# Superconductor–semiconductor phase transition in a random field of defects

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A theoretical model for describing a superconductor–semiconductor phase transition induced by radiation defects or impurities has been proposed. The model is based on the localization of a Bose condensate of Cooper pairs in a random field created by defects. Expressions for the critical temperature and density of the condensate, which make it possible to describe and predict some experimental facts, have been derived.

## 1. INTRODUCTION

High-$T_c$ superconductors have been found to be far more sensitive to defects (particularly, radiation defects) than conventional superconductors. It has been established experimentally (see, for example, Refs. 1 and 2) that the critical temperature $T_c$ and the critical current $J_c$ (determined by resistive or inductive methods) decrease with increasing values of the concentration of defects $N$ (or, accordingly, the irradiation fluence $\Phi$) and vanish at a certain critical value, while the resistivity increases without bound in the normal state. It has also been shown that the Hall concentration of carriers remains virtually unchanged.

Several hundred experimental reports devoted to the influence of ion, neutron, electron, and other kinds of irradiation on the properties of high-$T_c$ superconductors have been published so far (see, for example, Refs. 2 and 3). An analysis of the data reveals[2] that the dependence of the reduced temperature $T_c/T_{c0}$ ($T_{c0}$ is the critical temperature before irradiation) on the reduced fluence is a universal function for all kinds of irradiation and for various types of samples and superconductors. Nonmagnetic impurities have a similar influence.[4]

The foregoing suggests that a superconductor–semiconductor phase transition is induced by defects when $T_c$ and $J_c$ vanish at the critical concentration $N_c$.

The fundamental difference between the behavior of high-$T_c$ superconductors in a field of defects and that of other superconductors should be noted.[2]

In this report we propose a model describing this phase transition. It is based on the localization of a Bose condensate of Cooper pairs in a random field of defects or impurities.

Several theoretical studies, in which attempts were made to describe a superconductor–semiconductor transition on the basis of the phenomenon of electron localization, have been published (see Refs. 6–10). However, it was shown in Refs. 6 and 7 that $T_c$ does not vanish even under the conditions of an Anderson insulator. The studies employing the scaling approach (see Refs. 8–10) did not yield concrete results that could be compared with experiment.

## 2. FORMULATION OF THE PROBLEM. FUNDAMENTAL EQUATIONS

We start with the Bogolyubov–de Gennes equations[11]

$$\varepsilon_n u_n(\mathbf{r}) = \hat{H}_0 u_n(\mathbf{r}) + \Delta(\mathbf{r}) v_n(\mathbf{r}), \tag{1}$$

$$\varepsilon_n v_n(\mathbf{r}) = -\hat{H}_0^* v_n(\mathbf{r}) + \Delta^*(\mathbf{r}) u_n(\mathbf{r}), \tag{2}$$

$$\Delta(\mathbf{r}) = V \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r})(1 - 2n(\varepsilon_n)), \tag{3}$$

where the one-particle Hamiltonian

$$\hat{H}_0 = -\nabla^2/2m - \varepsilon_F + U(\mathbf{r}), \quad \hbar = 1 \tag{4}$$

describes electrons moving in a random potential $U(\mathbf{r})$ created by randomly distributed defects, and the remaining notation is standard.

In the limit of small values of the order parameter $\Delta(\mathbf{r})$ and its derivatives, we can make the transition from (1)–(4) to an equation of the Ginzburg–Landau type[11]

$$\Delta(\mathbf{r}) = K_0(\mathbf{r})\Delta(\mathbf{r}) + \tfrac{1}{2} K_1(\mathbf{r}) \nabla^2 \Delta(\mathbf{r}) + K_2(\mathbf{r}) \Delta(\mathbf{r}) |\Delta(\mathbf{r})|^2, \tag{5}$$

where

$$K_0(\mathbf{r}) = \int K(\mathbf{r},\mathbf{r}') d^d r', \tag{6}$$

$$K_1(\mathbf{r}) = \int (\mathbf{r}-\mathbf{r}')^2 K(\mathbf{r},\mathbf{r}') d^d \mathbf{r}', \quad K_2(\mathbf{r})$$

are random functions in the general case. In fact,

$$K(\mathbf{r}_1,\mathbf{r}_2) = \frac{V}{\beta} \sum_{i\omega_n} G(r_1 r_2, i\omega_n) G(r_1 r_2, -i\omega_n) \tag{7}$$

can be expressed in terms of the exact one-particle Green's functions

$$G(\mathbf{r}_1 \mathbf{r}_2 \omega) = \sum_n \frac{\psi_n(\mathbf{r}_1)\psi_n^*(\mathbf{r}_2)}{\omega - \varepsilon_n} \tag{8}$$

for an electron moving in a random field $U(\mathbf{r})$. Equations like (5)–(8) have been derived in several studies (see, for example, Refs. 12 and 10).

