Superconducting classes in metals with spectrum anomalies at the Fermi surface

A. N. Vasil'chenko and A. V. Sokol

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR
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A symmetry approach is taken to analyze the properties of an anisotropic superconducting state in a metal having spectrum anomalies at the Fermi surface. The temperature dependence of the electron specific heat of the superconductor is derived for a transition accompanied by a change in the topology of the Fermi surface. It is also shown how degeneracy of the electron spectrum on the Fermi surface changes the pattern of zeros of the energy gap. A possible relationship between the effects considered and the superconductivity in metal oxides is discussed.

1. INTRODUCTION

There have been recent reports that the superconducting transition in the compound $Y_1Ba_2Cu_3O_7$ is split[1] and is accompanied by an anomaly in the orthorhombic distortion.[2] These facts might imply an anisotropy of the superconducting pairing,[2–4] so attention is drawn to the causes of the anomalies of the nontrivial superconductivity in the new materials. In the present paper we wish to discuss one of these anomalies.

Most metal-oxide conductors, particularly $Y_1Ba_2Cu_3O_7$, belong to symmetry group D_4, which is lowered to D_2 by a slight distortion of the lattice. The superconducting classes and the form of the order parameter were listed in Ref. 5 for the most common crystal groups and in Ref. 6 for an expanded D_2 and D_4 band scheme. Results on the state density near the Fermi surface were also reported in Ref. 5. That state density determines the temperature dependence of the electronic characteristics of the superconductor (in particular, the electron component of the specific heat). In the situtation studied in Ref. 5 the maximum symmetry of a point on the Fermi surface corresponds to a symmetry plane or axis. This is the case for an arbitrary position of the Fermi surface. In the new superconductors the band structure is quite complex and has yet to be analyzed experimentally. Numerical calculations of the carrier spectrum[7–10] show that the Fermi surface may pass through a high-symmetry point in the compounds $Y_1Ba_2Cu_3O_7$, $La_{2-y}X_yCuO_4$ (X = Ba, Sr), and $Bi_2Sr_2CaCu_2O_8$. This situation corresponds to a Lifshitz transition of order 2.5 (Ref. 11). Since calculations of that sort ignore electron-electron correlations, which are strong in the high-temperature superconductors, they are probably of only qualitative validity in this case. Nevertheless, by varying the pressure and the number of carriers (the doping) one can expect to find a Lifshitz transition in these materials. The effect of a topological transition on superconductivity has been studied previously (Ref. 12, for example) for a trivial symmetry of the order parameter. It turned out that in the ordinary BCS model the spectrum anomalies of the Fermi surface raised the transition temperature slightly.

There is thus some reason to believe that the electron spectrum in these new materials has anomalies, at the Fermi surface and that the order parameter is anisotropic. The electron state density near the Fermi surface, which determines the temperature dependence of electronic properties (e.g., the specific heat), can then be found from symmetry considerations, without reference to the pairing mechanism. The existence of spectrum anomalies at the Fermi surface causes far-reaching changes in the results derived in Ref. 5, so the corresponding calculations must be repeated. The expressions derived here will be valid in the temperature (or energy) interval $\varepsilon_0 - \varepsilon_F \ll T \ll T_c$, where ε_0 is the energy of an electron at the anomaly point and T_c is the superconducting transition temperature. This temperature interval can be quite broad because of the high values $T_c \sim 50$–100 K in the new materials.

2. METHOD

As usual, we assume that the superconductivity is induced by a large sheet of the Fermi surface and that the order parameter sets in near the symmetry point $\mathbf{k}_0$. We write the basis functions of the degenerate representation in the form $\psi_{m\alpha}(\mathbf{k})$, where a Latin letter specifies the number of the function in the representation, and a Greek letter specifies the spin. Generalizing the customary approach (Ref. 13, for example), we write the matrix Hamiltonian

$$\hat{H} = \begin{pmatrix} \varepsilon_{\alpha\beta}^{mn}(\mathbf{k}) & \Delta_{\alpha\beta}^{mn}(\mathbf{k}) \\ \Delta_{\beta\alpha}^{nm*}(k) & -\varepsilon_{\alpha\beta}^{mn}(-\mathbf{k}) \end{pmatrix}. \tag{1}$$

We assume that the crystal has an inversion center and no magnetic structure. We then have $\varepsilon_{\alpha\beta}{}^{mn}(\mathbf{k}) = \delta_{\alpha\beta}\varepsilon^{mn}(\mathbf{k})$, $\varepsilon^{mn}(\mathbf{k}) = \varepsilon^{mn}(-\mathbf{k})$. Near the point $\mathbf{k}_0$, of interest we can replace the matrix $\varepsilon^{mn}(\mathbf{k})$ by its expansion in powers of $\mathbf{k} - \mathbf{k}_0$. By virtue of the symmetry of the crystal, the coefficients of this expansion can be expressed in terms of a few constants.

