsilon,k)],$$
$$\Delta_t(p)=T\sum_{\varepsilon}\int\frac{k\,dk}{4\pi}V_p(p,k)[F_{(+)}(i\varepsilon,k)-F_{(-)}(i\varepsilon,k)]. \tag{16}$$

For simplicity we shall assume that the anisotropic part of the interaction is factored

$$V_p(p,\ k)=\lambda_p u(p)u(k)\vartheta_p\vartheta_k \tag{17}$$

and that the functions $u(p)$ are the same as in Eq. (12). Then, assuming that

$$\Delta_{s,\,t}(p,\ T)=u(p)\Delta_{s,\,t}(T) \tag{18}$$

and confining our attention only to temperatures close to T_c, we obtain the system of linear equations

$$\begin{pmatrix}\Delta_s\\ \Delta_t\end{pmatrix}=\begin{pmatrix}2\lambda_s I_0 & \lambda_s(I_{(+)}-I_{(-)})\\ -\lambda_p(I_{(+)}-I_{(-)})/2 & -\lambda_p I_0\end{pmatrix}\begin{pmatrix}\Delta_s\\ \Delta_t\end{pmatrix}, \tag{19}$$

where, to within an error amounting to δ, we have

$$I_{(\pm)}=-T\sum_{\varepsilon}\int\frac{p\,dp}{2\pi}\frac{u^2(p)\vartheta_p}{(i\varepsilon)^2-\xi^2_{(\pm)}}\approx[1\mp(1+2\beta)\delta]I_0,$$
$$I_0=(m/2\pi)\ln(2\omega_D\gamma/\pi T),\quad \ln\gamma=0.577. \tag{20}$$

The condition of solvability of this system determines T_c and the ratio[1)]

$$\frac{\Delta_t}{\Delta_s}\approx\delta(1+2\beta)\frac{\lambda_p/2\lambda_s}{1+\lambda_p/2\lambda_s}. \tag{21}$$

The temperature of the transition is given equally accurately by the following expression from the BCS theory:

$$T_{BCS}=(2\omega_D\gamma/\pi)\exp(-\pi/m\lambda_s).$$

It is shown in Ref. 4 that this applies also to the function $\Delta_s(T)$. Thus, the matrix $\Delta_{\alpha\beta}$ is governed entirely by one complex function $\Delta_s(p,T)$, although it may contain different (singlet and triplet) spinor structures.

The main consequence of the above expressions is the appearance of a difference between the energy gaps on two Fermi circles. In the absence of the anisotropic interaction V_p this follows from the fact that $u(p)$ varies: it follows from Eq. (18) that

$$\Delta_s(p_{(-)})-\Delta_s(p_{(+)})\approx 2\delta\beta\Delta_s(T). \qquad (22)$$

It is clear from Eq. (15) that allowance for the anisotropy increases the difference further by $2\Delta_t$. Therefore, to first order in the spin–orbit interaction the excitation energies of quasiparticles with different helicities are different, i.e., the helical symmetry is destroyed dynamically.

The splitting of the excitation spectrum in superfluid Fermi systems was predicted earlier (see, for example, Ref. 5 and the literature cited there, and also a much earlier study[6] dealing with the exchange analysis of a dynamic group of superfluid He^3). In that case and in our case the reason for the appearance of this effect in the final analysis is related to the spin–orbit interaction. The only difference is that in Ref. 5 the system exhibited a triplet state as well as vector pairing when the energy of a quasiparticle could depend on the projection of its spin along the condensate symmetry axis. In the situation under discussion the splitting is of different geometrical nature: it is due to the loss of spatial parity and it exists also for singlet pairing, when the scalar condensate does not have any preferred spatial direction.

4. PARAMAGNETIC SUSCEPTIBILITY

We now consider paramagnetic properties of the ground state. We begin with the spin susceptiblity χ of the system.