Next, with no loss of generality, we assume that only $K_0(\mathbf{r})$ is a random function, i.e., we set

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$$K_0(\mathbf{r})=\langle K_0(\mathbf{r})\rangle+\delta K_0(\mathbf{r}),\quad \langle K_0(\mathbf{r})\rangle=K_0, \tag{9}$$

$$K_1(\mathbf{r})\to\langle K_1(\mathbf{r})\rangle=K_1,\quad K_2(\mathbf{r})\to\langle K_2(\mathbf{r})\rangle=K_2. \tag{10}$$

When these assumptions are taken into account, Eq. (5) takes the form

$$\tfrac{1}{2}K_1\nabla^2\Delta(\mathbf{r})+(K_0-1)\Delta(\mathbf{r})+\delta K_0(\mathbf{r})\Delta(\mathbf{r})$$
$$+K_2\Delta(\mathbf{r})|\Delta(\mathbf{r})|^2=0. \tag{11}$$

The coefficients $K_0$, $K_1$, and $K_2$ were found for weak disorder in Ref. 13, for strong localization in the self-consistent approximation in Ref. 7, and with the aid of scaling theory in Ref. 6.

When the critical temperature and current are calculated from (11), the term containing $\delta K_0(\mathbf{r})$ is usually omitted. This is equivalent to assuming that the order parameter is self-averaging (see Ref. 11). It has been shown that $T_c$ and the current then do not vanish even in an Anderson insulator phase.[6,7] Therefore, the self-averaging approximation is inadequate for describing the phase transition.

We next take into account the contribution of $\delta K_0(\mathbf{r})$, which turns out to be decisive. Rewriting Eq. (11) as

$$\frac{1}{2m}\nabla^2\psi(\mathbf{r})+\psi(\mathbf{r})[\widetilde{E}+\widetilde{U}(\mathbf{r})+\alpha|\psi(\mathbf{r})|^2]=0, \tag{12}$$

where

$$\psi(\mathbf{r})\equiv\Delta(\mathbf{r}),\quad \widetilde{E}=(K_0-1)/mK_1,$$
$$\widetilde{U}(\mathbf{r})=\delta K_0(\mathbf{r})/mK_1,\quad \alpha=K_2/K_1m$$

reveals its similarity to the nonlinear Schrödinger equation with an assigned energy $\widetilde{E}$ in a random field $\widetilde{U}(\mathbf{r})$. By definition

$$\langle\widetilde{U}(\mathbf{r})\rangle=0, \tag{13}$$

and the correlator in the white-noise approximation

$$\langle\widetilde{U}(\mathbf{r})\widetilde{U}(\mathbf{r}')\rangle=\mathscr{D}\delta_d(\mathbf{r}-\mathbf{r}') \tag{14}$$

can be calculated for specific cases.

If the nonlinear term in (12) is neglected, the equation for a condensate of Cooper pairs

$$\frac{1}{2m}\nabla^2\psi(\mathbf{r})+[\widetilde{E}+\widetilde{U}(\mathbf{r})]\psi(\mathbf{r})=0 \tag{15}$$

together with (13) and (14) has the same form as the corresponding system for an electron in the random field $\widetilde{U}(\mathbf{r})$. The equation for the discrete problem (in a lattice) is equivalent to the Anderson model, if $\widetilde{U}(\mathbf{r})$ is compared with the energy at a lattice site $\varepsilon_i$, and

$$\mathscr{D}=W^2/12, \tag{16}$$

where $W$ is the width of the distribution function in energy,

$$P(\varepsilon)=\frac{1}{W}\begin{cases}1, & |\varepsilon|<W/2,\\ 0, & |\varepsilon|>W/2,\end{cases} \tag{17}$$

$$\langle\varepsilon_i\rangle=0,\quad \langle\varepsilon_i\varepsilon_j\rangle=\delta_{ij}W^2/12.$$

