Physica C 497 (2014) 67–76

Contents lists available at ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

High-temperature superconductivity and normal state in the Holstein-t-J model

E.E. Zubov *

O.O. Galkin Institute for Physics and Engineering, NASU 72, R. Luxemburg Str., Donetsk 83114, Ukraine

ARTICLE INFO

Article history:
Received 12 August 2013
Accepted 7 November 2013
Available online 15 November 2013

Keywords:
t-J model
Polaron
Superconductivity

ABSTRACT

A possible origin of the high-temperature superconductivity in cuprates has been suggested. It is supposed that electron–phonon interaction determines the strong correlation narrowing of the electron band. It provides the conditions for the formation of a singlet electron pair coupled by exchange interaction. For the pure t-J model it has been proved that these electron pairs are destroyed by a strong effective kinematic field. The detailed analysis of an influence of the Holstein polaron excitations upon normal and superconducting properties of the strongly correlated electrons was made. A calculated critical temperature of the superconductivity and gap function are in good agreement with experimental data for cuprates.

1. Introduction

In the 21st century a phenomenon of the high-temperature superconductivity in cuprates continues to attract the attention of many researches [1]. There are a tremendous number of suggested mechanisms of this phenomenon. In any case there is not a such theory which would describe all properties of this complicated state. In this work we have centered on the main peculiarity which in our opinion might help to illuminate the origin of high-T_{SC} in cuprates. The electron–phonon coupling is supposed to be not essential in the Cooper electron pairings. But this interaction forms the polaron excitations which play an important role in the correlation narrowing of the electron band. In that case it is necessary to differentiate the collectivized electrons in metals and ones in doped cuprates. Indeed, in metals there is wave electron states with a possibility of the site double occupancy. But their hole states is virtual. And that's why we have the partition function $\exp(\varepsilon_{\mathbf{k}\sigma}/T)+\exp(\varepsilon_{\mathbf{k}-\sigma}/T)$ for electron excitations $\varepsilon_{\mathbf{k}\pm\sigma}$. In cuprates a coordinate representation is realized for electron wave functions and we have the partition function $1+\exp(\varepsilon_{\sigma}/T)+\exp(\varepsilon_{-\sigma}/T)$ with electron levels $\varepsilon_{\pm\sigma}$ and hole state.

The cuprates belong to class of the strongly correlated electron system. In work [2] an effective Hamiltonian of the t-J model was suggested based on the use of Gutzwiller projection operator. It allowed to exclude the upper Hubbard band with double site occupancy by electrons and essentially to simplify an investigation of the strongly correlated electron systems. In work [3] a mean field approximation of the t-J model was developed to study the high-temperature superconductivity. In this work a fundamental idea about spin pairing via electron exchange interaction was formulated. Unfortunately, authors were not taken into account the essential difference between metal and strongly correlated electrons. Using Bogolyubov's u–v transform of the Hamiltonian they obtained the equation for gap function to be similar in BCS theory.

In this work we propose to divide the mean field BCS type Hamiltonian into uniform and nonuniform parts. The perturbation theory was built with uniform unperturbed Hamiltonian. The nonuniform part is neglected since it has a weak influence on the hopping integral. A hopping term of the total t-J Hamiltonian is considered as perturbation in the limit of a weak doping with u–v transformed creation and destruction operators. The abnormal mean values to be proportional the superconductive gap function were calculated. It has been obtained the condition on values of the chemical potential and exchange parameter. With account of the correlation band narrowing we make the conclusion about impossibility of HTSC in the pure t-J model.

In what follow we include into consideration the electron–phonon interaction. The evidences for a presence of one and its important role in the strongly correlated systems were emphasized in works [4–6]. In view of the fact that Hamiltonian of electron–phonon coupling is nonuniform many authors simplify the kinematic part by simple renormalization of the hopping integral [6] or use the theory of Eliashberg for collectivized metal electrons [4]. In former case it gives rise to drastic suppression of the electron band and is responsible for the absence of HTSC in a system without interaction of polarons. The simplest form of the Holstein Hamiltonian for polarons needs to be considered with uniform electron–phonon interaction and Einstein phonon mode. One can provide the exact unitary transform to separate fermion and boson degree

* Tel.: +380 623429624.
E-mail address: zubov@fti.dn.ua

0921-4534/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physc.2013.11.005

of freedom. It allows to build the subsequent perturbation theory of the strongly correlated electron system with Holstein's polarons.

