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1992 J. Phys.: Condens. Matter 4 3283

(http://iopscience.iop.org/0953-8984/4/12/018)

J. Phys.: Condens. Matter 4 (1992) 3283–3288. Printed in the UK

Superconductivity of narrow-band metals in a model of multichannel scattering on electron density fluctuations

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Received 11 October 1991

Abstract. We consider the possibility that superconductivity (SC) may arise in narrow-band metals owing to electron–electron correlations. Consideration is given also to the superconductivity suppression mechanisms which are caused by the same correlations (spin fluctuations, or transition to dielectric phase). A new approach is proposed to describe high-T_c SC by introducing the Nambu field in the functional integral scheme. A stable superconducting state is realized in a rather small region of parameters: hole concentration and Hubbard repulsion. A method is proposed for approximating an interacting system by means of some simple multichannel models.

1. Introduction

We discuss the superconductivity (SC) that arises in systems with a narrow band, of width w, owing to the intratomic electron repulsion U in region $U \leqslant w$ [1]. The consideration is based on the Hubbard model in the functional integral technique (in its simplest Gaussian form). This permits introduction of relatively independent channels of multiple particle–particle and particle–hole scattering [2]. Significantly, the final results depend on the specification of the general Hubbard system at the level of the free-energy functional. Novel results are obtained as a result of the introduction of a fluctuating Nambu field that acts on the anomalous electron density component. The non-equivalency of the various scattering channels, which is due to the rather complicated electron structure of high-T_c superconductors, is very important for our consideration. We discuss both factors that lead to SC and those that suppress it. The latter factors include strong spin-density fluctuations and the appearance of a dielectric gap in the normal excitation spectrum.

2. Formalism

Let us consider the Hubbard model with the Hamiltonian

$$H = H_0 + H_1 \qquad H_0 = \sum_{ks} \varepsilon_k n_{ks} \qquad H_1 = \sum_{ks} U n_{js} n_{j-s} \tag{1}$$

where n_{ks} is the operator of electron numbers in a Bloch state with energy ε_k and spin projections $s = +, -$ and n_{js} is the same operator for a site j.

0953-8984/92/123283 + 06 $04.50

Let us write H_1 as a sum of the squares of the operators ρ:

$$H_1 = \sum_j (u_0\rho_{0j}^2 - u_z\rho_{zj}^2 + u_y^x\rho_{yj}^{x2}) \tag{2}$$

where

$$\rho_{0,z} = (\bar{a}_+a_+ \pm \bar{a}_-a_-)/2 \qquad \rho_y^x = (\bar{a}_+\bar{a}_- - a_-a_+)/2\mathrm{i},$$

and $\bar{a}_s$ and a_s are the creation and annihilation operators, respectively, on site j. Note that ρ_{0j} and ρ_{zj} are the standard operators of the charge and spin electron densities and ρ_{yj}^x is an operator describing an anomalous density matrix component.

Equations (1) and (2) tell us that the constants u_0, u_z and u_y^x are consistent with the equation

$$u_0 + u_z + u_y^x = 2U. \tag{3}$$

The Stratonovich–Hubbard transformation [3] allows us to replace the initial system (1) by an equivalent ensemble of electrons that are in fluctuating (in time τ and space R_j) fields $[V] = V_{\beta j}^{\alpha}(\tau)$:

$$H_1 \to H_1[V] = \sum_j (V_{0j}(\tau)\rho_{0j}(\tau) + V_{zj}(\tau)\rho_{zj}(\tau) + V_{yj}^x(\tau)\rho_{yj}^x(\tau)). \tag{4}$$

Each field configuration $[V]$ has a weight determined by its free energy. The field-averaged values can be calculated in explicit form in the quadratic (Gaussian) approximation for the energy functional.

