

Energy Gap Induced by Impurity Scattering: New Phase Transition in Anisotropic Superconductors

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It is shown that layered superconductors are subjected to a phase transition at zero temperature provided the order parameter reverses its sign on the Fermi surface but its angular average is finite. The transition is regulated by an elastic impurity scattering rate $1/\tau$. The excitation energy spectrum, being gapless at the low level of scattering, develops a gap as soon as the scattering rate exceeds some critical value of $1/\tau_*$.

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It has been shown recently that nonmagnetic impurities may destroy the d -wave superconductivity in the same manner as magnetic impurities do it in the s -wave conventional superconductors [1–3]. However, this pure d -wave scenario is not supported by the existent experimental data, at least in YBaCuO samples, subjected to radiation damage or doping [4]. One might anticipate that T_c should drop abruptly above a certain critical concentration of the defects. Instead, the critical temperature has been found just to decrease gradually in the whole range of a residual resistivity variation. The above discrepancy has been considered as a compelling counterargument against the whole idea of exotic pairing in this compound. However, in this Letter we make the case that the above-mentioned experimental results do not, in fact, contradict the alleged nontrivial structure of the order parameter (OP), provided the latter is determined by the symmetry of the crystal and, hence, deviates from the exact d -wave form. In this situation, as will be demonstrated below, an initially gapless excitation spectrum of a clean superconductor may acquire a gap due to a scattering of electrons by nonmagnetic impurities. An elastic scattering gives rise to this paradoxical effect, once the OP in the clean material possesses the nodes on the Fermi surface, whereas its angular average still does not vanish, and the scattering rate exceeds some critical value.

The results of recent Josephson tunneling experiments [5] and the measurement of critical temperature versus residual resistivity variation [4] may be interpreted as an evidence in favor of this very structure of the OP. Indeed, the Josephson tunneling data in the corner geometry imply the sign reversal of the OP on the Fermi surface. On the other hand, as already mentioned, the growth of the residual resistivity is accompanied by a slow decrease of critical temperature. This type of behavior rules out the nullification of the OP averaged over the Fermi surface as we shall show later.

It should be noted that recent measurements of a Josephson current in the c direction by Sun *et al.* [6] do

not conform easily with the phase alternating OP. The values of the net current found in this experiment for the heavily twinned samples in plain geometry are several orders of magnitude higher than theoretically estimated. The interpretation of these results may prove to be a subtle matter, however. A possible source of the finite Josephson current could be a symmetry violation caused by surface defects and the surface itself together with the phase self-adjustment. For other plausible scenarios on this effect see Ref. [7]. For now we assume that the OP sign reversal, as well as the nonzero value of $\langle \Delta \rangle$, is reliably established in the experiments cited above [4,5].

We analyze the problem in the framework of the anisotropic BCS model. The OP is determined by the self-consistency equation

$$\Delta(\phi) = T \sum_n \int V(\phi, \phi') \frac{\tilde{\Delta}_n(\phi')}{\sqrt{\tilde{\eta}_n^2 + \tilde{\Delta}_n^2(\phi')}} \frac{d\phi'}{2\pi}. \quad (1)$$

Here the summation goes over the Matsubara imaginary frequencies, whereas the integration is restricted to the Fermi surface, which is presumed to be a cylinder. The kernel $V(\phi, \phi')$ describes the interaction of electrons on the Fermi surface. The renormalized Matsubara frequency $\tilde{\eta}_n$ and the frequency-dependent OP $\tilde{\Delta}_n(\phi)$ are related to the corresponding bare quantities $\eta_n = (2n + 1)\pi T$ and $\Delta(\phi)$ via the Abrikosov-Gor'kov (AG) equations

$$\tilde{\eta}_n - \frac{\tilde{\eta}_n}{\tau} \langle [\tilde{\eta}_n^2 + \tilde{\Delta}_n(\phi)^2]^{-1/2} \rangle = \eta_n, \quad (2)$$

$$\tilde{\Delta}_n(\phi) - \frac{1}{\tau} \langle \tilde{\Delta}_n(\phi) [\tilde{\eta}_n^2 + \tilde{\Delta}_n(\phi)^2]^{-1/2} \rangle = \Delta(\phi). \quad (3)$$

The angular brackets in the AG equations denote the angular average. For the sake of simplicity we consider isotropic scattering only. For the same reason we have disregarded any dependence of the OP and the electronic interaction potential on the c component of momentum.

