Vortices with half magnetic flux quanta in "heavy-fermion" superconductors

V. B. Geshkenbein and A. I. Larkin
Landau Institute for Theoretical Physics, Academy of Sciences of U.S.S.R., Moscow, U.S.S.R.

A. Barone
Dipartimento di Fisica Nucleare Struttura della Materia e Fisica Applicata, Università di Napoli, Napoli, Italy and Istituto di Cibernetica del Consiglio Nazionale delle Ricerche, Arco Felice (Napoli), Italy
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It is shown that in "heavy-fermion" superconductors a new vortex state can occur characterized by the existence of half magnetic flux quanta. Vortices in polycrystals should exist even in the absence of an externally applied magnetic field. The internal structure of the vortices is also investigated.

INTRODUCTION

The so-called "heavy-fermion" behavior observed in various substances is one of the most stimulating topics of condensed matter physics which have attracted the attention of both theoretical and experimental investigators during the last years. Experimental data on superconducting cerium- and uranium-based intermetallic compounds such as $CeCu_2Si_2$, UBe_{13}, and UPt_3 (Ref. 1) suggest that an "unusual" pairing of electrons can take place.

In this context tunneling between spin "singlet" and hypothetical "triplet" superconductors has been investigated for many years[2] together with proximity effect between such systems.[3] More recently, the limits of using pair tunneling as a probe to differentiate between even- and odd-parity states (e.g., Ref. 4) and results of rather sophisticated experiments[5] have been discussed by several authors.

In the case of unusual pairing, the order parameter should belong to the nontrivial representation of the crystal symmetry group.[4–8] This circumstance leads to quite interesting consequences. In this article we show that in these superconductors there exist vortices with a half magnetic flux quantum.[9] We shall demonstrate that in a single crystal these vortices may exist only on the domain walls between different degenerate superconducting states whereas in a polycrystalline sample, vortices can occur at the intersection of the three boundaries between three crystal grains (the line L at which three crystalline grains are in contact). In this case these vortices are energetically favored and they exist even in the absence of an externally applied magnetic field. We shall refer only to nonmagnetic superconducting phases.

Let us show first that a system of an S-P-S sandwich (S and P stand for usual and unusual superconductor, respectively) closed by a superconducting loop (Fig. 1) will contain half magnetic flux quanta, namely $(n+\frac{1}{2})\Phi_0$.

As is known,[5] the order parameter of a superconductor can be expressed as

$$\Delta_{\alpha\beta}(\mathbf{k},X)=\sum_i \eta^i \psi^i_{\alpha,\beta}(\mathbf{k}) \ , \qquad (1)$$

where η^i is an order parameter which can be in general function of temperature T and coordinate X_i, and $\psi^i_{\alpha\beta}(\mathbf{k})$ is the basis function of the representation which contains the angular dependence of the momentum. The usual normalization condition for $\psi(\mathbf{k})$ is $\int |\psi(k)|^2 d\Omega=1$. If in the superconductive phase there exists only one function $\psi^i(i=1)$, then η belongs to the one-dimensional representation. Let us consider a system of two superconductors, one usual (S) and one unusual (P), coupled by tunneling. The free energy of such a system of two weakly-coupled superconductors is given by

$$F=\mathrm{Re}\int \Delta_1\Delta_2^* G_1 G_1 \,|\,T\,|^2 G_2 G_2 \, d\mathbf{k}_1\, d\mathbf{k}_2 = A\ \mathrm{Re}\eta_1\eta_2^* \ , \qquad (2)$$

where Δ_1 and Δ_2 are the order parameters in the S- and P-type superconductors, respectively. The coefficient A is a function of the orientation of the barrier with respect to the crystal axes (it is also temperature dependent). A is an odd function of n (unit vector normal to the surface of contact) since Δ_1 and Δ_2 are even and odd functions of $\mathbf{k}_1$ and $\mathbf{k}_2$, respectively. Here our reference system is provided by the crystal axes. For example if we assume the order parameter Δ_2 to be a pseudoscalar $[\Delta_2\sim(\mathbf{k},\boldsymbol{\sigma})]$ we can write for the case of a crystal of cubic symmetry[8]