The simplest equations are obtained in the local approximation, which is quite acceptable for chaotic fluctuations [4]. The equations for the normal self-energy part (SEP) Σ and the anomalous SEP Δ have the forms

$$\begin{aligned} \Sigma(\mathrm{i}\omega_n) &= T\sum_{n'} [\Gamma(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'}) + \tilde{\Gamma}(\mathrm{i}\omega_n + \mathrm{i}\omega_{n'}]G(\mathrm{i}\omega_{n'}) \\ \Delta(\mathrm{i}\omega_n) &= T\sum_{n'} D(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'})F(\mathrm{i}\omega_{n'}) \end{aligned} \tag{5}$$

with $\omega_n = 2\pi nT$ being the thermodynamic frequencies. The normal single-site Green function G and the anomalous single-site Green function F are related to Σ and Δ by the standard equations [1]

$$\begin{aligned} G(\varepsilon) &= \tfrac{1}{2}[1 + (\varepsilon - \Sigma_a)/r]G^0(r - \Sigma_s) + (r \to -r) \\ F(\varepsilon) &= (\Delta/2r)G^0(r - \Sigma_s) + (r \to -r) \end{aligned} \tag{6}$$

where

$$r = \{[\varepsilon - \Sigma_a(\varepsilon)]^2 - \Delta^2(\varepsilon)\}^{1/2} \qquad \Sigma_{s,a} = [\Sigma(\varepsilon) \pm \Sigma(-\varepsilon)]/2$$

$$G^0(\varepsilon) = \int \mathrm{d}\varepsilon', \nu^0(\varepsilon')/(\varepsilon - \varepsilon')$$

and $\nu^0(\varepsilon)$ is the density of states (DOS) of non-interacting electrons.

The normal effective single-site interaction $\Gamma + \tilde{\Gamma}$ and the pairing effective single-site interaction D are determined by the contribution of three scattering channels which

arise as a result of the fluctuations in the electron-exchanging charge (u_0 channel), the spin density u_z and the anomalous density u_y^x. Thus,

$$\begin{aligned}\Gamma(\varepsilon) &= [u_0^2\chi(\varepsilon)/2]/[1 + u_0\chi(\varepsilon)] + [u_z^2\chi(\varepsilon)/2]/[1 - u_z\chi(\varepsilon)]\\ \tilde{\Gamma}(\varepsilon) &= -[u_y^{x\,2}\tilde{\chi}_s(\varepsilon)/2]/[1 + u_y^x\tilde{\chi}_s(\varepsilon)]\\ D(\varepsilon) &= U - [u_0^2\chi(\varepsilon)/2]/[1 + u_0\chi(\varepsilon)] + [u_z^2\chi(\varepsilon)/2]/[1 - u_z\chi(\varepsilon)]\\ &\quad - [u_y^{x\,2}\tilde{\chi}_s(\varepsilon)/2]/[1 + u_y^x\tilde{\chi}_s(\varepsilon)].\end{aligned} \tag{7}$$

The local electron–hole susceptibility $\chi(i\omega_n)$ and the electron–electron susceptibility $\tilde{\chi}(i\omega_n)$ are given by

$$\left.\begin{matrix}\chi(i\omega_n)\\ \tilde{\chi}(i\omega_n)\end{matrix}\right\} = \pm T\sum_{n'} G(i\omega_n \pm i\omega_{n'})G(i\omega_{n'}). \tag{8}$$

3. Results

Because of the singular behaviour of the anomalous Green function $F(\varepsilon \to 0) \propto \Delta(0)i\nu(0)/\varepsilon$, the non-trivial solution of the second equation (5) arises only provided that $D(0) < 0$. According to (7), this condition can be obtained owing to the u_y^x channel if

$$u_{cr2} \leqslant u_y^x \leqslant u_{cr1} < 0. \tag{9}$$

The value $u_0 > 0$ corresponds to the repulsion of charge fluctuations. The second critical value u_{cr2} follows from the requirement that the Gaussian approach be stable: $1 + u_y^x\tilde{\chi}(0) > 0$.