The susceptibility can be found in a homogeneous magnetic field **H** by writing down the spin magnetic moment to five + order in the field:

$$\mathbf{M}=-T\sum_{\varepsilon}\int\frac{d^2p}{(2\pi)^2}\mu_B\operatorname{Tr}\hat{\sigma}\hat{G}(i\varepsilon,\mathbf{p},\mathbf{H}), \qquad (23)$$

i.e., we can find a linear correction to the Green's function $\hat{G}$. Therefore, in the mass operator $\hat{M}$ in Eq. (6) we must also include the Zeeman energy and, if it differs from zero, a linear correction to the order parameter:

$$\hat{M}_{(1)}(\mathbf{H})=\begin{pmatrix}\mu_B\boldsymbol{\sigma}\mathbf{H} & \hat{\Delta}_{(1)}(\mathbf{p},\mathbf{H})\\ \hat{\Delta}^{+}_{(1)}(\mathbf{p},\mathbf{H}) & -\mu_B\boldsymbol{\sigma}^t\mathbf{H}\end{pmatrix}. \qquad (24)$$

It is then found that χ is a sum of the four diagrams in Fig. 2.

The equation for the correction $\hat{\Delta}_{(1)}(\mathbf{p},\mathbf{H})$ is obtained by integration of the self-consistent condition with respect to the Zeeman energy, which gives the results shown in Fig. 3. The contribution of the first two diagrams in Fig. 3 is

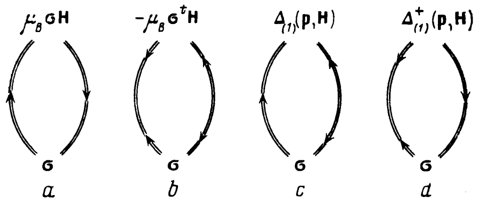

FIG. 2.

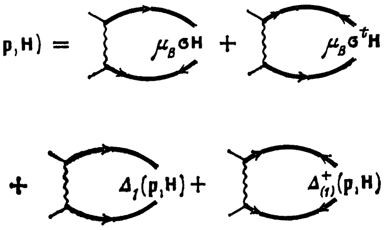

FIG. 3.

$$-T\sum_{\varepsilon}\int\frac{d^2k}{(2\pi)^2}V^{\alpha\beta|\gamma\rho}(\mathbf{p},-\mathbf{k})$$

$$\times\sum_{\mu,\nu=(\pm)}[\hat{\Pi}^{(\mu)}(\mathbf{k})\mu_B\boldsymbol{\sigma}\mathbf{H}\hat{\Pi}^{(\nu)}(\mathbf{k})g]_{\rho\gamma},$$

$$[G_{(\mu)}(i\varepsilon,k)F_{(\nu)}(i\varepsilon,k)-F_{(\mu)}(i\varepsilon,k)G_{(\nu)}(-i\varepsilon,k)]. \qquad (25)$$

It is clear from Eqs. (4) and (5) that this expression includes terms

$$\left\{\begin{matrix}g_{\gamma\rho}\\ \hat{k}^l(g\sigma^i)_{\gamma\rho}\end{matrix}\right\}[\hat{\Pi}^{(\mu)}(\mathbf{k})\boldsymbol{\sigma}\mathbf{H}\hat{\Pi}^{(\nu)}(\mathbf{k})\hat{g}]_{\rho\gamma}, \qquad (26)$$

which can be calculated from the relation

$$A_{ij}^{(\mu\nu)}\equiv\operatorname{Tr}\hat{\Pi}^{(\mu)}(\mathbf{k})\sigma_i\hat{\Pi}^{(\nu)}(\mathbf{k})\sigma_j$$
$$=\begin{pmatrix}P_iP_j & \delta_{ij}-P_iP_j+ie_{ijn}P_n\\ \delta_{ij}-P_iP_j-ie_{ijn}P_n & P_iP_j\end{pmatrix},\quad \mathbf{P}(\mathbf{k})=[\hat{\mathbf{k}}\mathbf{c}]. \qquad (27)$$

Hence, it is clear that the contribution made to Eq. (25) by the isotropic part of the interaction is governed by the traces (Tr) in the first line of Eq. (26) and it vanishes as a result of angular averaging.

