Effect of impurities on phase transitions in quasi-one-dimensional conductors

A. I. Larkin and V. I. Mel'nikov

L. D. Landau Theoretical Physics Institute, USSR Academy of Sciences
(Submitted May 6, 1976)
Zh. Eksp. Teor. Fiz. **71**, 2199–2203 (December 1976)

It is shown that in quasi-one-dimensional conductors impurities suppress not only the dielectric transition but also the superconducting transition. Impurities with a slowly-varying potential do not affect the size of the region in which short-range order exists in the one-dimensional case, but decrease the amplitude for coherent hopping of a pair of electrons from filament to filament. As a result, the temperature of the superconducting transition is decreased but remains finite for any concentration of quasi-classical impurities. Impurities that can backscatter an electron decrease the region of the existence of short-range order in the one-dimensional case. Because of this, in the quasi-one-dimensional case the superconducting transition temperature should vanish at a certain concentration of impurities.

PACS numbers: 71.55.−i, 71.40.+n, 74.10.+v

In the majority of quasi-one-dimensional compounds there is no superconducting transition, since a phase transition to the dielectric state occurs at a higher temperature. The opinion has been expressed that suppression of the dielectric transition by impurities could facilitate the appearance of superconductivity. The basis for this was that nonmagnetic impurities have no effect on the superconducting transition in three-dimensional conductors. Below it is shown that in quasi-one-dimensional conductors impurities suppress not only the dielectric transition but also the superconducting transition. This is connected with the inapplicability of quasi-one-dimensional conductors of the BCS formula for the superconducting transition temperature. In the three-dimensional case the transition temperature is determined by the density of electron states, which depends weakly on the impurity concentration. In the quasi-one-dimensional case it is determined by the amplitude for hopping of a pair of electrons from filament to filament and by the form of the one-dimensional correlation function.

In the one-dimensional case we shall distinguish two types of impurity. If the potential of the impurities is slowly varying, the scattering by them occurs quasi-classically. In this case actual scattering of an electron does not occur and the effect of the impurities reduces to the appearance of a random phase of the electron wavefunction. As was shown by Zawadowski, [1] such impurities do not affect the thermodynamics of a one-dimensional system, in which, however, phase transitions are in any case absent. A finite transition temperature is obtained as a consequence of three-dimensional effects, which establish a coherent state over the whole volume. The impurities induce an independent phase shift on each filament, as a result of which the coherence decays and the transition temperature decreases. If the potential of the impurities is sufficiently steep we cannot neglect scattering with change of the electron momentum. As shown below, such impurities have a significantly stronger effect on the superconducting transition temperature, which vanishes at a certain impurity concentration.

In the self-consistent field approximation with respect to the interaction of electrons on different filaments, for the temperature of the dielectric transition we have the equation[2]

$$V\int \Pi(x)e^{2ip_Fx}\,dx=1, \tag{1}$$

where V is the interaction of electrons on neighboring filaments, and $\Pi(x)$ is the correlator of the densities for electrons situated on the same filament.

The Fourier components of the density operators with momentum $2p_F$ appear in the expression (1). Taking quasi-classical impurities into account reduces to multiplying $\Pi(x)$ by

$$\exp\left[-\frac{2i}{v_F}\int_0^x u(x')\,dx'\right],$$

where $u(x)$ is the random potential created by the impurities. After averaging over the impurities this factor acquires the form $e^{-x/l}$, where l is the mean free path.

For weak electron–electron interaction $g\ll 1$ there is a region of small $x\ll ae^{1/g}$ (a is the lattice constant) in which the interaction is unimportant. In this region,

$$\Pi(x)=\frac{2T\cos 2p_Fx}{v_F^2\,\mathrm{sh}(2\pi T|x|/v_F)}. \tag{2}$$

At low temperatures the right-hand side of Eq. (1) is equal to $V(\pi v_F)^{-1}\ln(l/a)$, and therefore, if $l<a\exp(\pi v_F/V)$, Eq. (1) has no solution at any temperature and the phase transition is absent. The result obtained applies to the case when the interaction of electrons on different filaments is of the same order of magnitude as the interaction in the same filament. Under these conditions the result coincides with that obtained in the review by Bulaevskiĭ. [3]

In another limiting case, when the interaction V of electrons on different filaments is weaker than their interaction gv_F in the same filament, we must substitute into Eq. (1) the correlator $\Pi(x)$ calculated with allowance for this interaction[2]:

$$\Pi(x) \approx \frac{1}{v_F x}\left(\frac{x}{ae^{1/g}}\right)^{2-1/\alpha}, \tag{3}$$

where the parameter α depends on the interaction g, and $1-\alpha \approx g/2$ for $g \ll 1$. Then the condition on the mean free path l under which the phase transition is certainly absent takes the form

$$l < ae^{1/g}\left(\frac{v_F(1-\alpha)}{V}\right)^{\alpha/(2\alpha-1)}. \tag{4}$$

This inequality was derived under the assumption that the impurities are quasi-classical and backward scattering does not occur. It is physically obvious that the action of impurities of a general kind is not weaker. Thus, for a sufficiently small mean free path the dielectric transition disappears.

