Spontaneous breaking of rotational symmetry in superconductors†

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We show that homogeneous superconductors with broken spin/isospin symmetry lower their energy via a transition to a novel superconducting state where the Fermi-surfaces are deformed to a quasi-ellipsoidal form at zero total momentum of Cooper pairs. In this state, the gain in the condensation energy of the pairs dominates over the loss in the kinetic energy caused by the lowest order (quadrupole) deformation of Fermi-surfaces from the spherically symmetric form. There are two energy minima in general, corresponding to the deformations of the Fermi-spheres into either prolate or oblate forms. The phase transition from spherically symmetric state to the superconducting state with broken rotational symmetry is of the first order.

In the original Bardeen-Cooper-Schrieffer (BCS) theory of bulk superconductivity, the condensate wavefunction describes a quantum coherent state which is invariant under spatial and time (particle-hole) reversal transformations.\textsuperscript{1} External perturbations which act on discrete quantum variables, like the spin of the fermions, break the particle-hole symmetry. A typical example is a metallic superconductor in a high magnetic field where the Pauli paramagnetism induces an asymmetry in the populations of the spin-up and spin-down electrons. The superconducting state is quenched via a first order phase transition once the splitting in the energy spectrum of spin-up and spin-down electrons becomes of the order of the pairing gap in the unpolarized state.\textsuperscript{2} The crossover from the BCS to the normal state can be understood in terms of the phase-space overlap between the fermionic states located at the top of their individual Fermi-surfaces. The pairing gap is maximal for the symmetric (unpolarized) state with perfectly overlapping Fermi-surfaces. As these are driven apart by the “polarizing field” the phase-space available for the pairing decreases and the gap is successively suppressed. At finite temperatures the smearing of the Fermi-surfaces increases the phase-space overlap and hence the critical field at which the superconductivity is quenched.

The superconducting state sustains larger asymmetries if the translational symmetry is broken. Larkin and Ovchinnikov and Fulde and Ferrell (LOFF) argued that the crossover from the BCS to the normal state, as the Fermi-surfaces are driven apart by the polarizing field, occurs via a spatially inhomogeneous superconducting phase.\textsuperscript{3, 4} The Cooper pairs carry a finite total momentum in the LOFF phase, i.e., the centers of the Fermi-spheres are shifted allowing for a partial phase-space overlap.

This paper suggests an alternative mechanism of breaking the symmetry which is based on a deformation of the spherical Fermi-surfaces, to the lowest order, into quasi-ellipsoidal form. If the total momentum of the Cooper pairs is zero, as we shall assume in the following, the deformation spontaneously breaks the rotational symmetry. The novel superconducting phase maintains its stability due to the dominance of the condensation energy of the Cooper pairs over the loss in the kinetic energy of the system caused by the deformation of the Fermi-surfaces. We shall assume that there is a single axis along which the symmetry is broken, although more complicated patterns of symmetry breaking are possible (simultaneous breaking of the rotational and translational symmetries, higher order multipole deformations of Fermi-surfaces, etc). Note that deformed or non-spherical Fermi-surfaces are common for electrons in solids; here we treat systems which are homogeneous in the normal state, i.e., any deformations of the spherical shape of the Fermi-surfaces would correspond to a metastable state.

We start with the BCS-Gorkov equations in energy-momentum representation

\[
\sum_{\gamma} \left( \begin{array}{cc} \omega - E_{\alpha\gamma} & -\Delta_{\alpha\gamma} \\ -\Delta_{\alpha\gamma}^\dagger & \omega + E_{\alpha\gamma} \end{array} \right) \left( \begin{array}{c} G_{\gamma\beta}^\dagger \\ F_{\gamma\beta}^\dagger \end{array} \right) = \delta_{\alpha\beta} \mathbf{i}, \quad (1)
\]

where \(G_{\gamma\beta}(\omega, p)\) and \(F_{\gamma\beta}(\omega, p)\) refer to the full normal and anomalous retarded propagators, \(\Delta_{\alpha\gamma}(\omega, p)\) is the anomalous self-energy, and the diagonal matrix elements of the first matrix correspond to the inverse of free-single particle propagators; the Greek indices \(\alpha, \beta \ldots = 1, 2\) label the two different species, and \(\omega\) and \(p\) refer to the particle energy and momentum. (Note that the center-of-mass momentum of particles is zero). Suppose that the rotational symmetry is broken by a deformation of the Fermi-surfaces from spherical form. The quasiparticle spectrum of species \(\alpha\) can be parameterized, then, as

\[
E_\alpha = \frac{p^2}{2m_\alpha} - \mu_\alpha \left( 1 - \epsilon_\alpha \cos^2 \theta \right), \quad (2)
\]

where \(\mu_\alpha\) are the chemical potentials of the particles in the undeformed state, \(\theta\) is the angle between the particle momentum \(p\) and the axis of symmetry breaking; the deformation of the Fermi-sphere in Eq. is truncated at the lowest order non-trivial axisymmetric deformation, which is described by the \(l = 2, m = 0\) term of the Legendre polynomials associated with an expansion in spherical harmonics. The constant energy surfaces of quasiparticle