$$A(n)=Af(\mathbf{n}) \ ,$$

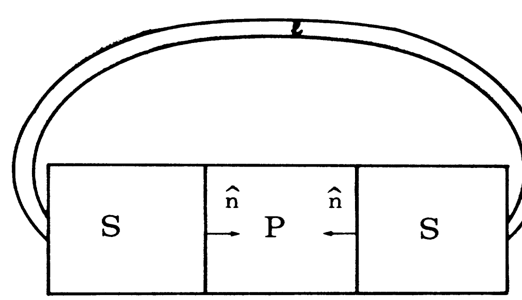

FIG. 1. Sketch of a sandwhich structure S-P-S (see text) closed by a superconducting loop.

where

$$f=n_x n_y n_z(n_x^2-n_y^2)(n_y^2-n_z^2)(n_z^2-n_x^2)$$

with the resulting angle dependence of the Josephson current, $I_j(\phi)=Af\sin\phi$, ϕ being the relative phase across the boundary.

Let us observe that a minimum of the free energy does not occur necessarily for $\phi=0$. Indeed, if we consider a structure such as that sketched in Fig. 1, the minima of the free energy at the *S-P* and *P-S* boundaries will correspond to the values $\phi=0$ and $\phi=\pi$, respectively. Thus the minima of the free energy in our system occur at values of magnetic flux equal to $(n+\frac{1}{2})\Phi_0$, where Φ_0 is the flux quantum.

It is worth observing that the expression of the free energy we used is written under the assumption of equal critical temperatures for the two superconductors. Such an assumption allows a more clear discussion of the topic. It is worth noting that this is a limit which, however, does not affect what follows since everything else is essentially symmetric in character and valid for arbitrary $T_c \neq T_c'$.

POLYCRYSTALLINE STRUCTURES

Let us discuss the case when the nontrivial order parameter η belongs to the one-dimensional representation of the crystal symmetry group.[5] In this case in a single crystal the Ginzburg-Landau equation has the same form as in conventional superconductors, and vortices, as usual, carry one magnetic flux quantum. Let us consider the boundary between two crystal grains. Near T_c the contribution to the free energy of this boundary, which depends on the phase difference ϕ of the order parameter is, as we have seen, equal to $F_{12}=A\,\mathrm{Re}\eta_1\eta_2^*$ where η_1 (η_2) is the order parameter in the crystal grain 1 (2). Here both η_1 and η_2 refer to unusual superconductors. For nontrivial representations, transformations of the symmetry group of the crystal 1 exist under which the order parameter η changes sign. The free energy is invariant, so the coefficient A has to change sign under such a transformation; consequently its sign depends upon the choice of the coordinate axes in the first and second crystal grains. For two crystal grains we can always choose these axes so that the coefficient A is negative and the minimum of F corresponds to the phase difference ϕ equals to zero.

If we consider three border planes of three crystal grains the situation can be different. The energy associated with the boundaries between the three grains is

$$F=F_{12}+F_{23}+F_{31}$$
$$=\mathrm{Re}(A_{12}\eta_1\eta_2^*+A_{23}\eta_2\eta_3^*+A_{31}\eta_3\eta_1^*)\ . \tag{3}$$