A superconducting transition in the quasi-one-dimensional case can occur only when there are electron hops from filament to filament. We find the transition temperature in this case using the formula (38) of the paper[2] by Efetov and one of the authors:

$$W\int G(x,\tau)\,dx\,d\tau = 1, \tag{5}$$

where W is the amplitude for hopping of a pair of electrons from filament to filament and $G(x, \tau)$ is the correlator of superconducting pairs in one filament.

The correlator $G(x, \tau)$ is not changed by quasi-classical scattering. Therefore, as in the "clean" case,[2] we obtain the following relation between the transition temperature and the parameter W:

$$(T_c/\Delta)^{2-\alpha} = Wv_F/\Delta^2, \tag{6}$$

where Δ is the magnitude of the gap, determined by the BCS formula.

The amplitude W decreases with increase of impurity concentration. This follows from the expression

$$W_{ij} = J^2\int d\omega\, dx \langle F_{i\omega}(x) F_{j\omega}^+(x')\rangle, \tag{7}$$

where J is the amplitude for an electron to hop from filament to filament, i and j are the labels of neighboring filaments, $F_{i\omega}(x)$ is the Gor'kov function, and the angular brackets denote averaging over the positions of the impurities.

When quasi-classical impurities are taken into account the function $F_{i\omega}(x)$ is multiplied by

$$\exp\left(\frac{i}{v_F}\int_0^x u_j(x')\,dx'\right),$$

where $u_j(x)$ is the potential of the impurities in the j-th filament. Averaging independently over the positions of the impurities in each filament, we obtain

$$W \approx \frac{J^2}{v_F^2}\int\frac{d\omega}{2\pi}\frac{\Delta^2}{\omega^2+\Delta^2}\int\exp\left[-\frac{2|x|(\omega^2+\Delta^2)^{1/2}}{v_F}-\frac{|x|}{l}\right]dx \approx \frac{J^2\Delta\tau}{v_F}$$
$$\left(\tau = \frac{l}{v_F}\right). \tag{8}$$

It follows from formulas (6) and (8) that with increase of the concentration of quasi-classical impurities the superconducting transition temperature decreases but remains finite for any concentration of impurities. Impurities that can scatter an electron backward have a significantly stronger effect on the superconducting transition temperature, since they change not only W, in accordance with formula (8), but also the law of decrease of the function $G(x, \tau)$ with distance.

As in the clean case,[2] we shall assume that the behavior of $G(x, \tau)$ at large distances is determined by slow fluctuations of the phase:

$$G(x,\tau) = \left(\int e^{-F[\varphi]}D\varphi\right)^{-1}\int e^{i\varphi(x,\tau)-i\varphi(0,0)}e^{-F[\varphi]}D\varphi, \tag{9}$$

where the functional $F[\varphi]$ is calculated under the assumption that a local superconducting state exists, and is equal to

$$F[\varphi] = \frac{K}{2}\int\left[\left(\frac{\partial\varphi}{\partial\tau}\right)^2 + v_s^2\left(\frac{\partial\varphi}{\partial x}\right)^2\right]dx\,d\tau, \tag{10}$$

where K is the density of states at the Fermi level and Kv_s^2 is the superfluid density. It follows from formulas (9) and (10) that, at large distances,

$$G(x,\tau) \approx (v_s/\Delta)^\alpha (x^2+v_F^2\tau^2)^{-\alpha/2}, \tag{11}$$
$$\alpha = 2(\pi K v_s)^{-1}. \tag{12}$$

For $\alpha < 2$, large distances $R \sim v_s/T$ are important in the integral (5), and for the transition temperature we obtain the formula (6).

It seems natural that $G(x, \tau)$ will fall off faster in the dirty limit than in the clean limit. There are two conceivable possibilities for the law of decrease of $G(x, \tau)$. The first is that the impurities lead to the disappearance of the long-wavelength sound excitations. In this case the correlator $G(x, \tau)$ falls off exponentially at large distances and the integral in the expression (5) converges even at zero temperature, so that for small W and a not very small concentration of impurities the superconducting transition is absent. The second possibility is that the long-wavelength sound excitations continue to exist even in the presence of impurities, which, in this case, change the parameter α in formula (11). In fact, the coefficient of $(\partial\varphi/\partial x)^2$ in the free energy (10) is proportional to the superfluid density, i.e., to the correlator of the electron velocities. Even in the three-dimensional case this correlator decreases with increase of impurity concentration. We shall show that in the one-dimensional case it decreases still faster.