## 3. LOCALIZATION OF A BOSE CONDENSATE OF COOPER PAIRS

In the one-dimensional case, the solutions of (13)–(15) are known to be localized states. This means that for any $\widetilde{U}(\mathbf{r})$ a condensate of Cooper pairs is localized, and a nondecaying current is impossible. In the three-dimensional case (and possibly the two-dimensional case) an Anderson transition occurs, i.e., localized and delocalized states exist, and the energy $E_c$ separating them depends on the degree of disorder $W$. For example, numerical calculations in the Anderson model[14,15] give

$$W_c/E_c=\chi_2=6.1,\quad W_c/E_c=\chi_3=14.4 \tag{18}$$

for a two-dimensional square lattice and a three-dimensional cubic lattice, respectively. From (18) and (16) we have

$$E_c=\widetilde{E}=\frac{K_0(T)-1}{mK_1}=\frac{2\sqrt{3}\mathscr{D}^{1/2}}{\chi_d}, \tag{19}$$

where $\chi_d$ is a numerical factor that depends on the dimensionality of the space $d$. Since $\widetilde{E}$ and $\mathscr{D}$ are temperature-dependent, (19) is the equation for a certain critical temperature $T=T_s$, above which all states are localized.

The coefficients $K_0$ and $K_1$ and correlator (14) have been calculated in several studies (see Refs. 13 and 10). The expressions obtained in the dirty limit ($T_c\tau\ll1$) are

$$K_0=V\rho\ln\frac{\widetilde{\omega}}{T},\quad \mathscr{D}^{1/2}=\frac{V\widetilde{\delta}}{\xi_0^dT_cmK_1}, \tag{20}$$

$$\xi_0^2=v_F^2\tau/T_c,\quad 1/\tau=2\pi N|U_0|^2\rho,\quad \widetilde{\delta}\sim1, \tag{21}$$

where $\xi_0$ is the low-temperature coherence length, $U_0$ is the Fourier component of the potential of a defect, $\rho$ is the density of electronic states, and $v_F$ is the velocity of an electron on the Fermi surface.

From Eqs. (20) and (19) we can derive an equation for the temperature $T_s$, above which the Bose condensate is completely localized,

$$1-\frac{T_s}{T_c}=\frac{\chi_d\widetilde{\delta}}{\xi_0^dT_c\rho}. \tag{22}$$

Hence we obtain an expression for $T_s$ in the three-dimensional case

$$T_s=T_c\left[1-\frac{\sqrt{3}\pi^2}{30}\left(\frac{T_c}{\varepsilon_F}\right)^{1/2}\frac{\widetilde{\delta}}{(\varepsilon_F\tau)^{3/2}}\right] \tag{23}$$

and an expression for the two-dimensional case

$$T_s=T_c\left[1-\frac{\sqrt{3}\pi\widetilde{\delta}}{6\varepsilon_F\tau}\right]=T_c\left[1-\frac{\sigma_c}{\sigma}\right], \tag{24}$$

where $\sigma_c=e^2\sqrt{3}\widetilde{\delta}/6$, $\sigma$ is the conductivity, and $e$ is the charge of the electron.

We introduced the special notation $T_s$ for the transition temperature to distinguish it from $T_c$, which may be defined as the temperature above which $\Delta=\psi=0$. In the situation under consideration, the order parameter $\psi$ is not equal to zero at $T_c>T>T_s$, but a superconducting current is impossible. Therefore, $T_s$ is the temperature above which a nonzero resistivity can be measured experimentally by a resistive or inductive method. Since $1/\tau$ is proportional to the concentration of defects, $T_s$ decreases with increasing $N$ according to (24) and (23).