By definition,

$$\Delta_{\alpha\beta}{}^{mn}(\mathbf{k}) = -\Delta_{\beta\alpha}{}^{nm}(-\mathbf{k}). \tag{2}$$

If we write the order parameter in its usual form ($\boldsymbol{\sigma}$ are Pauli matrices)

$$\hat{\Delta}_{\alpha\beta} = [\delta_{\tau\beta}\hat{\zeta} + (\boldsymbol{\sigma}_{\tau\beta}\hat{\mathbf{d}})]\, i\sigma_{\beta\tau}^{y}, \tag{3}$$

we find the following results in the even case ($P = 1, g$) and the odd case ($P = -1, u$) for the matrices $\hat{\zeta}$ and $\hat{\mathbf{d}}$:

$$\zeta^{mn}(\mathbf{k}) = P\zeta^{nm}(\mathbf{k}), \quad \mathbf{d}^{mn}(\mathbf{k}) = -P\mathbf{d}^{nm}(\mathbf{k}). \tag{4}$$

We see that if there is a degeneracy the order parameter will not be purely singlet or triplet.

We denote by $\mathbf{C}$ a rotation from the point group of the crystal. We define the matrices C_B and C_V as follows:

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$$\mathbf{C}[\psi_{m\alpha}(\mathbf{k})]=C_B{}^{mn}U_{\alpha\beta}{}^{c}\psi_{n\beta}[\mathbf{C}(\mathbf{k})],$$
$$\mathbf{C}[\mathbf{k}_i]=C_V{}^{ij}\mathbf{k}_j. \tag{5}$$

Here $U_{\alpha\beta}{}^{C}$ is the spin rotation matrix; i.e., we are assuming that the spin-orbit coupling is strong and that the spins are "frozen" in the lattice. In this case $\hat{\mathbf{d}}$ transforms under the rotation as an ordinary vector. The rules for the transformation of the order parameter under a rotation are

$$\mathbf{C}[\zeta^{mn}(\mathbf{k})]=C_B{}^{mp}C_B{}^{nl}\zeta^{pl}(\mathbf{C}[\mathbf{k}]),$$
$$\mathbf{C}[d_i{}^{mn}(\mathbf{k})]=C_B{}^{mp}C_B{}^{nl}C_V{}^{ij}d_j{}^{pl}(\mathbf{C}[\mathbf{k}]). \tag{6}$$

Time reversal is equivalent to taking the Hermitian adjoints of $\hat{\zeta}$ and $\hat{\mathbf{d}}$.

The complete group of the order parameter is $G\times U(1)\times R$, where G is the point group of the crystal, $U(1)$ are gauge transformations, and R is time reversal. Its subgroups (superconducting classes) were listed in Ref. 5 for all point groups. Using the laws given above for the transformation of the order parameter, we can write an expansion of the order parameter in powers of $\mathbf{k}-\mathbf{k}_0$ in terms of a few constants. The spectrum of the superconducting carriers near $\mathbf{k}_0$ is determined by Hamiltonian (1). Examining all the "suspect" points in this fashion, we can calculate the density of states near the Fermi surface and other electronic characteristics.

3. NONDEGENERATE CASE

To illustrate the situation we consider the following example. We assume that a metal has a symmetry group D_{2h} or D_{4h}. Near $\mathbf{k}=0$ the energy of an electron in a normal metal is

$$\varepsilon_0(\mathbf{k})=\varepsilon_0(0)+\sum_i k_i{}^2/2m_i. \tag{7}$$

For the group D_{4h} we have $m_x=m_y$. We assume that by varying the pressure or the doping we can make $\varepsilon_0(0)$ small in comparison with the temperature (the energy is reckoned from ε_F). In this case the metal is at the point of a topological transition that corresponds to the formation of a new cavity of the Fermi surface if the product $m_x m_y m_z$ is positive or to the formation of a bridge if it is negative. In the former case, we are forced to assume the existence of a large Fermi-surface sheet responsible for the metallic behavior and the superconductivity. We assume that the effective masses m_i are on the order of the free mass. Everywhere below we will be discussing the electron specific heat, whose temperature dependence corresponds unambiguously to the dependence of the state density on $\varepsilon-\varepsilon_F$. As was shown in Ref. 11, the component of the specific heat corresponding to the vicinity of the point $\mathbf{k}=0$ is $C\sim\gamma T^{3/2}/\varepsilon_F{}^{1/2}$ (the constant γ is equal to C_{norm}/T, and ε_F is of atomic order of magnitude). In a normal metal at reasonable temperatures, $T\ll\varepsilon_F$, this component is much smaller than C_{norm}. Below the superconducting transition temperature, however, this momentum region may become important.

