On the theory of gauge symmetry of superconductors

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All superconducting structures which are possible from the viewpoint of gauge symmetry and which exhibit nontrivial violation of gauge symmetry are determined. These are 58 nonmagnetic structures, 73 ferromagnetic structures, and 113 antiferromagnetic structures. Some new effects are predicted for "exotic" superconductors.

INTRODUCTION

As is well known, the phenomenon of superconductivity is conditioned by a spontaneous breakdown of gauge symmetry. The Hamiltonian of the electrons in the metal is invariant with respect to a gauge transformation of the electron creation and annihilation operators. This is simply a mathematical expression of the conservation of electron number. A superconducting state changes under such a transformation and is transformed into another equivalent state. Therefore a superconductor is characterized by a complex function ψ , the phase of which is the degeneracy parameter. In normal superconductors the ψ function does not undergo any change for pure crystal transformations (rotations, reflections, and translations). Recently Gor'kov and Volovik [1] have called attention to a new class of superconductors, in which the order parameter changes under some crystal transformations. It was shown in [1] that quite unusual physical properties will be observed, properties which are determined by the nontrivial way in which gauge symmetry is violated. Gor'kov and Volovik [1] have given an extension of the Landau-Ginzburg theory for this new class of superconductors and have formulated the general problem of determining all possible ways in which the gauge symmetry can be violated. The method of solving this problem proposed in Ref. [1] is, however, cumbersome and, as will follow from the results to be presented below, it needs to be augmented.

In place of a formal search for the set of combinations of usual and gauge transformations which make up the symmetry groups, in the present paper the complete solution of the problem posed in Ref. [1] is obtained by a method developed by Andreev and the present author [2] for the investigation of the exchange symmetry of magnetic materials. This simplifies the problem considerably, since it suffices to consider the one- and two-dimensional representations of the symmetry group of the crystal. It was shown that many superconducting structures which would be possible from the point of view of their symmetry turn out to be in principle unstable. This is a general effect for systems with continuous degeneracy (e.g., exchange magnetic materials, liquid crystals). An equivalence is established between many structures of coexistence of ordinary superconductivity with some type of magnetic ordering, coexistence which has been discussed in the literature long ago.

Since the phenomenon of superconductivity is observed only at low temperatures there is no hope of obtaining supeconductors with especially small relativistic effects. Therefore we shall not consider independent rotations of the spin space. Thus we will deal with the exact magnetic-gauge symmetry of the superconductors.

GAUGE SYMMETRY

A derivation of the gauge symmetry groups and the investigation of a series of general properties of states with broken gauge symmetry is possible without having a detailed knowledge of the structure of the space of arguments η of the function ψ which characterizes the superconductor. What is important is that these arguments (for example, the electron momenta) should be subject to definite changes under the action of crystallographic transformations. Let the group Gbe the group of crystallographic symmetry of the superconductor, i.e., the symmetry group of the microscopic charge density, and in general of all the physical characteristics which do not change under gauge transformations and under a change of the sign of time, R. We call attention to the fact that, in general, the group G differs from the symmetry group of the normal state. Thus, for instance, if the phase transition of the second kind into the superconducting state (cf. [1]) corresponds to a three-dimensional representation of the symmetry group of the normal state, then the crystal symmetry is necessarily lower after the transition.

We expand the function $\psi(\eta)$ in terms of physically irreducible representations (cf. [4] §96) of the group G

$$\psi(\eta) = \sum_{n} \psi_{n\alpha}(\eta), \qquad (1)$$

where the functions $\psi_{n\alpha}(\eta)$ transform according to the nth representation and the index α labels the functions belonging to this representation. The following remark must be made about the functions $\psi_{n\alpha}(\eta)$. According to the rules of quantum mechanics the state described by the function ψ goes over into the state described by the complex conjugate function ψ^* under time reversal R. In the case when there exists a gauge transformation $C_{\delta} = \exp(i\delta\partial/\partial\varphi)$ for which its action together with R does not modify the wave function ψ the state is nonmagnetic. This is possible only when the function ψ has the form

$$\psi = \chi(\eta) e^{i\varphi}, \tag{2}$$

where the function $\chi(\eta)$ is real. Such a state cannot be characterized by nonvanishing expectation values of the physical quantities which are invariant under gauge transformations but change when the sign of the time changes, such as the current density or magnetization density. If the function ψ is intrinsically complex, i.e.,