The problem of taking into account the nonlinear term in (12) (i.e., the interaction occurring during localization) is difficult and has not been solved completely. This interaction is known to result in shielding of the random potential and certain other effects. Such shielding causes a decrease in the effective value of $W_c$ in (19). In addition, the term $\alpha\psi|\psi|^2$ makes it possible to describe the temperature dependence. In the absence of disorder, this dependence is known to be given by the relation

$$|\psi|^2 \simeq 9.4 T_c(T_c - T). \tag{25}$$

If $\widetilde{U}(\mathbf{r})$ is nonzero, an evaluation can be performed in the following manner. Averaging (12) and taking into account that $\langle \widetilde{U}(r)\psi(r)\rangle = 0$ (Ref. 16), we obtain

$$\frac{1}{2m}\nabla^2\langle\psi\rangle + \widetilde{E}\langle\psi\rangle - \alpha\langle\psi|\psi|^2\rangle = 0, \tag{26}$$

whose integration over space gives

$$\int \langle\psi|\psi|^2\rangle d^d r = \alpha^{-1}\widetilde{E}\int \langle\psi\rangle d^d r. \tag{27}$$

Bearing in mind the overall spatial uniformity of the condensate, we obtain an estimate of its density

$$\langle\psi|\psi|^2\rangle \sim \widetilde{E}\langle\psi\rangle/\alpha, \tag{28}$$

which indicates that the density of the condensate is proportional to the temperature difference $T_c - T$. If $T$ is below $T_s$, there exist two condensates: a localized condensate with a density $|\psi_l|^2$ and a delocalized condensate with a density $|\psi_p|^2$, so that the total density is

$$|\psi_l|^2 + |\psi_p|^2 = |\psi|^2. \tag{29}$$

## 4. DISCUSSION OF RESULTS. COMPARISON WITH EXPERIMENT

Equation (22) for $T_s$ is applicable to the two-dimensional and three-dimensional cases and is independent of the pairing mechanism. However, for conventional superconductors with a large concentration of electrons and a large Fermi energy $\varepsilon_F$, the parameters $\varepsilon_F\tau$ and $\varepsilon_F/T_c$ are very large, so that $T_s$ differs only slightly from $T_c$ [see (23)]. The situation is different in quasi-two-dimensional high-$T_c$ oxide superconductors: $\varepsilon_F$ is small, and $\varepsilon_F\tau$ may reach unity at a relative concentration of defects equal to $10^{-3}$ to $10^{-2}$. Therefore, we shall discuss only the two-dimensional case further. The critical temperature and the Fermi energy for a two-dimensional superconductor without defects are given by[17,18]

$$T_c = (2\varepsilon_F\varepsilon_a)^{1/2}, \quad \varepsilon_a = 2\widetilde{\omega}\exp(-2\pi/mV)\gamma^2/\pi^2, \tag{30}$$

$$\varepsilon_F = \frac{n\pi}{m}, \quad \gamma = \exp(0.577),$$

where $V$ is the attraction energy, $\widetilde{\omega}$ is the cutoff frequency of the attractive interaction ($\widetilde{\omega}$ is assumed to be large compared with $\varepsilon_F$ and $T_c$), $m$ is the mass of the electron, and $\varepsilon_a$ is the binding energy of a pair. Relations (30) hold provided $\varepsilon_F \gg \varepsilon_a$. Otherwise, according to Ref. 18, we have

$$T_c \simeq \varepsilon_F.$$

Utilizing the expression for $\tau$ [see (21)], from (24) we find

$$T_s = T_c - \beta N, \quad \beta = \frac{\pi^2\widetilde{\delta}|U_0|^2\rho T_c}{\sqrt{3}\varepsilon_F}, \tag{31}$$

$$T_c/\varepsilon_F = 2\varepsilon_a/T_c = (2\varepsilon_a/\varepsilon_F)^{1/2}, \quad \varepsilon_F \gg \varepsilon_a,$$

$$T_c/\varepsilon_F = 1, \quad \varepsilon_F \ll \varepsilon_a. \tag{32}$$

The concentration of radiation defects is proportional to the fluence of high-energy particles $N = \gamma\Phi$, so that

$$T_s = T_c - \widetilde{\beta}\phi, \quad \widetilde{\beta} = \beta\gamma. \tag{33}$$

The latter equality coincides with the corresponding relation in Ref. 5, which we obtained on the basis of qualitative arguments to describe $T_c(\Phi)$ in initially oxygen-deficient films.