*Phys. Rev. Lett. 88, 252503 (2002)
excitations defined by Eq. (2) represent quasi-ellipsoids of revolution with an ellipticity \(\epsilon_0\). For \(\epsilon_0 = 0\) the spectrum (2) is the true eigenstate of the unpaired, homogeneous system in the absence of external fields. (Note that the deformation described by Eq. (2) does not need to conserve the volume of the Fermi-sphere, as we impose a self-consistency condition for the total density of the system, see Eq. (3) below).

In the following we shall neglect the possible pairing among the same species (\(\Delta_{\alpha \alpha} = 0\)) so that only the off-diagonal elements of the anomalous self-energy matrix are non-zero. The quasiparticle excitation spectrum in the superconducting phase is determined in the standard fashion by finding the poles of the propagators in Eq. (1):

\[ \omega_{1,2} = E_A \pm \sqrt{E_S^2 + |\Delta|^2}, \]  

(3)

where the symmetric and anti-symmetric parts of the spectrum (which are even and odd with respect to the time-reversal symmetry) are defined as \(E_{S,A} = (E_1 \pm E_2)/2\). The solution of Eq. (1) can be written in terms of the eigenstates (3) as

\[ G_{1,2} = \frac{v_p}{\omega - \omega_{1,2} + i\eta} + \frac{v_p}{\omega - \omega_{2,1} + i\eta}, \]  

(4)

\[ F = u_p v_p \left( \frac{1}{\omega - \omega_1 + i\eta} - \frac{1}{\omega - \omega_2 + i\eta} \right), \]  

(5)

where the Bogolyubov amplitudes are

\[ u_p^2 = \frac{1}{2} + \frac{E_S}{2\sqrt{E_S^2 + |\Delta|^2}}, \quad v_p^2 = \frac{1}{2} - \frac{E_S}{2\sqrt{E_S^2 + |\Delta|^2}}. \]  

(6)

The mean-field approximation to the anomalous self-energy yields the gap equation

\[ \Delta(p) = 2 \int \frac{d\omega' dp'}{(2\pi)^3} V(p, p') \text{Im} F(\omega', p') f(\omega'), \]  

(7)

where \(V(p, p')\) is the bare interaction \[17\], \(f(\omega) = [\exp(i\omega\beta) + 1]^{-1}\) is the Fermi distribution function and \(\beta\) is the inverse temperature. The \(\omega\) integration is straightforward in the quasiparticle approximation, since the frequency dependence of the propagator is constrained by the on-shell condition. For \(S\)-wave interactions the potential depends only on the absolute magnitude of the quasiparticle momenta. In this case the gap equation simplifies to

\[ \Delta(p) = \int \frac{dp'}{(2\pi)^2} V(p, p') \int d\cos \theta' \frac{\Delta(p')}{2\sqrt{E_S^2 + \Delta(p')^2}} [f(\omega_1) - f(\omega_2)]. \]  

(8)

Note that the deformation of the Fermi-surfaces enters the gap equation as a parameter which is determined by the minimum of the ground state energy of the superconducting phase. For strongly coupled superconductors the gap equation (8) is supplemented by the normalization condition for the net density \(\rho \equiv \rho_1 + \rho_2\) at a constant temperature. The densities of the species are given by

\[ \rho_{1,2} = -2 \sum \int \frac{dp}{(2\pi)^3} \text{Im} G_{1,2}(\omega, p) f(\omega) \]  

\[ = \sum \int \frac{dp}{(2\pi)^3} \left\{ v_p^2 f(\omega_{1,2}) + v_p^2 f(\omega_{2,1}) \right\}, \]  

(9)

where the summation is over the discrete quantum variables. The second equality follows in the quasiparticle approximation.