Let us first examine the behavior of the critical temperature with respect to the variation of the scattering rate. In

the vicinity of critical line Eqs. (1)–(3) may be linearized and the infinitesimal order parameter may be eliminated. The result reads

$$1 = g(T, \tau) \langle [1 - f(T, \tau) \hat{V}]^{-1} \bar{V}(\phi) \rangle. \quad (4)$$

Here we defined a linear operator \hat{V} related to the electronic interaction kernel

$$\hat{V} \psi(\phi) = \int V(\phi, \phi') \psi(\phi') \frac{d\phi'}{2\pi}. \quad (5)$$

This operator maps 1 onto the function $\bar{V}(\phi)$

$$\bar{V}(\phi) = \int V(\phi, \phi') \frac{d\phi'}{2\pi}. \quad (6)$$

The functions $f(T, \tau)$ and $g(T, \tau)$ in Eq. (4) are defined by the following expressions:

$$f(T, \tau) = T \sum_n \frac{1}{|\eta_n| + 1/\tau}, \quad (7)$$

$$g(T, \tau) = T \sum_n \frac{1}{|\eta_n| (1 + |\eta_n| \tau)}. \quad (8)$$

The summation in the expression for $f(T, \tau)$ is limited by an ultraviolet cutoff, $\eta_n < \bar{\epsilon}$. The latter is related to the critical temperature T_{c0} of the clean superconductor as follows:

$$T_{c0} = (2\gamma \bar{\epsilon} / \pi) \exp(-\pi / V_0), \quad (9)$$

where V_0 is the maximal eigenvalue of the operator \hat{V} and γ is a logarithm of the Euler constant. In the dirty limit ($T_{c0} \ll 1/\tau$) the approximate solution of Eq. (4) reads

$$T_c = (2\gamma \bar{\epsilon} / \pi) \exp(-\pi / \langle \bar{V} \rangle) (\bar{\epsilon} \tau)^{\kappa-1}, \quad (10)$$

where $\kappa = \langle \bar{V}^2 \rangle / \langle \bar{V} \rangle^2$. Within the same approximation $\Delta(\phi) \propto \bar{V}(\phi)$. Hence, the exponent κ may be expressed in terms of the OP: $\kappa = \langle \Delta^2 \rangle / \langle \Delta \rangle^2$. The power law (10) has been derived by Hohenberg [8] under the assumption of a weak anisotropy. We have found that it is the high scattering level that really matters. Notice that the exponent κ becomes infinite when $\langle \Delta \rangle \rightarrow 0$. A more scrupulous analysis [1–3] shows that if $\langle \Delta \rangle = 0$, the critical temperature vanishes at some finite scattering rate proportional to the critical temperature of the clean superconductor, $1/\tau_c = 2\gamma T_{c0} / \pi$.

Equation (10) might be interpreted directly as the relation between the critical temperature and the residual resistivity, $T_c(\rho) \propto \rho^{1-\kappa}$, provided that the effective number of carriers does not depend substantially on the concentration of defects.

Let us study Eqs. (1)–(3) at a temperature equal to zero. In this case the summation in Eq. (1) should be replaced by integration over the continuous variable η , and the domain of functions $\tilde{\eta}(\eta)$ and $\tilde{\Delta}(\phi, \eta)$ extends into the whole positive half axis of the same variable. We are interested in the behavior of the above functions at $\eta \rightarrow 0$. The values $\tilde{\eta}(0)$ and $\tilde{\Delta}(\phi, 0)$ determine the density of states (DOS) on the Fermi surface, vanishing if $\tilde{\eta}(0) = 0$.