The contribution of the anisotropic part of the interaction is determined primarily by angular integration of the lower row of Eq. (26). If $\mu=\nu$, the expression for $A_{ij}^{(\mu\nu)}$ is even in k and, consequently, it drops out. If $\mu\neq\nu$, we have

$$\int\frac{d\hat{k}}{2\pi}\hat{k}^l\left\{\begin{matrix}A_{ij}^{(+-)}\\ A_{ij}^{(-+)}\end{matrix}\right\}H^j=\frac{i}{2}[(\mathbf{c}\mathbf{H})\delta^{il}-c^iH^l]\left\{\begin{matrix}1\\ -1\end{matrix}\right\}. \qquad (28)$$

The remaining scalar part of Eq. (25) is then

$$[G_{(+)}(i\varepsilon)F_{(-)}(i\varepsilon)-F_{(+)}(i\varepsilon)G_{(-)}(-i\varepsilon)]-[G_{(-)}(i\varepsilon)F_{(+)}(i\varepsilon)$$
$$-F_{(-)}(i\varepsilon)G_{(+)}(-i\varepsilon)]=\frac{(\Delta_s-\Delta_t)2\xi_{(+)}-(\Delta_s+\Delta_t)2\xi_{(-)}}{[(i\varepsilon)^2-E^2_{(+)}][(i\varepsilon)^2-E^2_{(-)}]}$$
$$\approx 4\frac{\Delta_s\alpha p-\Delta_t\xi_0}{[(i\varepsilon)^2-E^2]^2} \qquad (29)$$

accurate to within corrections quadratic in δ.

A consistent allowance for the second two diagrams in Fig. 3 reduces to simple renormalization of the expression obtained in this way, so that the result is

$$\hat{\Delta}_{(1)}(\mathbf{p},\mathbf{H})=\frac{m\lambda_p}{1+\lambda_p/2\lambda_s}\left(\frac{\alpha p_0}{T_c}\right)i\mu_B[(\mathbf{c}\mathbf{H})(\hat{\mathbf{p}}\boldsymbol{\sigma})$$
$$-(\hat{\mathbf{p}}\mathbf{H})(\mathbf{c}\boldsymbol{\sigma})]\hat{g}K(T), \qquad (30)$$

where

$$K(T)=\begin{cases}\gamma/\pi, & T\ll\Delta_s\\ (\Delta_s/T)(7\zeta(3)/4\pi^3), & \Delta_s\ll T.\end{cases}$$

The presence of i in the above expression ensures invariance of the time inversion operator.

We shall now calculate the susceptibility. In the expression for the contribution of the diagrams a and b in Fig. 2

$$-\mu_B{}^2T\sum_\varepsilon\int\frac{d^2p}{(2\pi)^2}\mathrm{Sp}\{\sigma^i\hat{G}(i\varepsilon,\mathbf{p})\boldsymbol{\sigma}\mathbf{H}\hat{G}(i\varepsilon,\mathbf{p})$$

$$+\sigma^i\hat{F}(i\varepsilon,\mathbf{p})(-1)\boldsymbol{\sigma}^t\mathbf{H}\hat{F}^+(i\varepsilon,\mathbf{p})\}\tag{31}$$

we shall separate the matrix structure of the Green's functions using Eq. (15); we shall follow this by application of the relation (26) and carry out angular integration, which gives

$$-\mu_B{}^2T\sum_\varepsilon\int\frac{p\,dp}{2\pi}H^j\left[2A\delta^{ij}+\frac{1}{2}B(\delta^{ij}-c^ic^j)\right],\tag{32}$$