Let us assume that a superconducting order parameter corresponding to a nontrivial phase has arisen in the crystal. Because of the electron-photon interaction, an order parameter is also imposed near the point $\mathbf{k}=0$. Since the branch of the spectrum is not degenerate, an even order parameter (g) corresponds to $S=0$, and an odd one (u) to $S=1$. The basis

TABLE I. Specific heat of a superconductor at low temperatures: the components from various regions of reciprocal space.

Class		$\gamma^{-1}C$ ($k\ll k_F$), $m_x m_y m_z>0$	$\gamma^{-1}C$ ($k\ll k_F$), $m_x m_y m_z<0$	$\gamma^{-1}C$ ($k\sim k_F$)
$D_4\times R$	g	$T_c e^{-T/T_c}$	$T_c e^{-T/T_c}$	$T_c e^{-T/T_c}$
$D_2\times R$	u	$T^{3/2}/\varepsilon_F{}^{1/2}$, $T>T_1$ $T^3\varepsilon_F/T_c{}^3$, $T<T_1$	T^2/T_c, $T>T_1$ $T^3\varepsilon_F/T_c{}^3$, $T<T_1$	$T_c e^{-T/T_c}$
$D_4(C_4)\times R$	g	$T^{3/2}/\varepsilon_F{}^{1/2}$	$T^{5/4}/T_c{}^{1/4}$	T^2/T_c
	u	$T^{3/2}/\varepsilon_F{}^{1/2}$	$T^{4/3}/T_c{}^{1/3}$	$T^3/T_c{}^2$
$D_4(D_2)\times R$	g	$T^{3/2}/\varepsilon_F{}^{1/2}$,	$T^{3/2}/T_c{}^{1/2}$	T^2/T_c
$D_2(U_2)\times R$ $D_2(C_2)\times R$	u	$T^{3/2}/\varepsilon_F{}^{1/2}$, $T>T_1$ $T^{5/2}\varepsilon_F{}^{1/2}/T_c{}^2$, $T<T_1$	T^2/T_c, $T>T_1$ $T^{5/2}\varepsilon_F{}^{1/2}/T_c{}^2$, $T<T_1$	$T^3/T_c{}^2$
$D_4(E)$	g	$T^{3/2}/\varepsilon_F{}^{1/2}$	$T^{3/2}/T_c{}^{1/2}$	T^2/T_c
	u	$T^{3/2}/\varepsilon_F{}^{1/2}$, $T>T_1$ T^2/T_c, $T<T_1$	T^2/T_c	$T^3/T_c{}^2$

2) *Note.* Here $C(k\ll k_F)$ is the component of the specific heat which comes from the vicinity of the point $k=0$ if $\varepsilon(0)=0$. The case $m_x m_y m_z>0$ corresponds to the formation in the course of the topological transition of a small cavity on the Fermi surface. The case $m_x m_y m_z$ corresponds to the formation of a bridge between two sheets of the Fermi surface. Here $C(k\sim k_F)$ is the component which comes from a large sheet of the Fermi surface (from Ref. 5). The temperature T_1 is $T_1=T_c{}^2/\varepsilon_F$, where ε_F is of the atomic order of magnitude.

functions in this case are no different from those given in Ref. 5, which dealt with the situation in which the position of the Fermi level is arbitrary, and the maximum symmetry of a point on the Fermi surface corresponds to a rotational axis or a mirror-image plane. A zero of the energy gap arises at this point if this element enters the superconducting class along with a gauge transformation. Correspondingly, there are only two possibilities for the temperature dependence of the specific heat: T^3 (an axial phase) or T^2 (a planar phase). We now assume that the Fermi suface passes through the point $\mathbf{k} = 0$. Since this point is invariant under all operations of the point group, the number of possibilities for the temperature dependence of the specific heat increases sharply (Table I). The temperature $T_1 = T_c^2/\varepsilon_F$ is much lower than T_c. The case $D_4(C_4)\times R$, $m_x m_y m_z < 0$ (a bridge) is the most interesting in our opinion. The expansion of the order parameter in powers of the momentum begins with k^4 (a singlet) and k^3 (triplet) in this class, so there is a substantial volume in the reciprocal space in which the order parameter is small. The exponent in the power-law temperature dependence of the specific heat is therefore close to unity (respectively 5/4 and 4/3).

If the point at which the topological transition occurs lies at the boundary of the Brillouin zone, we need to examine the small symmetry group of this point, which obviously contains an inversion.