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$$\psi = \{\chi'(\eta) + i\chi''(\eta)\}e^{i\varphi}, \tag{3}$$

where the real functions χ' and χ'' are linearly independent, then the state will be magnetic. Therefore the functions $\psi_{n\alpha}$ in the expansion (1) may appear either in the form (2) or in the form (3), where in the latter case the functions $\chi'_{n\alpha}$ and $\chi''_{n\alpha}$ which realize the same representation, transform independently.

The gauge symmetry of the superconductor is completely determined by the set of functions $\psi_{n\alpha}$ which appear in the expansion (1). The maximum number of such sets is severely restricted. Indeed, let us form out of the functions $\psi_{n\alpha}$ the scalar quadratic forms $\psi_{n\alpha}\psi_{m\beta}^* + \psi_{n\alpha}^*\psi_{m\beta}$. These do not change under gauge transformations and under a change of the sign of time, since in an equilibrium state they must be invariant with respect to the group G. On the other hand, these quantities transform under the direct product of the representations n and m. Since only unitary representations participate in the expansion (1), the representation $n \otimes m$ contains the identity representation only if n coincides with m. Therefore

$$\psi_{n\alpha}\psi_{m\beta}^* + \psi_{n\alpha}^*\psi_{m\beta} = a_n(\eta)\delta_{nm}\delta_{\alpha\beta}, \tag{4}$$

where the $a_n(\eta)$ are some functions which are invariant under the group G. The condition (4) is satisfied in the following three essentially distinct cases:

1) The function ψ of the form (2) transforms according to the identity representation. This is the usual superconducting state.

2) The function ψ of the form (2) transforms according to a one-dimensional representation different from the identity representation. The gauge symmetry group of this superconductor consists of the crystallographic transformations which do not change the function ψ , and the products of a gauge transformation C_{π} by a crystallographic transformation which changes the sign of the function ψ . These groups are obviously isomorphic to the magnetic symmetry groups of antiferromagnetic materials. 3) The function ψ has the form (3) where the functions χ' and χ'' transform according to either the same two or according to two different one-dimensional representations, or they realize a two-dimensional representation. Such a superconductor is characterized by magnetic ordering. Of the two components of the ψ -function

$$\psi'(\eta) = \chi'(\eta) e^{i\varphi}, \qquad \psi''(\eta) = i\chi''(\eta) e^{i\varphi}$$

one can form the gauge invariant quadratic form

$$\psi'\psi''^* - \psi'^*\psi'', \tag{5}$$

which changes sign under a change of the sign of time and in the above cases transforms according to a one-dimensional representation. The symmetry of the form (5) obviously defines a magnetic symmetry group of the state described by it. We note that in superconductors in which the symmetry of the form (5) allows for magnetization, in Landau-Ginzburg theories one must introduce the magnetic field into the energy not only in the usual manner, via the vector potential, but also directly, by means of a term $im_i H_i(\psi'\psi''* - \psi'*\psi'')$. Then one can convince oneself that a situation becomes possible where in a magnetic field superconductivity appears earlier than without the magnetic field (cf. the A_1 -phase-in superfluid He³).

Many magnetic superconductors do not satisfy a stability criterion analogous to the well known Lifshitz criterion in the theory of phase transitions of the second kind. We represent the functions $\psi'(\eta)$ and $\psi''(\eta)$ in the form

$$\psi'(\eta) = \psi'\chi'(\eta), \quad \psi''(\eta) = \psi''\chi''(\eta),$$

where the real functions $\chi'(\eta)$ and $\chi''(\eta)$ transform according to the appropriate irreducible representations and ψ' and ψ'' are parameters which do not depend on η . Further we assume, as usual, that the parameters ψ' and ψ'' (and not the functions χ' and χ'') realize the representation under consideration. Then for small long-wave deviations from equilibrium the energy of the system can be expanded in powers of the variations $\delta\psi'$ and $\delta\psi''$. The structure will be unstable if there exists an expression invariant with respect to the group G of the form