where

$$A=G_{(+)}(i\varepsilon,p)G_{(-)}(i\varepsilon,p)+F_{(+)}F_{(-)},$$

$$B=(G_{(+)}-G_{(-)})^2+(F_{(+)}-F_{(-)})^2$$

$$=-2A+(G^2_{(+)}+F^2_{(+)})+(G^2_{(-)}+F^2_{(-)}).$$

The quantity A can be reduced to

$$A=-\frac{1}{2}\frac{(\xi_{(+)}-\xi_{(-)})^2+(\Delta_{(+)}-\Delta_{(-)})^2}{[(i\varepsilon)^2-E^2_{(+)}]\,[(i\varepsilon)^2-E^2_{(-)}]}$$

$$+\frac{2(i\varepsilon)^2+E^2_{(+)}+E^2_{(-)}}{[(i\varepsilon)^2-E^2_{(+)}]\,[(i\varepsilon)^2-E^2_{(-)}]}$$

$$+\frac{i\varepsilon(\xi_{(+)}+\xi_{(-)})}{[(i\varepsilon)^2-E^2_{(+)}]\,[(i\varepsilon)^2-E^2_{(-)}]}.\tag{33}$$

The third term in Eq. (33) can be dropped, because it is canceled out in summation over the frequency, whereas the second term leads to

$$\left(\frac{1/2}{(i\varepsilon)^2-E^2_{(+)}}+\frac{E^2_{(+)}}{[(i\varepsilon)^2-E^2_{(+)}]^2}\right)$$

$$+\left(\frac{1/2}{(i\varepsilon)^2-E^2_{(-)}}+\frac{E^2_{(-)}}{[(i\varepsilon)^2-E^2_{(-)}]^2}\right)$$

$$-\frac{(i\varepsilon)^2[E^2_{(+)}-E^2_{(-)}]^2}{[(i\varepsilon)^2-E^2_{(+)}]^2[(i\varepsilon)^2-E^2_{(-)}]^2}.\tag{34}$$

Since

$$-T\sum_\varepsilon\left\{\frac{1}{(i\varepsilon)^2-E^2}+\frac{2E^2}{[(i\varepsilon)^2-E^2]^2}\right\}=[4T\,\mathrm{ch}^2(E/2T)]^{-1},\tag{35}$$

we can see that the contributions of the first and second terms in Eq. (34) disappear separately in the limit $T\to0$. Therefore, they can be omitted in calculating the susceptibility of the ground state.

For the same reason the contributions of the second and third terms to the function B tend to zero. Thus, in the limit $T\to0$, Eq. (31) is asymptotically equal to

$$-T\sum_\varepsilon\int\frac{p\,dp}{2\pi}\mu_B{}^2H^j(\delta^{ij}+c^ic^j)A,\tag{36}$$

where up to terms of order $\varkappa^2$ inclusive we have

$$A\approx-\frac{1}{2}\frac{(\xi_{(+)}-\xi_{(-)})^2+(\Delta_{(+)}-\Delta_{(-)})^2}{[(i\varepsilon)^2-E^2]^2}$$

$$-\frac{(i\varepsilon)^2(E^2_{(+)}-E^2_{(-)})^2}{[(i\varepsilon)^2-E^2]^4}\tag{37}$$

and $E^2=\xi_0^2(p)+\Delta_s^2$. Therefore, the sum of the diagrams a and b in Fig. 2 assumes the following form in the limit $T\to0$:

$$\mu_B{}^2[H^i-c^i(\mathbf{cH})]\int\frac{p\,dp}{2\pi}E^{-3}\left\{(\xi_{(+)}-\xi_{(-)})^2+(\Delta_{(+)}-\Delta_{(-)})^2-\frac{(E^2_{(+)}-E^2_{(-)})^2}{4E^2}\right\}.\tag{38}$$

The expressions in the braces, considered in the same approximation, is

$$(\xi_{(+)}-\xi_{(-)})^2\frac{\Delta_s^2}{E^2}+(\Delta_{(+)}-\Delta_{(-)})^2\frac{\xi_0^2}{E^2}$$

$$-2\frac{\xi_0\Delta_s}{E^2}(\xi_{(+)}-\xi_{(-)})(\Delta_{(+)}-\Delta_{(-)}).\tag{39}$$

It follows from Eqs. (15) and (20) that the main contribution to the integral with respect to the parameter Δ_s/μ originates from the first term in Eq. (39).