Next we turn to the thermodynamic properties of the superconducting state. At a fixed density and temperature the relevant thermodynamic potential is the free energy:

\[ F_{\rho,\beta} = U - \beta^{-1} S, \]  

(10)

where \(U\) is the internal energy and \(S\) is the entropy. In the mean-field approximation the entropy is given by the expression

\[ S = -k_B \sum \int \frac{d^3p}{(2\pi)^3} \left\{ f(\omega_1) \ln f(\omega_1) + f(\omega_1) \ln \tilde{f}(\omega_1) ight\} \]  

\[ + f(\omega_2) \ln f(\omega_2) + \tilde{f}(\omega_2) \ln \tilde{f}(\omega_2) \}, \]  

(11)

where \(\tilde{f}(\omega_\pm) = [1 - f(\omega_\pm)], k_B\) is the Boltzmann constant. The internal energy, defined as the grand canonical statistical average of the Hamiltonian, is

\[ U = \sum \int \frac{d^3p}{(2\pi)^3} \left\{ n_1(p) E_1(p) + n_2(p) E_2(p) \right\} \]  

\[ + \int \frac{d^3p'}{(2\pi)^3} V(p, p') \nu(p) \nu(p') \right\}, \]  

(12)

where

\[ n_{1,2}(p) = v_p^2 f(\omega_{1,2}) + v_p^2 f(\omega_{2,1}), \]  

(13)

\[ \nu(p) = u_p v_p [f(\omega_1) - f(\omega_2)]. \]  

(14)

The first term in Eq. (12) is the kinetic energy while the second term includes the mean field interaction among the particles in the condensate. The true ground state of the system minimizes the free energy difference \(\delta F_{\rho,\beta}\) between the superconducting and normal states (the free energy in the normal state follows from Eqs. (11) and (12) when \(\Delta = 0\)).

The deformations of the Fermi-spheres can be described in terms of the “conformal deformation” \(\epsilon = (\epsilon_1 + \epsilon_2)/2\) and the “relative deformation” \(\delta\epsilon = (\epsilon_1 - \epsilon_2)/2\). Then, the symmetric and anti-symmetric parts of the energy spectrum can be written as

\[ E_S \equiv \frac{p^2}{2m} - \mu \left[ 1 + \epsilon \cos^2 \theta \left( 1 + \frac{\delta \epsilon \delta \mu}{\epsilon \mu} \right) \right], \]  

(15)

\[ E_A \equiv -\delta \mu + (\mu \epsilon \epsilon + \epsilon \delta \mu) \cos^2 \theta, \]  

(16)
where \( \mu = (\mu_1 + \mu_2)/2, \delta \mu = (\mu_1 - \mu_2)/2 \) (here we ignore the difference in the masses of the spin/isospin up and down quasi-particles). Equations 3, 4 and 10 form a closed system, which determines the pairing gap and the ground state energy of a superconductor for constant density asymmetry \( \alpha = (\rho_1 - \rho_2)/(|\rho_1| + |\rho_2|) \). The values of the deformation parameters \( \delta \epsilon \) and \( \epsilon \) are obtained by requiring that the free-energy attains its minimum. Note that in the weak coupling limit Eqs. 3 and 10 decouple and one may solve for \( \Delta \) as a function of \( \delta \mu \) instead of \( \alpha \). Apart from the fact that \( \alpha \), rather than \( \delta \mu \), is the measurable quantity, there is an additional reason for solving the full set of equations. The gap equation alone is symmetric under exchange \( E_A \rightarrow -E_A \), which implies that the solutions are symmetric under the simultaneous change of the signs of \( \delta \mu \) and \( \delta \epsilon \). Eq. 9, however, does not have this symmetry and the solutions are distinct under the sign transformation above.

As a specific example, which illustrates the solutions above, we consider isospin-singlet (neutron-proton) pairing in nuclear matter in the \( ^3S_1 - ^3D_1 \) channel 3, 4, 5. The gap in the isospin symmetric case is \( \Delta_{00} = 12 \text{ MeV} \) if we use as the bare interaction the Argonne potential and ignore the renormalization of the mass of the particles in the normal state due to interactions. The modification of the particle self-energy in nuclear medium (see for a review 3) affect the absolute magnitude of the gap and rescale its dependence on the parameters. Clearly, with these approximations, our model is schematic, however we do not expect qualitative changes when renormalization of the interaction and the bare mass are included.

The BCS solutions for the \( n-p \) pairing has been studied for the homogeneous (translationally and rotationally) invariant state under isospin asymmetric conditions 6, and 11, and the inhomogeneous state with broken translational symmetry 13 (the nuclear analogy of the LOFF phase. (The flavor asymmetric \( < q q > \) condensate in high density QCD is another example of strongly coupled superconductor where the breaking of translational symmetry plays a role 14). Consistent with the assumption \( \Delta_{00} = 0 \) above we ignore the \( n-p \) pairing in the \( ^1S_0 \) channel 15.

Fig. 1 shows the pairing gap as a function of the density asymmetry \( \alpha \) and the relative deformation \( \delta \epsilon \). The gap is normalized to its value for \( \delta \alpha = 0 = \delta \epsilon \).