We are going to prove the following three statements concerning the DOS on the Fermi surface: (1) Let

$\langle \Delta(\phi) \rangle \neq 0$ and $\Delta(\phi)$ does not change its sign on the Fermi surface. Then $\tilde{\eta}(0) = 0$ for any τ . (2) Let $\langle \Delta(\phi) \rangle = 0$. Then $\tilde{\eta}(0) > 0$ for any $1/\tau \geq 1/\tau_c = 2\gamma T_{c0} / \pi$. (3) Let $\langle \Delta(\phi) \rangle \neq 0$ but $\Delta(\phi)$ is a sign alternating function of the angle ϕ . Then $\tilde{\eta}(0) = 0$ for $1/\tau > 1/\tau_*$ but $\tilde{\eta}(0) > 0$ for $1/\tau < 1/\tau_*$. The equation for τ_* as a functional of $\Delta(\phi)$ will be derived below.

Before proceeding to the proof let us remark that according to Eq. (2) the following separation of variables takes place:

$$\tilde{\Delta}(\phi, \eta) = \Delta(\phi) + \sigma(\eta), \quad (11)$$

and the AG equations may be rewritten in terms of the function $\sigma(\eta)$ just defined:

$$\frac{\eta}{\tilde{\eta}(\eta)} = 1 - \frac{1}{\tau} \langle [\Delta(\phi) + \sigma(\eta)]^2 + \tilde{\eta}(\eta)^2 \rangle^{-1/2}, \quad (12)$$

$$\sigma(\eta) \frac{\eta}{\tilde{\eta}(\eta)} = \frac{1}{\tau} \langle \Delta(\phi) [\Delta(\phi) + \sigma(\eta)]^2 + \tilde{\eta}(\eta)^2 \rangle^{-1/2}. \quad (13)$$

The first proposition stems from Eqs. (12) and (13) straightforwardly. Indeed, let $\tilde{\eta}(0) \neq 0$, then the average (denoted by angular brackets) on the right-hand side (rhs) of Eq. (13) must vanish at $\eta = 0$. The latter is impossible, however, if $\Delta(\phi)$ does not reverse its sign. Hence, even if $\Delta(\phi)$ has nodes but is non-negative in the whole domain $0 \leq \phi < 2\pi$ (the case studied in [3]) $\tilde{\eta}(0) = 0$.

Let us skip the second statement for a moment and consider the case when the OP in a clean superconductor does reverse its sign but its angular average is finite.

We study, first, the limit of small impurity concentration [$\langle \Delta(\phi) \rangle \gg 1/\tau$]. Substituting the ratio $\eta / \tilde{\eta}(\eta)$ from Eq. (12) into Eq. (13) and then collecting terms proportional to $1/\tau$ in the latter one can find out that $\sigma = O(1/\tau)$. In other words, renormalization of the OP is small. In particular, its nodes remain almost at their original locations. However, renormalization of frequency is not small due to the logarithmic divergence of the term, proportional to $1/\tau$ in the rhs of Eq. (12) at $\tilde{\eta}(\eta) = 0$. A closer examination of the function $\eta / \tilde{\eta}(\eta)$ [inverse to $\tilde{\eta}(\eta)$], which can be extracted from Eq. (12), shows that it departs from the coordinate origin with an infinite negative derivative and, after reaching its minimum, crosses the abscissa axis at $\tilde{\eta}_0 = \Delta'_L \exp(-\tau \Delta'_L / 2)$. Here

$$1/\Delta'_L = 1/|\Delta'_1| + 1/|\Delta'_2|,$$

$$\ln \Delta'_L = \frac{|\Delta'_1| \ln |\Delta'_1| + |\Delta'_2| \ln |\Delta'_2|}{|\Delta'_1| + |\Delta'_2|},$$

and $\Delta'_{1,2}$ denote the derivatives of the order parameter at its nodes. Among the two roots, only $\tilde{\eta}_0$ resides on the physical sheet [9]. The first part of the statement (3) is proved.

In the opposite, dirty, limit ($1/\tau \gg T_{c0}$) the asymptotic solution of Eqs. (12) and (13) reads

$$\tilde{\eta}(\eta) = \eta \left\{ 1 + \frac{1}{\tau} [\langle \Delta(\phi) \rangle^2 + \eta^2]^{-1/2} \right\}, \quad (14)$$

$$\sigma(\eta) = \frac{1}{\tau} \langle \Delta(\phi) \rangle [\langle \Delta(\phi) \rangle^2 + \eta^2]^{-1/2}. \quad (15)$$