We thus obtain

$$\chi_{ij}=(m\mu_B{}^2/3\pi)(\alpha p_0/\Delta_s)^2(\delta_{ij}+c_ic_j).\tag{40}$$

We can show that the contributions of the diagrams c and d in Fig. 2 are small in terms of the weak coupling parameter $m\lambda_p\ll1$. Since Eq. (40) is derived by the linear response method, it is valid if the Zeeman energy u_BH is less than all the other characteristic energies, including the spin–orbit energy αp_0.

An analogy with Ref. 7 should be pointed out here: it is shown in Ref. 7 that in the case of ordinary superconductors with an undisturbed spin degeneracy an allowance for the spin–orbit scattering by impurities also makes the spin susceptibility finite.

5. VELOCITY-SPIN CORRELATION FUNCTION

Another paramagnetic property of the system in question is the contribution of the Zeeman interaction to the superfluid current. The velocity operator $\hat{\mathbf{v}}(\mathbf{p})$ in this case is not a polar vector: it also has a spin (axial) component

$$\hat{\mathbf{v}}(\mathbf{p})=\mathbf{p}/m+\alpha[\mathbf{c}\boldsymbol{\sigma}].\tag{41}$$

To first order the magnetic field the average electron velocity

$$V_z=T\sum_\varepsilon\int\frac{d^2p}{(2\pi)^2}\mathrm{Tr}\,\hat{\mathbf{v}}(\mathbf{p})\hat{G}(i\varepsilon,\mathbf{p};\mathbf{H})\tag{42}$$

is given by the sum of the four diagrams in Fig. 4, which are analogous to the diagrams in Fig. 2. The contribution of the diagrams a and b is

$$V_z{}^i(a+b)=T\sum_\varepsilon\int\frac{d^2p}{(2\pi)^2}\mathrm{Sp}\,v^i(\mathbf{p})\sum_{\mu,\nu=\pm}\Pi^{(\mu)}(\mathbf{p})\mu_B\boldsymbol{\sigma}\mathbf{H}\Pi^{(\nu)}(\mathbf{p})$$

$$\times[G_{(\mu)}(i\varepsilon,p)G_{(\nu)}(i\varepsilon,p)+F_{(\mu)}(i\varepsilon,p)F_{(\nu)}(i\varepsilon,p)]\tag{43}$$

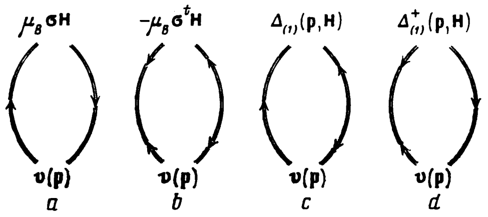

FIG. 4.

If we simplify Eq. (43) by retaining only the first term in the velocity operator, it then follows from

$$\operatorname{Tr} \Pi^{(\mu)}(\mathbf{p})\boldsymbol{\sigma}\mathbf{H}\Pi^{(\nu)}(\mathbf{p})=\delta^{(\mu\nu)} \operatorname{sign} \mu([\hat{\mathbf{p}}\mathbf{c}]\,\mathbf{H}) \tag{44}$$

that the expression in the square brackets in Eq. (43) occurs in the response only if $\mu = \nu$. It follows from Eq. (35) that at low temperatures this contribution tends to zero and, consequently, only the contribution of the spin part $\mathbf{v}(\mathbf{p})$ remains in Eq. (43) and this contribution can be expressed in an obvious manner in terms of the spin susceptibility

$$\mathbf{V}_z(a+b)=-\alpha\frac{m\mu_B}{3\pi}\left(\frac{\alpha p_0}{\Delta_s}\right)^2[\mathbf{cH}],\quad T\ll\Delta_s. \tag{45}$$

