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Off-Diagonal Nonmagnetic Disorder in *s*- and *d*-Wave Superconductors

M. Michalik and K.I. Wysokiński

Institute of Physics, M. Curie-Skłodowska University
Radziszewskiego 10, 20-031 Lublin, Poland

The previously developed approach to study off-diagonal disorder has been extended and applied to both *s*- and *d*-wave superconductors. The derived equations allow the self-consistent solution of the problem. For a special case of negative U centres embedded in non-superconducting host we have calculated their critical concentration for the appearance of superconductivity and found it equal to ≈ 0.4. For $x > x_{\rm cr}$ the order parameter continuously increases to its maximal value at $x = 1$.

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1. Introduction

The study of disordered superconductors has a long history. On experimental side it started with early work of Shalnikov [1], Buckel [2], and others, while theoretical ideas have been developed by Anderson [3], Abrikosov and Gorkov [4, 5] and many others [6–10]. Nowadays the reaction of superconductors against the impurities intentionally introduced into them is the first indication of the non *s*-wave symmetry of the order parameter.

Here we shall combine BCS approach to superconductivity with coherent potential approximation (CPA) technique to study off-diagonal disorder [11]. We calculate such characteristics of the superconducting system as the gap function and the density of quasiparticle states and the critical concentrations for a system to become superconductor. For this purpose we assume that the negative U centres are being introduced into otherwise insulating host.

In the next section we briefly present the model, remind the general approach and show the results for the density of states and the dependence of the superconducting gap on disorder. We end up with discussion and conclusions.

2. The model, approach, and results

The disordered superconducting alloy of the A_xB_{1-x} type is described by the following Hubbard model formulated in Wannier function representation:

$$H = \sum_{ij\sigma} \hat{t}_{ij} c^+_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (\epsilon_i - \mu) c^+_{i\sigma} c_{i\sigma} + \sum_i U_i c^+_{i\uparrow} c_{i\uparrow} c^+_{i\downarrow} c_{i\downarrow} + \sum_{i,j} V_{ij} n_i n_j, \quad (1)$$

in which site energies ϵ_i are random quantities taking on values $\epsilon_{\rm A}$ or $\epsilon_{\rm B}$ depending on whether site i is occupied by an atom of A or B type. In Eq. (1) $c^+_{i\sigma}$, $(c_{j\sigma})$ is the creation (annihilation) operator of spin σ electron at site i, $n_i = \sum_\sigma c^+_{i\sigma} c_{i\sigma}$, μ is the chemical potential. Both U_i and V_{ij} are here effective attraction parameters [12] leading to s- or d-wave superconducting instability in the system. $\hat{t}_{ij}$ denote random hopping integrals taking on three values $\hat{t}^{\rm AA}_{ij} = \alpha t_{ij}$, $\hat{t}^{\rm AB}_{ij} = \hat{t}^{\rm BA}_{ij} = \gamma t_{ij}$, and $\hat{t}^{\rm BB}_{ij} = \beta t_{ij}$ according to the type of atoms (A or B) occupying sites i and j, respectively. t_{ij} is the periodic hopping integral taking on nonzero value — t for sites i, j being nearest neighbours. In this paper we are interested in cases ($U_i \neq 0$, $V_{ij} = 0$; s-wave symmetry) or ($U_i = 0$, $V_{ij} \neq 0$; d-wave symmetry) only.

For s-wave symmetry the (local, but fluctuating) order parameter Δ_i has to be calculated in a self-consistent way. The CPA equations for the matrix self-energy $\hat{\sigma}$ and $\hat{G}$ of disordered superconductor read [13]

$$\sum_i c_i (\hat{1} - \hat{U})^{-1} = \langle \hat{G} \rangle_i, \quad (2)$$

$$\hat{U} = \hat{z} - \hat{\sigma} - \langle \hat{G} \rangle_i \quad (3)$$

$$\langle \hat{G} \rangle_i = \int (\hat{g}_i - \hat{t}(k)) {\rm d}^3 k, \quad (4)$$

where $i = {\rm A}, {\rm B}$, $c_{\rm A} = x$, $c_{\rm B} = 1 - x$ and $\hat{t}(k)$ denotes the Fourier transform of $\hat{t}$. The 4×4 matrix $\hat{\sigma}$ is a diagonal self-energy, $\langle \hat{G} \rangle_i$ conditionally averaged Green's function (the condition being that the atom of type i occupies a given site and other sites are described by an effective medium $\hat{\sigma}$).