$$K_i(\psi'\partial_i\psi''^*+\psi'^*\partial_i\psi''-\psi''^*\partial_i\psi'-\psi''\partial_i\psi'^*), \qquad (6)$$

where ∂_i denotes differentiation with respect to the coordinates. Indeed, let us consider a small deviation from the homogeneous state of the form

$$\delta \psi = i \psi \delta \varphi(\mathbf{r}),$$

where $\delta \varphi$ is a slowly varying function of the coordinates. Since at each point of space such a variation reduces to a gauge transformation, the change of the local part of the energy (i.e., the part that does not contain spatial derivatives) must vanish. The principal part of the variation of the energy is therefore determined by terms linear in the derivatives, such as those of Eq. (6), terms which obviously can always take on negative values. We note that the invariant (6) always exists when the magnetic quantity (5) transforms according to a representation contained in the vector representation of the group G, i.e., the symmetry would not forbid the existence of a spontaneous current.

The representations of the space groups can be realized by means of functions of the form

$$u_{\mathbf{q}}(\mathbf{\eta}')e^{i\mathbf{q}\mathbf{r}},\tag{7}$$

where η' consists of the set of variables η with the exception of the coordinate r. Indeed, as is well known [4], these representations are realized by functions of the form $u_{a}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}$, where $u_{q}(\mathbf{r})$ are functions periodic in the crystal lattice, but from the viewpoint of symmetry the dependence of u_a on r is necessary only for defining the transformation properties of u_q with respect to rotational elements of the group. We are interested only in one- and two-dimensional representations. Such representations can be characterized by wave vectors q which occupy a general position in the reciprocal cell only for crystals of the triclynic system. In crystals of the monoclynic system representations can be realized with wave vectors occupying a general position in the plane. Representations with a wave vector in general position on a symmetry axis are possible for noncubic crystals. In all these cases the representation is necessarily two-dimensional and the pair of corresponding functions (ψ', ψ'') transform under translations like the pair of functions sin q r and cos q r, i.e., the coordinate dependence of the ψ -function (3) is determined by the factor $e^{i\mathbf{q}\cdot\mathbf{r}}$, as it should be. The appearance of any other incommensurate structure will necessarily destroy the

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spatial periodicity of the crystal. The other structures can only be characterized by a wave vector q corresponding to distinguished points of the reciprocal cell.

From the analysis carried out by Lifshitz (Ref. 5) it is known that invariants of the form (6) are absent (for $q \neq 0$) only in representations which are characterized by wave vectors the components of which are definite fractions (1/2, 1/3, 1/4) of the periods of the reciprocal lattice. For incommensurate structures, however, the existence of invariants of the type (6) does not in all cases signify that there is an instability (cf. Ref. 2). Thus, if the wave vector q occupies a general position on the symmetry axis or a general position in the symmetry plane, then the invariants which are dangerous are those that contain derivatives with respect to the coordinate perpendicular to the symmetry axis or symmetry plane, respectively. We note that for some magnetic superconductors a peculiar piezo-effect becomes possible. Let the functions (ψ', ψ'') be such that there exists an invariant of the form

$$K_{ikj}u_{ik}(\psi'\partial_j\psi''^*+\psi'^*\partial_j\psi''-\psi''^*\partial_j\psi'-\psi''\partial_j\psi'^*),$$

where u_{ik} is the strain tensor. Then the deformed crystal will exhibit the instability described above, and the functions ψ' and ψ'' acquire a phase factor $e^{i\mathbf{q}\cdot\mathbf{r}}$, as is easily seen, where the vector $\mathbf{q} \sim u_{ik}$ is small as long as the deformations are small. Since there is no anisotropy which fixes the phase, the effect must lead to observable consequences, most conspicuously, to a Josephson current.