We can show that the contributions of the diagrams c and d at all temperatures is less than the contribution of the diagrams a and b in terms of the parameter $m\lambda_p \ll 1$.

We can conveniently calculate the contribution of the diagrams a and b near T_c by using the following circumstance. It follows from Eq. (45) that the response does not vanish when the gaps $\Delta_{(+)}$ and $\Delta_{(-)}$ coincide, so that in the lowest-order approximation in δ we can assume that $u(p)\equiv 1, \lambda_p = 0$. Then, Eqs. (15) yield the following identity

$$\begin{aligned}\partial\hat{G}(i\varepsilon,\mathbf{p})/\partial\mathbf{p}=&\hat{G}(i\varepsilon,\mathbf{p})\hat{\mathbf{v}}(\mathbf{p})\hat{G}(i\varepsilon,\mathbf{p})\\&+\hat{F}(i\varepsilon,\mathbf{p})\hat{\mathbf{v}}^t(-\mathbf{p})\hat{F}^+(-i\varepsilon,\mathbf{p}).\end{aligned} \tag{46}$$

It follows from it that, apart from the total derivative with respect to the momentum, the two terms in Eq. (43) are equal and, consequently,

$$\begin{aligned}V_z{}^i(a+b)=&2\mu_BT\sum_\varepsilon\int\frac{d^2p}{(2\pi)^2}\operatorname{Tr} v^i(\mathbf{p})\\&\times\sum_{\mu,\nu=\pm}\Pi^{(\mu)}(\mathbf{p})\boldsymbol{\sigma}\mathbf{H}\Pi^{(\nu)}(\mathbf{p})F_{(\mu)}F_{(\nu)}.\end{aligned} \tag{47}$$

Hence, it follows directly that the velocity–spin correlation vanishes in the normal phase. Using the inequalities (27) and (44), we can simplify this expression to

$$\begin{aligned}\mathbf{V}_z(a+b)=&2[\mathbf{cH}]\mu_BT\sum_\varepsilon\int\frac{p\,dp}{2\pi}\Big[\frac{p}{2m}(F_{(+)}^2-F_{(-)}^2)\\&+\frac{\alpha}{2}(F_{(+)}^2+F_{(-)}^2)+\alpha F_{(+)}F_{(-)}\Big],\end{aligned} \tag{48}$$

which is convenient for an analysis of the limit $\Delta_s \ll T_c$. In the integrals of the first two terms we have to go over to new integration variables $\xi_{(+)}$, which shows that the parameter α enters in them through δ, whereas in the third integral it enters through $\varkappa$. The terms linear in $\varkappa$ cancel out, so that we obtain

$$\mathbf{V}_z(a+b)=-\alpha m\mu_B[\mathbf{cH}]\left(\frac{\alpha p_0}{T_c}\right)^2\left(\frac{\Delta_s}{T_c}\right)^2\frac{31\zeta(5)}{32\pi^5}. \tag{49}$$

The paramagnetic contribution to the current does not mean that there is a constant current in the ground state. Since there is also the usual contribution proportional to the gradient of the condensate phase, it follows that in an infinite singly connected system the total current remains zero, but the condensate acquires a constant phase gradient.