Plugging this solution into Eq. (1) at $T = 0$ we derive the following quasilinear equation [12]:

$$\pi \Delta(\phi) = \ln(\tau \bar{\epsilon}) \hat{V} \Delta(\phi) - \ln(\tau \langle \Delta \rangle) \bar{V}(\phi) \langle \Delta \rangle. \quad (16)$$

Assuming that $V_0 \ln(\tau \bar{\epsilon}) \ll 1$, where V_0 is the maximal eigenvalue of the operator \hat{V} , as previously, its solution can be found explicitly:

$$\Delta(\phi) = \langle \Delta \rangle \frac{\bar{V}(\phi)}{\langle \bar{V} \rangle}, \quad \langle \Delta \rangle = \frac{2}{\tau} (\tau \bar{\epsilon})^\kappa \exp(-\pi / \langle \bar{V} \rangle). \quad (17)$$

From Eqs. (14) and (15) it follows that $\tilde{\eta}(0) = 0$ and $\sigma(0) = 1/\tau \gg \Delta$. Since the renormalized OP $\tilde{\Delta}(\phi)$ does not have any nodes, no divergence can arise in Eq. (12). In this way a self-consistency of the obtained solution is guaranteed.

Summarizing, $\tilde{\eta}(0) \neq 0$ in a clean superconductor, and it vanishes when a scattering rate substantially exceeds T_{c0} . Hence, there should exist some special value of $\tau = \tau_*$ at which $\tilde{\eta}(0)$ first turns into zero. Since $\sigma(0)|_{\tau=\tau_*} = 1/\tau_*$, the value of τ_* can be found as a functional of $\Delta(\phi)$ by means of the following equation:

$$\langle \Delta(\phi) \rangle / [\langle \Delta(\phi) \rangle + 1/\tau_*] = 0. \quad (18)$$

The above equation should be supplemented by the self-consistency and the AG equations (1), (12), and (13) with $\tau = \tau_*$. Using this ansatz one can find τ_* , at least in principle, as a functional of the OP in a clean superconductor.

To get more visible results we consider a limiting case $\langle \bar{V} \rangle^2 \ll \langle \bar{V}^2 \rangle$. If this strong inequality is satisfied, the average OP should be small compared to the amplitude of its variation, and one can expect that the dependence $T_c(\tau)$ is close to that for $\langle \Delta \rangle = 0$. It means that $T_c(\tau)$ reaches almost zero value as $\tau \rightarrow \tau_c$, but then has a powerlike tail: $T_c(\tau) \sim \tau^{\kappa-1}$ with $\kappa \gg 1$. Since the point τ_* separates the domain of τ with the d -like behavior from that of the s -like one, it is natural to conjecture that τ_* is close to τ_c . A direct calculation justifies this guess. Indeed, let $1/\tau_* \gg \sqrt{\langle \Delta^2 \rangle} \gg \langle \Delta \rangle$, then Eq. (18) yields

$$\tau_* = \langle \Delta \rangle / \langle \Delta^2 \rangle. \quad (19)$$

Plugging the solution of Eq. (16) into the expression for $\langle \Delta^2 \rangle$ of the above relation one gets

$$\tau_* \langle \Delta \rangle \left(\frac{1}{\pi} \ln(\tau_* \langle \Delta \rangle) \right)^2 \times \left\langle \left[\left(1 - \frac{1}{\pi} \ln(\tau_* \bar{\epsilon}) \hat{V} \right)^{-1} \bar{V}(\phi) \right]^2 \right\rangle = 1. \quad (20)$$

Since $\tau_* \langle \Delta \rangle$ is assumed to be small, $\ln(\tau_* \bar{\epsilon})/\pi$ must be close to the reciprocal maximal eigenvalue V_0^{-1} of

the operator \hat{V} in order to satisfy the above equation. Therefore, τ_* coincides with τ_c for $\langle \Delta \rangle^2 / \langle \Delta^2 \rangle \rightarrow 0$. This completes the proof of the statements (2) and (3).