![FIG. 1: The pairing gap as a function of the density asymmetry \( \alpha \) and the relative deformation \( \delta \epsilon \). The gap is normalized to its value for \( \delta \alpha = 0 = \delta \epsilon \).](image1)

The concentric circles correspond to the two populations of spin/isospin-up and down fermions in spherically symmetric state (\( \delta \epsilon = 0 \)), while the deformed figures correspond to the state with relative deformation \( \delta \epsilon = 0.64 \). The density asymmetry is \( \alpha = 0.35 \).

![FIG. 2: A projection of the Fermi-surfaces on a plane parallel to the axis of the symmetry breaking. The concentric circles correspond to the two populations of spin/isospin-up and down fermions in spherically symmetric state (\( \delta \epsilon = 0 \)), while the deformed figures correspond to the state with relative deformation \( \delta \epsilon = 0.64 \). The density asymmetry is \( \alpha = 0.35 \).](image2)

Solutions for the gap equation show the following features. For arbitrary constant \( \delta \epsilon \) the gap is maximal at \( \alpha = 0 \) and is suppressed as the asymmetry is increased. For constant \( \alpha \), \( \partial \Delta / \partial \delta \epsilon = 0 \) corresponds to a maximum at \( \delta \epsilon \neq 0 \) in the large \( \alpha \) limit. The position of the maximum is independent of \( \alpha \) and is located around \( \delta \epsilon = 0.5 \) in our model; this value also corresponds to the critical asymmetry \( \alpha_c \) at which the superconducting state vanishes. Note that for \( \alpha \) around \( \alpha_c \) the gap exists only in the de-
formed state. For $\alpha = 0$, Eqs. (8)-(10) are symmetric under exchange of the sign of deformation and so is the gap function. In particular, for $\alpha = 0$, the critical deformation for positive and negative deformations coincide. For finite $\alpha$ the dependence of the gap on the relative deformation depends on the sign of $\delta \epsilon$. In contrast to the positive range of $\delta \epsilon$, where the maximum value of the gap is attained at constant $\delta \epsilon$, for negative $\delta \epsilon$ the maximum increases as a function of the deformation and saturates around $\delta \epsilon \simeq 1$. Quite generally, to maintain the maximal phase space overlap, the system prefers to keep the sign of $\delta \mu$ opposite to that of $\delta \epsilon$. Fig. 2 shows a 2-dimensional projection of a configuration of deformed Fermi-surfaces for $\delta \epsilon = 0.64$ which minimizes the free-energy for fixed $\alpha = 0.35$.

The difference in the free-energies of the superconducting and normal states $\delta F$ as a function of the density asymmetry $\alpha$ and the relative deformation $\delta \epsilon$. The free-energy is normalized to its value for $\delta \alpha = \delta \epsilon = 0$.

The difference in the free-energies of the superconducting and normal states $\delta F$ is shown in Fig. 3. Owing to the symmetries of the underlying equations, $\delta F$ is symmetric with respect to the sign change of $\delta \epsilon$ when $\alpha = 0$. For finite $\alpha$‘s, a minor departure from the rotational invariant state leads to a decrease in $\delta F$ which develops two minima for either sign of $\delta \epsilon$. This behavior can be traced back to the increase of the potential energy with increasing gap (cf. Fig. 1). Note that, although there are non-trivial solutions to the gap equation in the large $\alpha$ limit for $\delta \epsilon \rightarrow -1$, these solutions do not lower the energy of the system. The superconducting phase becomes unstable for $\alpha > 0.4$ due to the increase in the kinetic energy caused by the large deformation of the Fermi-surfaces, so that $\delta F$ is a nearly even function of $\delta \epsilon$. An inspection of the latent heat associated with the phase transition at finite temperatures shows that this quantity does not vanish at the crossover from the spherically symmetric to the deformed superconducting state. Consequently, the phase transition associated with the breaking of the rotational symmetry is of the first order.

To summarize, this paper suggests a novel mechanism of symmetry breaking in superconducting system with particle-hole asymmetry. The lowest order (quadrupole) deformation of the Fermi-surfaces (at zero total momentum of the Cooper pairs) increases the phase-space overlap between the Fermi-surfaces of paired quasiparticles, which is otherwise depleted by the asymmetry in the particle/hole populations. As a result, the free-energy develops minima for finite deformations, since the gain in the (negative) pairing potential energy dominates the increase in the kinetic energy caused by the deformation. Since the deformed ground state spontaneously breaks the rotational symmetry, the dynamic properties of the superconducting state with deformed Fermi-surfaces such as the sound attenuation, the infrared absorption or the Meissner effect will be anisotropic. The results above do not depend on the nature of fields inducing the asymmetry in the fermion populations nor on the nature of the pairing forces and should be applicable to a wide range of fermionic systems.

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