We demonstrate how this occurs in the simplest situation when $\Delta_s \ll T_c$ and $\lambda_p = 0$. The presence of a phase gradient implies pairing with a nonzero momentum $\mathbf{Q}$, i.e., formation of a Cooper pair from electrons with quantum numbers $(\mathbf{p}+\mathbf{Q}/2,\ i\varepsilon)$ and $(\mathbf{p}+\mathbf{Q}/2,\ -i\varepsilon)$. Suitable modification of the Gor'kov scheme and linearization of the self-consistency equation for the order parameter $\Delta_{\alpha\beta}(H,Q) = \Delta(H,Q)g_{\alpha\beta}$ yields the condition for the appearance of a nonzero solution $\Delta(H, Q)$ in the form

$$\begin{aligned}1=-\lambda_sT\sum_\varepsilon\int\frac{d^2p}{(2\pi)^2}\operatorname{Tr}\Big\{&\hat{G}_0\Big(\mathbf{p}+\frac{\mathbf{Q}}{2},i\varepsilon;\mathbf{H}\Big)\\&\times\hat{g}(-1)\hat{G}_0{}^t\Big(-\mathbf{p}+\frac{\mathbf{Q}}{2},-i\varepsilon;\mathbf{H}\Big)\hat{g}^t\Big\},\end{aligned} \tag{50}$$

where

$$\hat{G}_0{}^{-1}\Big(\pm\mathbf{p}+\frac{\mathbf{Q}}{2},i\varepsilon;\mathbf{H}\Big)=i\varepsilon-H_0\Big(\pm\mathbf{p}+\frac{\mathbf{Q}}{2}\Big)-\mu_B\boldsymbol{\sigma}\mathbf{H}.$$

The right-hand side of Eq. (50) need be calculated only to first order in $\mathbf{H}$ and to second order in $\mathbf{Q}$. The perturbations will be assumed to be the Zeeman energy W_Z and part of the kinetic energy W_Q:

$$\hat{W}_Z=\begin{pmatrix}\mu_B\boldsymbol{\sigma}\mathbf{H} & 0\\ 0 & -\mu_B\boldsymbol{\sigma}^t\mathbf{H}\end{pmatrix},\quad \hat{W}_Q=\begin{pmatrix}\mathbf{v}(\mathbf{p})\mathbf{Q}/2 & 0\\ 0 & -\mathbf{v}^t(-\mathbf{p})\mathbf{Q}/2\end{pmatrix}. \tag{51}$$

The graphical representation of these perturbations can be found in Fig. 5. Using Eqs. (8) and (10), we can represent the expansion of the right-hand side of Eq. (50) in the form of a sum (Fig. 6)

$$R_0+R_{\mathbf{QH}}+R_{\mathbf{Q}^2}. \tag{52}$$

Comparing Eq. (52) with Fig. 4 and with the inequality of Eq. (43), we find that

$$\begin{aligned}&R_{\mathbf{QH}}=\mathbf{QV}_Z(a+b)/|\Delta_s|^2,\\&R_{\mathbf{Q}^2}=\mathbf{QV}_Q(a+b)/2|\Delta_s|^2,\end{aligned} \tag{53}$$

where $\mathbf{V}_Q(a+b)$ is found from the diagrams in Fig. 4 by replacing the perturbation W_Z with W_Q, and calculating all the diagrams near T_c to within $|\Delta_s|^2$. Since $\lambda_s > 0$, it follows that the sign of $\mathbf{Q}^2$ on the right-hand side of Eq. (50) is negative. Consequently, an instability of the normal state

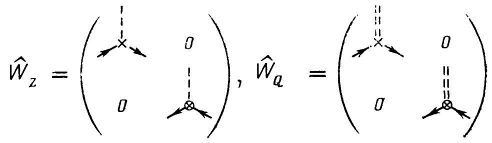

FIG. 5.

