ON SUPERCONDUCTIVITY IN THE THREE-BAND TWO-DIMENSIONAL REPULSIVE HUBBARD MODEL
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The three-band Hubbard model, known also as the Emery model, is investigated in the framework of thermal Green functions. It is shown that antiferromagnetic and superconductive states can exist in this model at appropriate doping and sufficiently low temperatures. In the two-dimensional repulsive case under consideration, superconductivity turns out to be possible due to the closeness of the Fermi level to one of the energy function saddle points and the pairing occurs in channels with odd angular momenta.

1. Introduction

This paper is devoted to the three-band two-dimensional (2D) repulsive Hubbard model, which seems to be a more realistic HTSC-candidate than the one-band Hubbard model investigated earlier [1-5]. The given paper is based on the results of [6, 7], where one can find more technical details.

Any HTSC-theory must explain the transition from antiferromagnetic behavior near half-filling to superconductivity at sufficiently high doping. For example, it is established by computer simulations that antiferromagnetic ordering exists at exact half-filling and disappears upon deviation from it, both in the one-band [8] and the three-band [9] repulsive Hubbard models. Application of the thermal Green function method to the simple 2D repulsive Hubbard model also demonstrates that antiferromagnetism exists at low doping and breaks down with increases in the doping parameter [1, 2].

A possible way of investigating superconductivity in the 2D repulsive Hubbard model was suggested in [2, 3]. As was shown in [4, 5], superconductivity in this model can exist if one of the Van Hove saddle points [10] lies in a close vicinity of the Fermi level. The type of Cooper pairing in such a state can be treated as a “superposition of pairings with odd angular momenta.” After the pioneer work [11], a lot of attention was attracted to the possible role of Van Hove singularities in increasing $T_c$ [12].

The aim of the present paper is to check whether the results obtained for the one-band case are still valid for the more complicated three-band system.

The paper is organized as follows. Section 2 contains an outline of the model. Here the perturbation scheme to calculate the Green functions is presented. Section 3 is devoted to the application of perturbation theory to the normal state of the system. Section 4 deals with antiferromagnetic ordering in the model in question, and in Section 5, we apply our approach to the superconducting state. The main results obtained in this work, as well as some prospects for further investigations, are discussed in the Conclusion, Section 6.

2. Outline of the model

The single-band repulsive Hubbard model exhibits the possibility of superconductive states with odd angular momenta pairing if the Fermi level is close to one of the Van Hove saddle points of the quasiparticle energy [1-5]. This model, however, can be considered only as a toy model for HTSC. Here, a more realistic three-band repulsive model is investigated which describes the quasi two-dimensional motion of electrons within the Cu–O$_2$ planes of high-$T_c$ oxides. The model accounts for the 2$p_x$, 2$p_y$ states of “oxygen” sites and the 3$d_{x^2-y^2}$ states of “copper” sites which are the most strongly hybridized [13]. It is appropriate to

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represent the face-centered lattice under consideration as consisting of three sublattices with \( N = L^2 \) sites in each (i.e., one corresponds to the “copper” sites, and the other two to the “oxygen” sites) so that the total number of sites is \( 3N \).

The corresponding Hamiltonian is of the type proposed by Emery [13] and is as follows:

\[
\hat{H} - \mu \hat{N} = -t_1 \sum_{\langle i,j \rangle, s} (d_{i,s}^+ p_{j,s} + p_{j,s}^+ d_{i,s}) - t_2 \sum_{\langle i,j \rangle, s} (d_{i,s}^+ p_{j,s} + p_{j,s}^+ d_{i,s}) \\
+ (\epsilon_d - \mu) \sum_{i,s} d_{i,s}^+ d_{i,s} + \epsilon_p \sum_{i,s} p_{i,s}^+ p_{i,s} + (\epsilon_p - \mu) \sum_{i,s} p_{i,s}^+ p_{i,s} \\
+ U_d \sum_i d_{i,s}^+ d_{i,s} + U_p \sum_{j_1} p_{j_1,s}^+ p_{j_1,s} + U_p \sum_{j_2} p_{j_2,s}^+ p_{j_2,s}.
\]

Here \( d_{i,s}^+ \), \( d_{i,s} \) are the operators of creation and annihilation of fermions with spin \( s = \uparrow, \downarrow \) at the “copper” sites \( i \), \( p_{j,s}^+ \), \( p_{j,s} \) are the corresponding Fermi operators at the “oxygen” sites \( j_k \) \((k = 1, 2)\). The Hamiltonian (2.1) accounts for hoppings between the nearest “copper” and “oxygen” sites \((t_1 \text{ and } t_2 \text{ are the hopping amplitudes})\) and also for on-site repulsion with the coefficients \( U_d \), \( U_p_1 = U_p_2 = U_p > 0 \). Repulsion between fermions at neighboring sites is neglected. The parameters \( \epsilon_d \), \( \epsilon_p_1 = \epsilon_p_2 = \epsilon_p \) are the band energies and \( \mu \) is the chemical potential.

It is more convenient to rewrite (2.1) in momentum representation using the standard Fourier transform with periodic boundary conditions, where the momenta take the values \( 2\pi n_i/L \), \( 1 \leq n_i \leq L \). It is suitable to introduce the notation

\[
\psi_{s}(\vec{k}) = \begin{pmatrix} d_{s}(\vec{k}) \\ p_{1,s}(\vec{k}) \\ p_{2,s}(\vec{k}) \end{pmatrix}, \quad \psi_{s}^{+}(\vec{k}) = \begin{pmatrix} d_{s}^{+}(\vec{k}) \\ p_{1,s}^{+}(\vec{k}) \\ p_{2,s}^{+}(\vec{k}) \end{pmatrix},
\]

for which (2.1) takes the form

\[
\hat{H} - \mu \hat{N} = \sum_{\vec{k}, s} \psi_{s}^{+}(\vec{k}) H_0(\vec{k}) \psi_{s}(\vec{k}) \\
+ N^{-1} \sum_{\alpha = 1}^{3} U_{\alpha} \sum_{\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4} \psi_{s}^{+}(\vec{k}_1) \psi_{s}^{+}(\vec{k}_2) \psi_{s}(\vec{k}_3) \psi_{s}(\vec{k}_4), \quad (2.2)
\]

where

\[
H_0(\vec{k}) = \begin{pmatrix} \epsilon_d - \mu & -T_1(\vec{k}) & -T_2(\vec{k}) \\ -T_1(\vec{k}) & \epsilon_p - \mu & 0 \\ -T_2(\vec{k}) & 0 & \epsilon_p - \mu \end{pmatrix},
\]

\[
T_i(\vec{k}) = t_i(1 + e^{ik_i}), \quad i = 1, 2, \quad U_1 = U_d, \quad U_2 = U_3 = U_p,
\]

and * means complex conjugation.

We shall use thermal perturbation theory [14] in the formalism of functional integration [15] to investigate models (2.1) and (2.2). To develop corresponding diagram technique, one has to define the action functional \( S \) and extract a “bare” action \( S_0 \) (the difference \( S - S_0 \) is a perturbation) from it. The explicit expression for \( S \) in our case looks as follows:

\[
S = S_0 + S_1, \quad S_0 = \sum_{p,s} \psi_{s}^{*}(p) G_0^{-1}(p) \psi_{s}(p),
\]

\[
S_1 = -\beta N^{-1} \sum_{\alpha = 1}^{3} U_{\alpha} \sum_{p_1 + p_2 = p_3 + p_4} \psi_{s}^{*}(p_1) \psi_{s}^{*}(p_2) \psi_{s}(p_3) \psi_{s}(p_4), \quad (2.3)
\]

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