The matrix $\langle \hat{G} \rangle_i$ is written as

$$\langle \hat{G} \rangle_i = \begin{pmatrix} G^{\rm AA}_{11} & 0 & F^{\rm AA}_{12} & 0 \\ 0 & G^{\rm BB}_{11} & 0 & F^{\rm BB}_{12} \\ F^{\rm AA}_{21} & 0 & G^{\rm AA}_{22} & 0 \\ 0 & F^{\rm BB}_{21} & 0 & G^{\rm BB}_{22} \end{pmatrix}_{ii} . \quad (5)$$

The order parameter is calculated as

$$\Delta_i = -U_i \frac{1}{\beta} \sum_n \exp({\rm i}\omega_n 0^+) F^{ii}_{12} \quad (6)$$

and the density of states $D(E) = -\frac{1}{\pi} {\rm Im}(G^{\rm AA}_{11} + G^{\rm BB}_{11})$. We have solved the CPA Eqs. (2–4) self-consistently together with the BCS Eqs. (5, 6) for the order parameter. The knowledge of $\hat{\sigma}$, $\langle \hat{G} \rangle_i$, and Δ_i enables the calculation of all characteristics of the system. For the numerical purposes we have assumed $T = 0$ K, the concentration of carriers $n = 1$ and the hopping parameter of the clean system to be an energy unit $t = 1$.

Disorder dependence of the density of states of s-wave and d-wave superconductors is shown in Fig. 1. The left panel shows the changes of the density of

states of s-wave and the right panel — the changes of d-wave superconductor with off-diagonal disorder. The diagonal disorder is measured by $\delta = \epsilon_{\rm A} - \epsilon_{\rm B}$ in units of t. $\delta = 0.4$ in both figures.

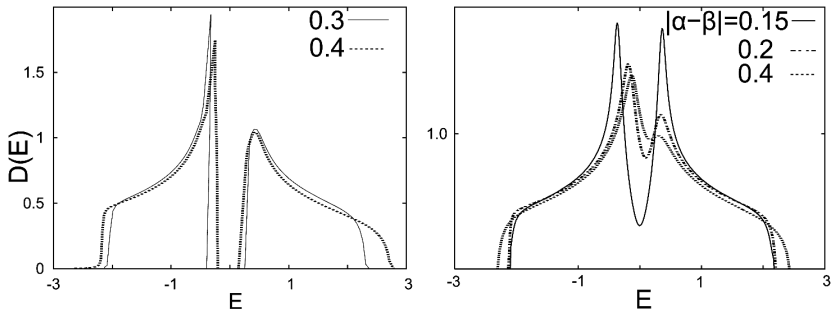

Fig. 1. Density of states of an A_xB_{1-x} alloy vs. energy E. The off-diagonal disorder is of the additive type $\gamma = (\alpha + \beta)/2$ with $\gamma = 1$ for $|\alpha - \beta| = 0.3$ (left panel — solid line) and 0.4 (dotted line). Right panel shows the density of states of d-wave superconductor with the same type of off-diagonal disorder. In both panels diagonal disorder $\delta = 0.4$.

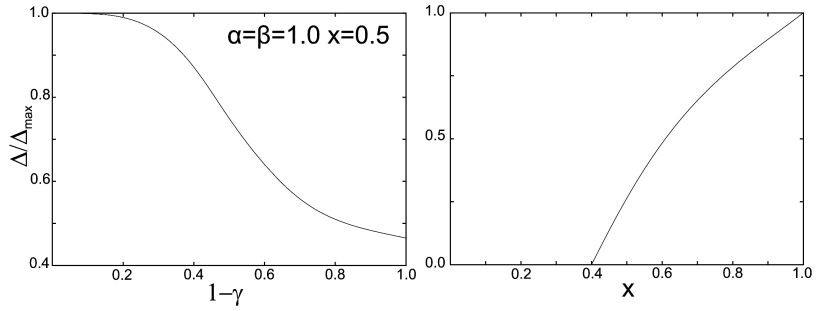

Fig. 2. Relative changes of Δ with disorder characterised by $\alpha = \beta = 1$ and $\gamma \neq 1$ (left panel) and with alloy concentration x (right panel) for $\beta = \gamma = 0$, $\alpha = 1$ and very large value of diagonal disorder. This set of parameters corresponds to superconducting centres A-type atoms embedded in an insulating host system. $\Delta_{\rm max}$ is the maximal value of the order parameter for a given set of parameters.

In Fig. 2 we show the dependence of the zero temperature gap on the disorder characterised by the value of γ (left panel) and concentration x of A-type atoms in an alloy (right panel). Let us note the existence of the critical concentration $x_{\rm cr} \approx 0.4$.

3. Summary and conclusions

In this paper we have combined the CPA formalism in the formulation of Blackman, Esterling, and Berk [11] with the BCS theory of superconductivity [12]

to get the self-consistent theory of superconducting alloys. Strong off-diagonal disorder effectively suppresses the d-wave superconductivity and only slightly the s-wave one in agreement with Anderson's "theorem" [3]. The interesting result is the existence of the critical concentration $x_{\rm cr}$ of superconducting element in non-metallic host which makes the system superconducting ($x_{\rm cr} \approx 0.4$). A more detailed study of the properties of superconducting alloys with off-diagonal disorder will be presented elsewhere [13].

Acknowledgments

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