For a fixed choice of the axes in grain 1, by choosing the coordinate axes in grains 2 and 3 we can assume the coefficients A_{12} and A_{13} to be negative. In this case the sign of the coefficient A_{23} will be fixed. By changing the coordinate axes in one grain, we change simultaneously the sign of two coefficients A, so the sign of the product $A_{12}A_{23}A_{31}$ is not arbitrary. This sign does not depend upon the choice of the coordinate axes; rather, it depends on the reciprocal orientation of the crystal grains. We show below that this sign may be positive or negative with probability of the order of one half. If it is negative, the minimum of the free energy corresponds to a state with equal and constant (spatially independent) phases of the order parameter. If the sign of the product $A_{12}A_{23}A_{31}$ is positive, the zero-current-carrying state corresponds to a maximum of the energy at one boundary. For not very small grains a current-carrying state is more favored. In such a state the phase of the order parameter changes in each grain. Indeed in formula (3) the parameter η in each term indicates the order parameter close to the boundary. More explicitly we indicate (see Fig. 2) with $\eta_{1(2)}$ and $\eta_{1(3)}$ the values of η_1 at the border with grains 2 and 3, respectively (analogously for η_2 and η_3); sufficiently far from the borderline of the three crystal grains, the phases of the order parameters at the different boundaries are independent (i.e., $\eta_{1(2)}\neq\eta_{1(3)}$). The minimum of the free energy is achieved if at one boundary (1-2, for example) the phase difference is π and at the others (2-3 and 3-1) such a phase difference is zero. This phase difference (π) results from the phase change in the whole volume of the grains. Let us denote by $\Delta\phi_i$ the phase change of the order parameter inside the ith crystal grain. Thus, by following a path around the border L and far enough from it, the phase difference will be

$$\Delta\phi=\Delta\phi_1+\Delta\phi_2+\Delta\phi_3=\pi\ . \tag{4}$$

In the volume of the grains we have

$$\mathbf{j}=\frac{c^2}{8\pi e\lambda_L^2}\left[\hbar\nabla\phi-\frac{2e}{c}\mathbf{A}\right]\ , \tag{5}$$

where λ_L indicates the London penetration depth.

Attention should be directed also to the limits of expression (5) which is actually valid only for one-dimensional representations of the cubic symmetry group. In the other cases the superconducting current density is a

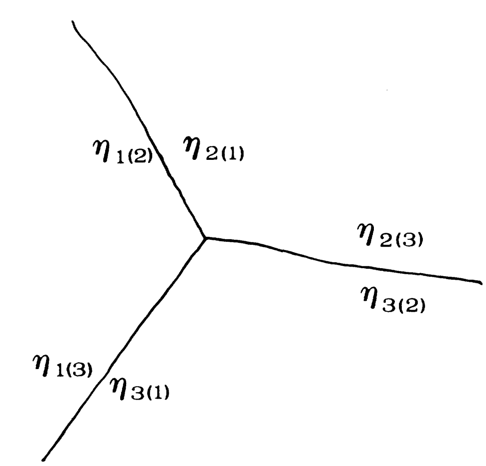

FIG. 2. Values of the order parameters at the grain boundaries.

tensor and there should be more than one penetration length.

This last circumstance should be taken into account also in connection with the lower degree of symmetry at the boundary. Moreover, let us observe that in the nonmagnetic case the components of the order parameter have equal phases. Thus the expression given here for the superconducting current density holds for a nonmagnetic phases without domain walls.

By choosing the contour in a region where the current is zero, we obtain that inside the contour there exists a half magnetic flux quantum. Indeed we have

$$\int H\, dS = \oint \mathbf{A}\cdot d\mathbf{l}\frac{\Phi_0}{2} = \frac{c\hbar\pi}{2e} \ . \tag{6}$$

Thus when the product $A_{12}A_{23}A_{31}$ is positive the free-energy minimum corresponds to the state with a vortex on the border line L of the three crystal grains. This vortex carries a half magnetic flux quantum.

Let us show that this product may have different signs depending on the mutual orientation of the three grains. Let us rotate the crystal lattice of grain 3 only, keeping the orientation of grains 1 and 2. Let us first study the case when η changes sign under some rotations. In this case A changes sign as well. The product $A_{12}A_{23}A_{31}$ changes sign when one of the coefficients A_{23} or A_{31} changes sign. A simultaneous change of the sign of both under rotation is unrealistic because A_{23} and A_{31} correspond to different boundaries and depend upon the orientation of these boundaries and crystal grains 2 and 1, accordingly.