These simple rules for the derivation of the gauge symmetry groups and the stability criterion are completely analogous to the corresponding results in the theory of exchange symmetry (Ref. 2). In [2], in addition to the crystallographic symmetry a role was played by the group of threedimensional rotations of spin space, whereas here we deal with rotations of a two-dimensional space (gauge transformations). Therefore it is not surprising that the gauge symmetry groups under discussion are isomorphic to a certain class of exchange symmetry groups, specifically, the structures characterized by one function $\psi(\eta)$ (cases 1 and 2) are associated with collinear magnetic materials, described by one magnetic vector, whereas those characterized by two functions $\psi'(\eta)$ and $\psi''(\eta)$ (case 3) correspond to noncollinear magnetic materials, characterized by two perpendicular magnetic vectors (cf. Ref. 2). Making use of this correspondence it is easy to effect a classification of all possible superconducting structures with q = 0 (cf. Ref. 2).

As an example we consider the crystalline class D_3 . The group D₃ has three irreducible representations: the identity representation A_1 (the corresponding parameters will be denoted by ψ_0 in the nonmagnetic case and by ψ'_0 and ψ''_0 for magnetic structures); the one-dimensional representation A_2 according to which the coordinate z (represented by the parameters ψ_z and ψ_z' , ψ_z'' , respectively) transforms; the twodimensional representation E, according to which the coordinates x and y transform (the parameters are ψ'_x and ψ''_y). The possible combinations of the representations are the following: $A_1: \psi_0; A_2: \psi_z; (A_1A_1): (\psi'_0, \pm \psi''_0); (A_2A_2): (\psi'_z, + \psi''_0); (A_2A_2): (A_2A_2):$ $\pm \psi_z''$; E: $(\psi_x', \pm \psi_y'')$; $(A_1 A_2)$: $(\psi_0', \pm \psi_z'')$. In the magnetic cases the notation $(\psi'_x \pm \psi''_y)$ corresponds to a twofold degeneracy produced by a violation of the $t \mapsto -t$ invariance. In this case there exist two Lifshitz invariants (6): the first

$$\psi_{x^{'}}\partial_{z}\psi_{y^{''}} *+\psi_{x^{'}} *\partial_{z}\psi_{y^{''}}-\psi_{y^{''}} *\partial_{z}\psi_{x^{'}}-\psi_{y^{''}}\partial_{z}\psi_{x^{'}} *$$

leads to an unstable E structure; the second

$$\psi_0'\partial_z\psi_z''$$
 *+ ψ_0' * $\partial_z\psi_z''-\psi_z''$ * $\partial_z\psi'-\psi_z''\partial_z\psi_0'$ *

leads to an unstable (A_1A_2) structure. Thus, the group D_3 has six structures which are admissible from the viewpoint of symmetry. However, only the following four among them are stable: $A_1, A_2, (A_1A_1), (A_2A_2)$.

The Appendix lists the results of an analogous analysis for all 32 crystal classes. In fact this "table" is constructed on the basis of the analogous "table" contained in our paper on exchange symmetry [2]. Here we have added only the twoparameter structures not taken into account in Ref. 2, structures which transform according to one one-dimensional representation (they are unstable only in polar crystals, when the identity representation is contained in the vector representation). The first number after a class symbol refers to the total number of structures which are possible from a symmetry viewpoint, the second gives the number of stable structures. The ferromagnetic structures, i.e., those for which the symmetry of the form (5) allows for a magnetization, are labeled with superscript F, whereas the antiferromagnetic ones are labeled by the superscript A. It should be kept in mind that the representations B_1 , B_2 , B_3 in the class \mathbf{D}_2 ; the representations B_{1g} , B_{2g} , B_{3g} and B_{1u} , B_{2u} , B_{3u} in the class \mathbf{D}_{2h} ; B_1 , B_2 in the classes \mathbf{C}_{2v} , \mathbf{C}_{4v} , \mathbf{D}_4 , \mathbf{D}_6 , \mathbf{C}_{6v} ; and B_{1g} , B_{2g} and B_{1u} , B_{2u} in the classes D_{4h} and D_{6h} are equivalent in the sense that they go over into each other under rotations of the coordinate axes. The replacement of these structures by one another leads to equivalent structures.