A non-zero region of parameters U and hole concentrations b exists which satisfies the inequalities (9) because $\tilde{\chi}(0; b) \geqslant \chi(0; b)$ for any hole concentration. For a rectangular DOS of unit width (here and henceforth used for illustrations), the local Cooper susceptibility $\tilde{\chi}(0; b) = 2\ln 2$ is always independent of b, while $\chi(0; b)$ decreases monotonically from the above value at $b = 0.5$ to zero at $b = 0$.

The inequality (9) is a necessary but insufficient condition for superconductivity. The point is that the large (resonance) negative effective interaction $\tilde{\Gamma}$ in the u_y^x channel also affects the normal averages. This can lead to a dielectric gap arising in the normal excitation spectrum. The negative interaction can bring the Fermi-level one-particle states outside the initial band, i.e.

$$\varepsilon - \mathrm{Re}[\Sigma_s(\varepsilon)] > \varepsilon_{max} \qquad \varepsilon \to \varepsilon_F = 0. \tag{10}$$

Since the damping on the Fermi level is absent ($\mathrm{Im}[\Sigma(\varepsilon)] \propto \varepsilon^2$), the DOS goes to zero.

The ground-state phase diagram is shown in figure 1 ($u_0 = 2U$; $u_z = -u_y^x = U$). The SC phase borders the dielectric phase (D) on one side and the paramagnetic phase with strong spin-density fluctuations (SF) on the other.

The characteristics of the SC state are shown in figure 2. The real part (full curve) of the pairing interaction $\mathrm{Re}[D(\varepsilon)]$ is determined mainly by the u_y^x channel and is of a highly resonant type. The gap function $\Delta(\varepsilon)$ closely reproduces the $D(\varepsilon)$ curve (with opposite sign) in the initial portion of the energy ε scale. It is the strong energy dispersion that causes the relative SC transition temperature to lower than that in the standard BCS theory: $2\Delta(0)/T_c \simeq 10$.

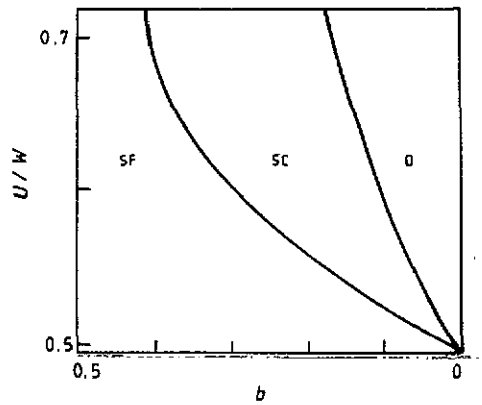

Figure 1. Phase diagram in coordinates of hole concentration b and intratomic repulsion U ($u_0 = 2U$; $u_z = -u_z^+ = U$).

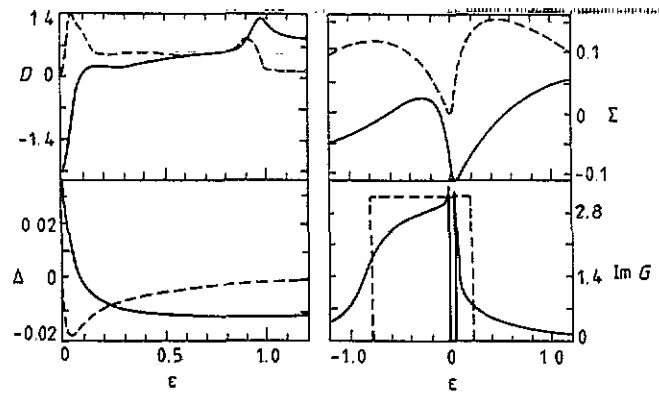

Figure 2. Effective pairing interaction D, the gap function Δ, the normal SEP Σ (——, real parts of advanced functions; – – –, imaginary parts of advanced functions), and the DOS $\nu = \mathrm{Im}\, G/\pi$ in the SC state ($b = 0.2$; $u_0 = 2U$; $u_z = -u_z^+ = U = 0.65$). The broken lines indicate the initial rectangular DOS.