To calculate the correlator of the velocities we shall make use of a technique proposed by Berezinskiĭ[4] for the calculation of the conductivity in a one-dimensional system. We expand the velocity correlator in a series in the interaction with the impurities and write each term of the series in the coordinate representation. The

Green function in the self-consistent field approximation has the form

$$\mathcal{G}(x,\varepsilon)=v_F^{-1}[\hat{A}e^{ip_F|x|}+\hat{B}e^{-ip_F|x|}]\exp\left[-|x|\left(\frac{\varepsilon^2+\Delta^2}{v_F^2}\right)^{1/2}\right], \qquad (13)$$

$$\begin{pmatrix}\hat{A}\\ \hat{B}\end{pmatrix}=\frac{1}{2(\varepsilon^2+\Delta^2)^{1/2}}\begin{pmatrix}-i[\varepsilon\pm(\varepsilon^2+\Delta^2)^{1/2}] & -\Delta\\ \Delta^* & i[\varepsilon\mp(\varepsilon^2+\Delta^2)^{1/2}]\end{pmatrix}, \qquad (14)$$
$$\varepsilon=(2n+1)\pi T.$$

It follows from the latter formula that $\hat{A}\hat{B}=\hat{B}\hat{A}=0$. Therefore, as in Berezinskiĭ's paper, [4] the correlator is represented by loops consisting of two lines. One of these contains only matrices $\hat{A}$, and the other contains only matrices $\hat{B}$. Since $(i\hat{A})^n=i\hat{A}$ and $(-i\hat{B})^n=-i\hat{B}$, the product of matrices in the correlator gives the factor

$$\mathrm{Sp}\,\hat{A}\sigma_z\hat{B}\sigma_z=\frac{\Delta^2}{\varepsilon^2+\Delta^2}. \qquad (15)$$

The factors $\exp[-x(\varepsilon^2+\Delta^2)^{1/2}/v_F]$ can be assigned to the impurity vertices, and then each diagram differs from the corresponding diagram of Berezinskiĭ's paper[4] by the replacement of $\omega/2$ by $i(\varepsilon^2+\Delta^2)^{1/2}$. Having made this replacement in the expression for the conductivity[4] in the regime $\tau\varepsilon\ll 1$, we obtain[1)]

$$Kv_s^2=\int_0^\beta d\tau\int dx\langle v(\tau,x)v(0,0)\rangle\approx 32\zeta(3)\pi^{-1}v_F(\Delta\tau)^2\ln\frac{1}{\Delta\tau}. \qquad (16)$$

This formula is applicable in the limit $\Delta\tau\ll 1$.

Impurities have little effect on K—the density of states at the Fermi surface. Substituting (16) into (12) we obtain

$$\alpha=\frac{\alpha_0}{\Delta\tau[32\zeta(3)\ln(1/\Delta\tau)]^{1/2}}, \qquad (17)$$

where α_0 is the value of α in the absence of impurities and ζ is the Riemann function. For weak interaction, α_0 is close to 1.

Thus, in the dirty limit $\Delta\tau\ll 1$ the parameter α is large, and, consequently, for $\tau<\tau_{\mathrm{crit}}\sim\Delta^{-1}$, the value of α exceeds 2. In this case the integral in formula (5) converges even at zero temperature, and, therefore, Eq. (5) for small W has no solution and the superconducting transition is absent.

The existence of a dielectric transition in quasi-one-dimensional conductors implies that the interaction of electrons on different filaments (V in Eq. (1)) is larger than the pair-hopping amplitude (W in formula (5)). By introducing a sufficiently large quantity of impurities it is possible to suppress the dielectric transition, but then, almost inevitably, the superconducting transition will also be suppressed. Only exotic impurities that either increase the probability of an electron hopping from filament to filament or do not scatter electrons backward could save the situation.

An obstacle to quantitative comparison with experiment is the difficulty of determining experimentally the mean free paths appearing in the expressions that we have obtained. Scattering by quasi-classical impurities does not affect the conductivity at all, while scattering with a change of momentum leads to localization of the electron and absence of conduction at low temperatures.

In certain quasi-one-dimensional conductors (KCP and salts of TCNQ with quinoline and acridine) internal disorder exists. It is evident that this disorder does not lead to a small mean free path, since a dielectric transition exists in all the compounds indicated. [3,6]

1)The numerical coefficient in this formula is written taking into account the results of Gogolin, Mel'nikov and Rashba. [5]

1A. Zavadovskiĭ (Zawadewski), Zh. Eksp. Teor. Fiz. **54**, 1429 (1968) [Sov. Phys. JETP **27**, 767 (1968)].
2K. B. Efetov and A. I. Larkin, Zh. Eksp. Teor. Fiz. **69**, 764 (1975) [Sov. Phys. JETP **42**, 390].
3L. N. Bulaevskiĭ, Usp. Fiz. Nauk **115**, 263 (1975) [Sov. Phys. Usp. **18**, 131].
4V. L. Berezinskiĭ, Zh. Eksp. Teor. Fiz. **65**, 1251 (1973) [Sov. Phys. JETP **38**, 620 (1974)].
5A. A. Gogolin, V. I. Mel'nikov, and É. I. Rashba, Zh. Eksp. Teor. Fiz. **69**, 327 (1975) [Sov. Phys. JETP **42**, 168].
6F. F. Igoshin, A. P. Kir'yanov, V. N. Topnikov, and I. F. Shchegolev, Zh. Eksp. Teor. Fiz. **68**, 1203 (1975) [Sov. Phys. JETP **41**, 597]; V. N. Topnikov and I. F. Shchegolev, Pis'ma Zh. Eksp. Teor. Fiz. **20**, 404 (1974) [JETP Lett. **20**, 182 (1974)].

Translated by P. J. Shepherd