The total number of structures with q = 0 which are possible from the standpoint of symmetry is 343. Of these 276 are stable. These are the 32 structures of normal superconductivity, the other structures with nontrivial violation of gauge symmetry-58 nonmagnetic structures, 73 ferromagnetic ones, and 113 antiferromagnetic structures. The other structures with $q \neq 0$ correspond to highly degenerate, really exotic superconductors. It is clear that for Cooper pairing the restructuring of the electron spectrum in such superconductors can occur only in certain bands on the Fermi surface, so that, on the one hand all Cooper pairs should have identical total momentum q, and on the other hand, the electrons in the pairs should remain close to the Fermi sur-

We stress the fact that all the results obtained here do not depend on specific models of the structure of the superconductors; therefore the picture developed here is common for any cases of breakdown of the gauge symmetry. Thus, for example, the possibility of Bose-Einstein condensation of bound states of four (or in general, of any even number) of electrons in a metal is in principle not excluded; neither is superfluidity in the system of null defects in a quantum crystal, or superfluidity of hydrogen dissolved in a metal. In the case of superconductors with Cooper pairing further important conclusions are possible (Ref. 1) regarding the oneparticle spectrum of the electrons. The modulus of the ψ function determines the gap in the electron spectrum. The symmetry of the ψ -function might imply its vanishing at certain points or along whole lines on the Fermi surface. This in turn implies power-law dependence on the temperature in

thermodynamics (Ref. 1), in contrast to the exponential laws encountered in usual superconductors. We note that the topology of the Fermi surface can be such that the electronic states for which symmetry would dictate a vanishing gap are absent altogether. Such a superconductor would be hard to distinguish from a usual superconductor.

We also note that it is possible to describe magnetic superconductors (ψ', ψ'') , in the cases where ψ' and ψ'' transform according to one-dimensional representations, in two essentially equivalent ways. On the other hand, they can be represented as the result of coexistence of two types of superconductivity, as was done above. With the same success one could have chosen as the order parameter another pair (ψ', M) , where M is a purely magnetic characteristic which transforms like the form (5). Thus, this symmetry also corresponds to the coexistence, e. g., of an ordered state of localized spins and superconductivity of conducting electrons.