Thus, we have discussed the possibility that a superconducting state may arise owing to the electron correlations described in the Gauss approximation for charge and spin-density fluctuations and also the anomalous density fluctuations (given by the Nambu field). The method that we have developed permits various multiple-scattering channels to be included in a unified theory. The distribution of the interactions between different channels is rather arbitrary in terms of the isotropic Hubbard model (only equation (3) must be satisfied). In fact, the choice of channel-constant values must correspond to the electron structure and interactions in real (non-isotropic and many-band) superconductors. One of the possible approaches to determining the channel distribution is presented in section 4.

Formally, the initial Hubbard interaction is written as a sum of several terms. One of them (anomalous fluctuations) leads to electron attraction, and the rest of the terms (charge and spin fluctuations) to electron repulsion. The energy (time) dependences of

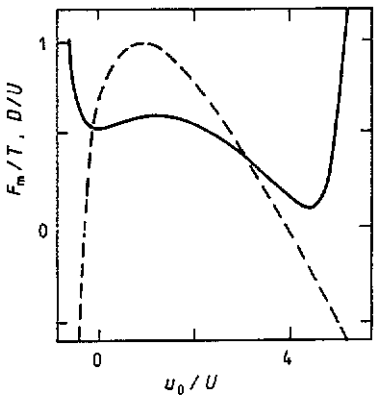

Figure 3. Model free energy F_m (——) and pairing interaction $D(0)$ (– – –) versus charge channel constant $u_{\parallel}$ ($u_z = 0$; $u_\uparrow^x = u_\uparrow^y = U - u_{\parallel}/2$; $U = 0.5$; $\chi(0) = 0.8\tilde{\chi}(0)$).

the interactions in the corresponding channels are such that the attractive interaction has a larger retardation than the repulsive one (the Cooper susceptibility $\tilde{\chi}$ is larger than the spin susceptibility χ). As a result, with the times being large (or small energy excitations) the attraction exceeds the repulsion, and the generation of Cooper pairs becomes possible.

4. Calculation of the channel weights by minimizing the free energy

Method of minimizing a model free energy for determining a relation between the charge and spin field constants was first introduced by Hirooka and Shimizu [5] in connection with the temperature itinerant magnetism problem. We use an analogous method for determining the channel weights.

According to the variational principle, the true free energy F is less the model energy F_m, i.e.

$$F \leqslant F_m = F_G + \langle \psi - \psi_G \rangle_G \tag{11}$$

where F_G is the free energy in the Gauss approximation.

For simplicity, we use the static approximation. For the charge fluctuation channel we have

$$\langle \psi_0 - \psi_{0G} \rangle_G = -\ln(1 - W_0^2) - W_0^2 \qquad W_0^2 = [u_0\chi(0)/2]/[1 + u_0\chi(0)]. \tag{12}$$

Of course, the true free energy F is independent of values of the constants u_0, u_z, u_y^x, etc, subject to the condition (3), but the model F_m acquires such a dependence. Minimizing F_m with respect to the values of u_α we obtain, according to (11), the best approximation for the interacting system on the class of relatively simple model systems.

Figure 3 illustrates the case $u_z = 0$, $u_y^x = u_y^y = \bar{u} = U - u_0/2$ ($U = 0.5$; $\chi(0) = 0.8\tilde{\chi}(0)$). It describes the combination of the well known channel of multiplex single-site electron–electron scattering and the channel of charge fluctuations. Here we have rejected the spin fluctuations in order to make the free energy a function of one variable. The full curve gives F_m versus u_0. The left-hand minimum is formed owing to the

contribution of the charge fluctuations (with $u_0 < 0$), while the right-hand minimum comes from the Nambu channel ($\bar{u} < 0$).

Of course, a situation is possible in which the curve $F_m(u_0)$ has only one minumum, but in any case the curve has a segment with a weak u_0 dependence. The broken curve shows the pairing interaction $D(0)$. In the present version, the $D(0)$ is negative in the point, where the free energy F_m has a minimum value, a fact which can lead to a superconductive state.

We do not quote results for different relations between the parameters. The main goal of this paper was to ascertain whether attraction and SC can arise owing to the electron–electron interaction.

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