It should be borne in mind that (31) and (32) hold provided $T_s$ does not differ excessively from $T_c$ [see (20)]. However, their behavior at $T_s \to 0$ remains qualitatively correct, since the contribution of the term with $T_s \simeq 0$ in (22) becomes small. Therefore, Eqs. (31) and (32) my be regarded as approximate interpolation formulas over the entire temperature range.

Expressions (31) and (32) enable us to qualitatively describe the phase transition and some of its properties:

1. The universal dependence of $T_s/T_{c0}$ on $\Phi/\Phi_0$

$$T_s/T_{c0} = 1 - \Phi/2\Phi_0, \quad \Phi_0 = T_{c0}/2\widetilde{\beta}, \tag{34}$$

which is close to the experimentally observed linear dependence.

2. The fact that $T_s$ vanishes at a certain critical value of the fluence $\Phi_c(0)$ (and, accordingly, of the concentration of defects or impurities)

$$\Phi_c(0) = 2\Phi_0 = T_{c0}/\widetilde{\beta}, \tag{35}$$

which is proportional to the concentration of carriers (and, therefore, $T_{c0}^2$ or $T_{c0}$) (see, for example, Refs. 2 and 5).

3. The appearance of nonzero resistivity at a finite temperature, if the fluence exceeds a certain value

$$\Phi_c(T) = (T_c - T)/\widetilde{\beta}. \tag{36}$$

4. The behavior of the rate of variation of $T_s(\Phi)$

$$\partial T_s/\partial\Phi = -\widetilde{\beta} \tag{37}$$

as a function of the oxygen deficiency. In particular, in samples with high values of $T_{c0}$, this rate decreases with increasing $T_{c0}$, while in oxygen-deficient samples ($\varepsilon_F \ll \varepsilon_a$) the slope no longer depends on $T_c$ [see Eq. (32)].

5. The universal dependence of $T_s$ on the London penetration depth $\lambda$ (Ref. 19), if it is taken into account that in the dirty limit $\lambda^{-2} \sim \tau$.

6. The observed deviations of the ratio $2\Delta/T_s$ and the temperature dependence of $\Delta(T)$ from those given by the

BCS theory [the large values of $2\Delta/T_s$ and weak dependence of $\Delta(T)$ as $T\to T_s$], which are attributable to the difference between $T_c$ and $T_s$.

7. A superconductor–semiconductor transition as the oxygen concentration (i.e., $\varepsilon_F$) is lowered at a fixed concentration of defects in a particular sample [see (31)].

The model under consideration predicts the existence of a localized Bose condensate ($\langle|\psi|^2\rangle\neq 0$) in the range $T_s<T<T_c$. The dependence of the order parameter $|\psi|^2$ on $\Phi$ should be measured to test this prediction. This can be accomplished in tunneling, ultrasonic or electromagnetic probing, and Andreev reflection experiments. When $\Phi>\Phi_c(T)$ [or $T_c>T>T_s(\Phi)$], effects caused by the gap in the spectrum of excitations should be observed, although the resistivity will be nonzero [$R(\mathrm{T})\neq 0$].

The localization of a Bose condensate is probably not the only factor which can alter the critical temperature. Another possible mechanism, which operates when there is weak localization, was proposed in Ref. 17 and is based on enhancement of the fluctuations of a Bose condensate as a result of scattering from defects, due to a decrease in the coherence length. The corresponding expression for $T_c$ is[17]

$$T_c/T_{c0}=1-m\varepsilon_a\eta/\varepsilon_F^2\tau,\quad \varepsilon_F\gg\varepsilon_a,\quad \eta\sim 1, \tag{38}$$

so that the rate of variation $\partial T_c/\partial\Phi$ is $\varepsilon_a/\varepsilon_F$ smaller than the rate given by Eq. (37). Therefore, when the fluence is small (and $\varepsilon_F\gg\varepsilon_a$), it may be expected that $T_s(\Phi)$ will have form (38) and will then be described by Eq. (37).

Another reason for variations in $T_c$ may be the effect of defects on the attraction energy. Numerical calculations of the binding energy $\varepsilon_s$ in two-dimensional $Cu_4O_8$ clusters with disorder[20] also predict that $\varepsilon_s$ will decrease and vanish as the degree of disorder rises. In those calculations the binding energy was calculated by exact diagonalization.

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