The properties of the AG equations, which have been just established, give us a clue for an investigation of the behavior of the angular-dependent DOS. The latter may be found via the solutions of the AG equations, analytically continued from the Matsubara sequence, defined on the upper half of the imaginary axis of the frequency complex plane, to the real axis according to

$$\frac{\nu_s(\epsilon, \phi)}{\nu_n(\epsilon, \phi)} = \text{Re} \{ \tilde{\epsilon}(\epsilon) [\tilde{\epsilon}^2(\epsilon) - \tilde{\Delta}^2(\phi, \epsilon)]^{-1/2} \}. \quad (21)$$

Here $\nu_s(\phi)$ and $\nu_n(\phi)$ denote the DOS in the superconducting and the normal states, respectively, and the functions $\tilde{\epsilon}(\epsilon)$ and $\tilde{\Delta}(\phi, \epsilon)$ represent the result of the analytical continuation mentioned above. Namely, $\tilde{\epsilon}(i\eta_n) = i\tilde{\eta}_n$, $\tilde{\Delta}(\phi, i\eta_n) = \tilde{\Delta}_n(\phi)$. At the Fermi level $\tilde{\epsilon}(0) = i\tilde{\eta}(0)$ for $1/\tau < 1/\tau_*$ and $\tilde{\epsilon}(0) = 0$ for $1/\tau > 1/\tau_*$. Hence, $\nu_s(\phi, 0)$ is finite for $1/\tau < 1/\tau_*$ and vanishes identically for $1/\tau > 1/\tau_*$. It also vanishes at $1/\tau = 0$. Therefore, it has a maximum at some $1/\tau < 1/\tau_*$.

It is natural to suppose that a gap in the excitation spectrum does persist for all $1/\tau > 1/\tau_*$. We can confirm this conjecture at least for $1/\tau \gg 1/\tau_*$. The solution (14) and (15) of the AG equations can be employed in this case with the same substitution $\eta = -i\epsilon$ and $\tilde{\eta} = -i\tilde{\epsilon}$. Plugging this solution into Eq. (21) and keeping the precision up to $\tau\Delta$, one derives exactly the same formula as for an isotropic superconductor [13] with the average value $\langle \Delta \rangle$ playing the role of the isotropic gap. This result agrees with the Anderson isotropization theorem [14]. Notice, however, that neither $\nu_s(\epsilon, \phi)$ nor the OP become isotropic even in the extra dirty limit.

Evaluation with a higher precision shows that the standard square root singularity in DOS turns into a finite maximum of the height $\sim (\langle \Delta \rangle \tau)^{-1/2}$, smeared over the interval $\delta\epsilon \approx \tau\Delta^2$ and varying with angle. Nevertheless, the threshold character of the DOS dependence on energy with the threshold approximately equal to $\langle \Delta \rangle$ remains unaffected.

We have shown that the gap vanishes at $1/\tau = 1/\tau_*$, and it also vanishes at $\tau = 0$. Therefore, the gap reaches its maximum value at some scattering rate $1/\tau > 1/\tau_*$.

Thus, we propose to look for a rather peculiar phase transition, which can exist at zero temperature and is regulated by impurity concentration. One can try to find it experimentally, scrutinizing the dependence of the quasiparticle tunneling rate or the temperature correction to the penetration depth on the residual resistivity in single crystals of YBaCuO, doped by Pr or subjected to the radiation damage. A transmutation of the gapless tunneling current-voltage characteristics at small resistivity into the curves with a threshold feature at higher values of residual resistivity and an analogous conversion of the temperature dependence of the penetration depth from the gapless to the activated one would clearly indicate the presence of the

transition. An ideal experimental setting would include controlling Josephson tunneling measurements in the corner geometry on the same samples to verify whether the OP changes its sign.

In conclusion, we have shown that a phase transition should take place at zero temperature and a special value of the impurity scattering rate $1/\tau_*$ in a layered superconductor, provided the OP in the clean limit does change its sign on the Fermi surface but its angular average is finite. We have argued that, according to the recent experimental observations, the OP with the required properties is likely to be an inherent feature, at least for YBaCuO. This transition is characterized by a gap generation in the excitation spectrum for $1/\tau > 1/\tau_*$. The energy gap grows from zero at $1/\tau = 1/\tau_*$ to its maximum at some $1/\tau < 1/\tau_*$ and vanishes again in the extra dirty limit. The DOS at the Fermi level turns into zero in the clean case and at $1/\tau = 1/\tau_*$, reaching its maximum at an intermediate value of $1/\tau$.

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