4. DEGENERATE CASE

We turn now to a case which is probably not pertinent to the new superconducting materials and which is of only methodological interest. We assume that in a crystal with a symmetry group D_{4h} there exists a sheet of the Fermi surface which corresponds to wave functions from a doubly degenerate representation E. Degeneracy is conserved along the entire symmetry axis C_4. The Fermi momentum along the C_4 axis is $\mathbf{k}_0 = (0, 0, k_0)$. The spectrum near $\mathbf{k}_0$ is

$$\varepsilon_\pm = \varepsilon_{A_1} \pm (\varepsilon_{B_1}^2 + \varepsilon_{B_2}^2)^{1/2}, \tag{8}$$

where

$$\varepsilon_{A_1} = (k_z - k_0) v_F + (k_x^2 + k_y^2)/2m_\parallel + (k_z - k_0)^2/2m_\perp,$$
$$\varepsilon_{B_1} = (k_x^2 - k_y^2)/2m_1, \quad \varepsilon_{B_2} = k_x k_y / 2m_2. \tag{9}$$

The Fermi surface consists of two sheets, which touch at the points $\pm\ \mathbf{k}_0$.

If there is a degeneracy, the order parameter is a 4×4

TABLE II. The order parameter at the degeneracy point.

Class		ζ	$\mathbf{d}$
$D_4\times R$	g	$\hat{\sigma}_0$	$\hat{\sigma}_y \mathbf{z}$
	u	$\hat{\sigma}_y$	$\hat{\sigma}_0 \mathbf{z}$
$D_4(C_4)\times R$	g	0	0
	u	0	0
$D_4^{(1)}(D_2)\times R$	g	$\hat{\sigma}_z$	0
	u	0	$\hat{\sigma}_z \mathbf{z}$
$D_4^{(2)}(D_2)\times R$	g	$\hat{\sigma}_x$	0
	u	0	$\hat{\sigma}_x \mathbf{z}$
$D_4(E)$	g	0	$\hat{\sigma}_y (\mathbf{x} + i\mathbf{y})$
	u	0	$d_0\sigma_0 (\mathbf{x} + i\mathbf{y}) + (d_z\hat{\sigma}_z + d_x i\hat{\sigma}_x)(\mathbf{x} - i\mathbf{y})$
$D_2(U_2)$	g	0	$\hat{\sigma}_y \mathbf{x}$
	u	0	$(d_0\hat{\sigma}_0 + d_z\hat{\sigma}_z)\mathbf{x} + d_x\hat{\sigma}_x \mathbf{y}$
$D_2(U_2')$	g	0	$i\hat{\sigma}_y (\mathbf{x} - \mathbf{y})$
	u	0	$(d_0\hat{\sigma}_0 + d_x\hat{\sigma}_x)(\mathbf{x} - \mathbf{y}) + d_z\hat{\sigma}_z (\mathbf{x} + \mathbf{y})$

2) *Note.* The form of the order parameter at the point $\mathbf{k}_0 = (0, 0, k_0)$ if the wave functions of the electrons transform under a two-dimensional representation E of group D_4. The Pauli matrices σ_1 and the unit matric σ_0 act on the indices which specify the basis functions of representation E. There is no energy gap at point $\mathbf{k}_0$ in classes $D_4(C_4)\times R - g, u$ and $D_4(E)\times R - g$.

matrix, and the carrier spectrum is determined by Hamiltonian (1). In this situation, even if there is a nontrivial symmetry element which leaves $\mathbf{k}_0$ invariant, the carrier spectrum at this point may nevertheless have a gap. Table II gives the order parameter at point $\mathbf{k}_0$ for classes from D_4. The Pauli matrices $\hat{\sigma}_i$ and the unit matrix $\hat{\sigma}_0$ act on the Latin indices in this case. The coefficient d_i are real. An energy gap appears at point $\mathbf{k}_0$ in all classes except $D_4(C_4)\times R - g$, u and $D_4(E) - g$. Interestingly, a gap also arises in the class $D_4(E) - u$, although in the absence of degeneracy the zero of the order parameter at point $\mathbf{k}_0$ is of a topological nature.

5. CONCLUSION

We have derived results on the low-temperature behavior of the specific heat for a superconductor at the point of a topological transition. A question which arises in this connection is that of making a comparison with experiment. Important evidence in favor of the existence of spectral features at the Fermi surface would be the observation of an anomaly in the specific heat as a function of the doping or the pressure. Unfortunately, at this point we are unaware of any such measurements, which would be rather complicated from the technical standpoint. The existence of such features along with an anisotropic superconductivity would lead to predictions regarding the behavior of the specific heat at the extremely low temperatures. Of greatest interest from this standpoint are phases in which the $C(T)$ dependence is approximately linear ($T^{5/4}$, $T^{4/3}$, $T^{3/2}$).

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