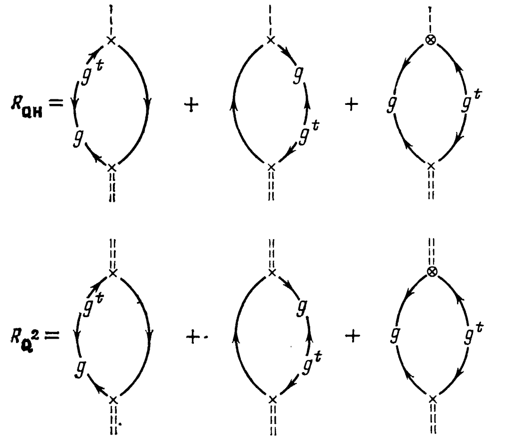

FIG. 6.

occurs primarily for those values of **Q** for which $R_{QH} + R_{Q^2}$ has a minimum. Setting the derivative with respect to **Q** to zero, we obtain the following equation for the determination of the function **Q**(**H**) near T_c:

$$\mathbf{V}_Z(a+b)+\mathbf{V}_Q(a+b)=0, \qquad (54)$$

which is expressed in diagram language in Fig. 7.

We can easily understand that the contribution to the average velocity made by the phase gradient is induced specifically by the interaction W_Q, i.e., it simply represents $\mathbf{V}_Q(a+b)$. Therefore, Eq. (54) means precisely that the total current vanishes. To lowest order in α we find from Eq. (54) near T_c

$$\mathbf{Q}(\mathbf{H})=\frac{m\mu_B}{p_0}[\mathbf{cH}]\left(\frac{\alpha m}{p_0}\right)\left(\frac{\alpha p_0}{T_c}\right)^2\frac{31\zeta(5)}{7\pi^2\zeta(3)}. \qquad (55)$$

Since $v_0Q/\mu_b H \sim \delta\varkappa^2 \ll 1$, we can ignore the influence of W_Q on the spin susceptibility.

A similar investigation of the general case of arbitrary temperatures allowing for the triplet part of the condensate is outside the scope of the present paper.

It should be mentioned that in the case of the spin susceptibility and the condensate phase the presence of the triplet part of the order parameter and the splitting of the energy gap are unimportant.

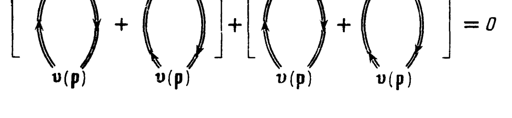

FIG. 7.

6. CONCLUSIONS

The above results can be applied to a two-dimensional defect, to a thin film when the central symmetry breaks down because of the van der Waals interaction with the substrate, or to a layer crystal with a noncentrosymmetric crystal symmetry group. If the unit cell contains an even number of conducting planes, as is true of the recently discovered high-temperature superconductors, this condition is not necessary because antipyroelectricity can be observed even in the presence of an inversion center. For example, the Cu–O planes in the superconducting compound $Ba_2YCu_3O_{7-\delta}$ are surrounded on one side by yttrium atoms and on the other by barium atoms. Although this feature of the compound in question has been the reason for the proposal of the model described above, certain difficulties may be encountered when the results obtained are applied specifically to $Ba_2YCu_3O_{7-\delta}$. The hypothesis of a weak tunnel coupling between two Cu–O layers is supported also by the experimental observation that replacement of the yttrium atoms separating such adjacent layers by magnetic gadolinium atoms has no significant influence on the critical temperature.[8] Evidence against this hypothesis may be the relatively small distance between the oxygen atoms in the two nearest layers and the directional nature of their valence orbitals.

It therefore follows that only a comparison of the experimental results with various consequences of the proposed model can determine the degree of its validity in the case of specific materials. An investigation of the possibility of the influence of pyroelectricity and ferroelectricity on superconductivity is moreover of intrinsic theoretical interest.

[1)] It is always assumed that $\lambda_s < |\lambda_p/2|$, so that the condensate is mainly of singlet nature. We can show that in the case of a weak interaction characterized by $m\lambda_{s,p} \ll 1$ the relationship (21) remains valid at all temperatures.

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