For pseudoscalar representations, the order parameter does not change under rotations, but changes sign under reflection. In this case the statement of the existence of a vortex is not general; rather it depends upon the boundary conditions at the border between two grains. For the usual diffusive case the coefficient A_{23} does not depend upon the reciprocal orientation of crystal axes 2 and 3; it depends only on their orientation with respect to the boundary between the grains (uncorrelation between $\mathbf{k}_1$ and $\mathbf{k}_2$) and is

$$A_{23} = af_2(n)f_3(-n) \ , \tag{7}$$

where $f_i(\hat{\mathbf{n}})$ is a function which depends on the projection of the vector (normal to the boundary) onto the crystal axes of the ith crystal grain. This function describes the angle dependence of the Josephson current between this and the usual superconductor, as discussed in the Introduction. Depending on the orientation of the crystal axes with respect to the boundary, this function may have different signs, as will A_{23}. Thus vortices can exist also in the pseudoscalar case.

The internal structure of the vortices depends upon the value of the coefficient A. We found this value at temperatures near T_c. The order parameter η decreases near the boundary within a distance and may be found from the integral equation

$$\Delta(\mathbf{K},X) = \int V(\mathbf{k},\mathbf{k}_1)\overline{GG}(\mathbf{k}_1,\mathbf{k}',X,X^1) \times \Delta(\mathbf{k}',X')d\mathbf{k}\, d\mathbf{k}'dX' \ . \tag{8}$$

The kernel of (8) decreases at distances of the order of ξ_0. Thus at distance $X \gg \xi_0$ from the boundary the expression for $\Delta(\mathbf{k},X)$ is given by (1). In the region $\xi_0 \ll X \ll \xi$, η satisfies the equation

$$\frac{d^2\eta(X)}{dX^2} = 0 \ . \tag{9}$$

The solution of this equation is a linear function. This solution must turn into the exact solution of the Ginzburg-Landau equation in the ith crystal (which is rigorously valid for $|x| \gg \xi_0$)

$$\eta(x) = \begin{cases} \eta_1 \left[\dfrac{X}{\xi}\right] & X > 0 \\ -\eta_2 \left[\dfrac{X}{\xi}\right] & X < 0 \end{cases} \ .$$

A linear solution on the different sides of the boundary has the form

$$\eta(x) = \begin{cases} \dfrac{1}{\xi}(\eta_1 X + \eta_1 a_1 \xi_0 + \eta_2 b \xi_0) & x \to +\infty \\ \dfrac{1}{\xi}(-\eta_2 x + \eta_2 a_2 \xi_0 + \eta_1 b \xi_0) & x \to -\infty \end{cases} \ .$$

The coefficients a_i and b depend upon the reciprocal location of the crystal grains and are determined from (8).

Since the only length parameter in this integral equation ξ_0, the coefficients a_i are of the order of unity, and b is of the order of the boundary transparency which we consider also to be of the order of unity. Let us write the expression for the current flowing through the boundary

$$j = C\, \mathrm{Im}(\eta^* \nabla \eta) = \frac{Cb\xi_0}{\xi^2} |\eta|^2 \sin(\phi_1 - \phi_2) \ , \tag{10}$$

where ϕ is the phase difference across the boundary C is a constant. Hence, even if the transparency of the boundary is of the order of unity, near T_c the critical current through the boundary is smaller than the despairing current by a factor ξ_0/ξ. On the other side the current is related to the free energy of the contact by the formula

$$j = \frac{2e}{\hbar}\frac{\partial F}{\partial \phi} \ ,$$

so the coefficient A in (2) is equal to

$$A = \frac{\hbar C}{2e}\frac{b\xi_0}{\xi^2} \ .$$

For the determination of phase and current distribution inside the vortex we must find the solution of the equation $\nabla \cdot j(\phi) = 0$ ($\Delta\phi = 0$) which is valid inside both volumes 1 and 2. The boundary condition is provided by Eq. (10)

$$\nabla_n \phi_1 = \nabla_n \phi_2 = \frac{b\xi_0}{\xi} \sin(\phi_1 - \phi_2) \ .$$