APPENDIX

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C_i. 5; 4. A_s; A_u; (A_sA_s)^F; (A_uA_u)^F. C_s. 5; 2. A'; A''.
    C_2. 5; 2. A; B.
    C_{2h}. 14; 10. A_g; B_g, A_u, B_u; (A_gA_g)^T; (B_gB_g)^P, (A_uA_u)^F, (B_uB_u)^P; (A_gB_g)^P,
        (A_uB_u)^T
  (A_uB_u)^{A_u}_{1}, (A_1A_2)^{F_1}, (B_1B_2)^{F_2}_{1}, (B_1^{A_2})^{F_3}_{1}, (B_1^{A_2})^{F_4}_{1}, (B_1^{A_2})^{F_4}_{1}, (B_1^{A_2})^{F_4}_{1}, (B_1^{A_2})^{A_2}_{1}, (B_1^{A_2})^{A_3}_{1}, (B_1^{A_2})^{A_4}_{1}, (B_1^{A_2}
    \mathbf{D}_{2d}, 15; 13. A_1, A_2, B_1, B_2; (E)^F; (A_1A_1)^A; (A_2A_2)^A, (B_1B_1)^A, (B_2B_2)^A; (A_1A_2)^F, (A_1B_1)^A, (A_2B_2)^A, (B_1B_2)^F.
      C_4. 6; 3. A; B; (AB)^A.
C4. 6; 3. A; B; (AB)^{A}.
C4. 16; 14. A_{g}; B_{g}, A_{u}, B_{u}; (E_{g})^{F}, (E_{u})^{F}; (A_{g}A_{g})^{F};
(B_{g}B_{g})^{F}, (A_{u}A_{u})^{F}, (B_{u}B_{u})^{F}; (A_{g}B_{g})^{A}, (A_{u}B_{u})^{A}, (A_{g}B_{u})^{A}, (B_{g}A_{u})^{A}.
C4. 11; 8. A_{1}; A_{2}, B_{1}; (A_{1}A_{1})^{F}; (A_{1}A_{2})^{F}; (A_{1}B_{1})^{A}; (A_{2}B_{1})^{A}, (B_{1}B_{2})^{F}.
D4. 11; 8. A_{1}; A_{2}, B_{1}; (A_{1}A_{1})^{A}; (A_{2}A_{2})^{A}, (B_{1}B_{1})^{A}; (A_{1}B_{1})^{A}, (A_{2}B_{1})^{A}.
D4. 23; 29. A_{1g}; A_{2g}, B_{1g}, A_{1u}, A_{2u}, B_{1u}; (E_{g})^{F}, (E_{u})^{F}; (A_{1g}A_{1g})^{A}; (A_{2g}A_{2g})^{A}, (B_{1g}B_{1g})^{A}, (A_{1u}A_{1u})^{A}, (A_{2u}A_{2u})^{A}, (B_{1u}B_{1u})^{A}; (A_{1g}A_{2g})^{F}, (A_{1g}A_{1g})^{A}, (A_{2g}B_{1g})^{A}, (B_{1g}B_{2g})^{F}, (A_{1u}A_{2u})^{F}, (A_{1u}B_{1u})^{A}, (A_{2u}B_{1u})^{A}, (B_{1u}B_{2u})^{F}, (A_{1g}A_{1u})^{A}, (A_{1g}B_{1u})^{A}, (A_{2g}A_{2u})^{A}, (A_{2g}B_{1u})^{A}, (B_{1g}A_{2u})^{A}, (B_{1g}B_{2u})^{A}, (B_{1g}B_{1u})^{A}.
C... 3: 1. A.
C<sub>3</sub>. 3; 1. \dot{A}.
S<sub>4</sub>. 7; 6. \dot{A}_{g}; \dot{A}_{u}; (E_{g})^{F}, (E_{u})^{F}; (A_{g}A_{g})^{F}; (A_{u}A_{u})^{F}.
C<sub>3v</sub>. 6; 4. \dot{A}_{1}; \dot{A}_{2}; (\dot{B})^{F}; (\dot{A}_{1}A_{2})^{F}.
D<sub>3</sub>. 6; 4. \dot{A}_{1}; \dot{A}_{2}; (\dot{A}_{1}A_{1})^{A}; (\dot{A}_{2}A_{2})^{A}.
D<sub>3d</sub>. 16; 14. \dot{A}_{1g}; \dot{A}_{2g}, \dot{A}_{1u}, \dot{A}_{2u}; (\dot{E}_{g})^{F}, (E_{u})^{F}; (\dot{A}_{1u}A_{2u})^{F}, (\dot{A}_{1u}A_{2u})^{A}, (\dot{A}_{2u}A_{2u})^{A}; (\dot{A}_{2u}A_{2u})^{A}; (\dot{A}_{1u}A_{2u})^{F}, (\dot{A}_{1u}A_{2u})^{F}, (\dot{A}_{1u}A_{2u})^{A}, (\dot{A}_{2u}A_{2u})^{A}.
D<sub>3h</sub>. 16; 14. \dot{A}_{1}; \dot{A}_{2}, \dot{A}_{1}, \dot{A}_{2}, \dot{A}_{1}, \dot{A}_{2}, \dot{A}_{1}, \dot{A}_{2}, \dot{A}_{2
        C<sub>3</sub>. 3; 1. A.
    \begin{array}{l} \textbf{C}_{6v}. \ 12; \ 9. \ A_{1}; \ A_{2}, \ B_{1}; \ (E_{2})^{F}, \ (E_{1})^{F}; \ (A_{1}A_{2})^{F}, \ (A_{1}B_{1})^{A}, \ (A_{2}B_{1})^{A}, \ (B_{2}B_{1})^{F}. \\ \textbf{D}_{6}. \ 12; \ 8. \ A_{1}; \ A_{2}, \ B_{1}; \ (A_{1}A_{1})^{A}; \ (A_{2}A_{2})^{A}, \ (B_{1}B_{1})^{A}; \ (A_{1}B_{1})^{A}, \ (A_{2}B_{1})^{A}. \\ \textbf{D}_{8h}. \ 34; \ 31. \ A_{18}; \ A_{2g}, \ B_{1g}, \ A_{1u}, \ A_{2u}, \ B_{1u}; \ (E_{1g})^{F}, \ (E_{2g})^{F}, \ (E_{1u})^{F}, \ (E_{2u})^{F}; \end{array}
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