The solution of the equation depends on the distance of the borderline of the three grains. As a result we get that at distances less than ξ^2/ξ_0 from the border L line of the three grains the phase has little change in the volume of the crystal grains and has "jumps" at the boundaries. At distances larger than $\xi^2/b\xi_0$ the phase has a jump on the boundary close to π, and a continuous change in the volume up to π. For heavy-fermion superconductors the Ginzburg-Landau parameter $x=\lambda_L/\xi\approx 50$. So if the boundary transparency is of the order of unit ($b\sim 1$) then $\xi^2/b\xi_0 \ll \lambda_L$ and the current distributions in the vortices at distances larger than $\xi^2/b\xi_0$ is as in the usual vortices. The energy of such vortex is four-times less than the energy of the usual vortices. If the transparency of the boundary b is small or the temperature is close to T_c then the opposite condition, $\lambda_L \ll \xi^2/b\xi_0$ holds. The current distribution in this case is like that occurring in Josephson junctions.[10] Currents and fields penetrate across the boundaries between the grains within a length (the Josephson penetration depth)

$$\lambda_J = \left[\frac{\lambda_L \xi^2}{b\xi_0} \right]^{1/2} . \tag{11}$$

So far we have considered the border lines of three crystal grains. In polycrystals these lines may end only at the surface of the sample. In the volume they can intersect and form loops. In the absence of externally applied magnetic field, the magnetic flux in the vortices may be directed along two different directions with a probability $\frac{1}{2}$. If the grain size and hence the distance between the vortices becomes less than the vortex size λ_L then it is meaningless to refer to a magnetic flux of "one" vortex. In the sample there must exist randomly distributed magnetic field with local amplitude of the order of $\Phi_0/4\pi\lambda_L^2$.

Let us consider now the case when the nontrivial order parameter belongs to multidimensional representations of the crystal symmetry group. This topic is quite complicated because domain walls may exist (even in a single crystal) between the different degenerate superconducting states. If there are no domain walls in the volume of the crystal grains, then there are no changes in the previous considerations except for the fact that the product of the coefficients A depends not only upon the mutual orientation of the crystal grains but also on the state in the degenerate representation. For different states belonging to one degenerate representation the coefficient A has different values; this result does not change our conclusions.

VORTICES AND DOMAIN WALLS

We can characterize the domain wall by some element $\hat{g}_w$ of the crystal symmetry group which transforms the order parameter from one side of the wall to the order parameter on the opposite side (for instance it may be a rotation of $\pi/2$ around the axis of the cube which rotates one tetragonal axis into another).

For some superconducting states it is possible after a number of rotations $\hat{g}$ to return to the original value of the order parameter η but with opposite sign. In this case a vortex with a half magnetic flux quantum does exist on the common line of the n domain walls. In this case domain walls play somewhat the same role of grain boundaries in polycrystals. For $n=2$ a vortex line will exist on the wall separating the two domains. The energy of such a vortex is positive (i.e., it requires applied field) but it is 4 times smaller than the energy of a "usual" vortex. Thus vortices with a half magnetic flux quantum can occur also in a single crystal.

There are superconducting phases in which it is impossible by whatever number of rotations to transform the order parameter η into $-\eta$. In this case there are no such vortices in single crystals; they can exist only in the polycrystals as previously discussed. Moreover, vortices can occur also on a crossing line between a domain wall and a grain boundary.

CONCLUDING REMARKS

In conclusion we expect that for "heavy-fermion" superconductors a new vortex state can occur which is characterized by the existence of half magnetic flux quanta. Half-quantum vortices can occur in single crystals depending on the symmetry properties of the order parameter in the superconducting phases. In polycrystals such vortices have negative energy and therefore should exist even in the absence of externally applied magnetic field. It would be of great interest to consider the possibility of a direct experimental observation of such a vortex structure by using a suitable "microscopy" technique or any other possible probe which could be envisaged.

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