The structure of the paper is as follows. In Section 2 we consider the Hamiltonian of pure t-J model in the superconducting state. It was separated the uniform mean field part with corresponding coefficients of u–v transform. It enables us in Section 3 to build the perturbation theory for strongly correlated electrons in the superconducting state. In particular, it was obtained the transformed Hubbard operators in coordinate representation using the Bogolyubov's u–v transform. As a result, the equation for gap function and conditions for the existence of the superconducting state were presented. In Section 4 the properties of normal state without electron–phonon coupling are considered. In the framework of the developed diagrammatic method it was shown the absence of superconductivity in a pure t-J model. In Section 5 a normal state of the cuprate d-electrons with polaron excitations is investigated to find the critical temperature of superconducting state. In this section it has been solved the problem of a frequency summation with infinity number of poles as implicit functions. The suggested method of an inverse function allowed to calculate the diagrammatic contributions for all polaron bands. In Section 5 the obtained equations are solved numerically that allowed to find the concentration dependencies of the critical temperature T_{SC} and gap function Δ versus temperature. The theoretical values of T_{SC} and Δ are in good agreement with experiment that supports the model to put forward by us.

2. Hamiltonian of the system

The Hamiltonian of the Holstein model with strongly correlated electrons takes the form:

$$\widehat{H} = \widehat{H}_f + \widehat{H}_b, \tag{1}$$

where the Fermi part, $\widehat{H}_f$, is expressed as follows:

$$\widehat{H}_f = \sum_{i,j} J_{ij}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_i n_j\right) - \mu\sum_{i\sigma} n_{i\sigma} + \widehat{V}, \tag{2}$$

Here, J_{ij} is the indirect exchange of the collectivized d-electrons with spins $\mathbf{S}_i$ and $\mathbf{S}_j$, $n_i = n_{i\sigma} + n_{i-\sigma}$ is the electron concentration on i-site, μ is the chemical potential. The perturbation $\widehat{V}$ is written as

$$\widehat{V} = \sum_{i,j,\sigma} t_{ij} c^+_{\sigma i} c_{\sigma j}(1-n_{i-\sigma})(1-n_{j-\sigma}), \tag{3}$$

where $c^+_{\sigma i}$ ($c_{\sigma j}$) creates (annihilates) an electron with spin σ on lattice site i, respectively, and t_{ij} is the hopping integral to be equal to t for nearest neighbors. The Hamiltonian (2) of t-J model reflects the strong electron correlations. In a weak doping level we will consider the part (3) as a perturbation.

The boson part of Hamiltonian (1) has a form similar to that used in the Holstein model of a small polaron:

$$\widehat{H}_b = -g\sum_i n_i(b^+_i + b_i) + \omega_0\sum_i b^+_i b_i, \tag{4}$$

where g is the electron–phonon coupling strength, b^+_i and b_i are the phonon creation and destruction operators, respectively. We will use the Einstein model where the phonon frequency ω_0 is assumed to be dispersion-free.

The Lang–Firsov unitary transform [7] $\widetilde{U} = \exp\left(\widetilde{S}\right)$ of Hamiltonian (4) allows to separate the boson and fermion operators in (4), where $\widetilde{S} = -\frac{g}{\omega_0}\sum_i n_i(b^+_i - b_i)$. As a result we have

$$\widehat{\widetilde{H}}_b = \widetilde{U}^{-1}\widehat{H}_b\widetilde{U} = \omega_0\sum_i b^+_i b_i - \xi\sum_i n_i, \tag{5}$$

where $\xi = g^2/\omega_0$ is the polaron binding energy. The unitary transformed perturbation $\widehat{V}$ is presented as

$$\widehat{V} = \sum_{\langle ij\rangle,\sigma} t_{ij}\tilde{c}^+_{i\sigma}\tilde{c}_{j\sigma}(1-n_{i-\sigma})(1-n_{j-\sigma}). \tag{6}$$

Here, the unitary transformed Fermi operators

$$\tilde{c}_{i\sigma} = Y_i c_{i\sigma}, \tag{7}$$

are product of Bose $Y_i = e^{\lambda(b^+_i - b_i)}$ and corresponding Fermi destruction operators, where $\lambda = g/\omega_0$. It is necessary to point out that first and second terms of the Hamiltonian (2) are not changed under transform $\widetilde{U}$.

One can separate in a Heisenberg part of the Hamiltonian (2) by standard manner a mean field to be connected with anomalous averages [3]. Then an unperturbed Hamiltonian takes the form

$$\widehat{H}_{0f} = \sum_{\langle ij\rangle\sigma}\left\{\Delta_{ij\sigma}c^+_{i\sigma}c^+_{j-\sigma} + \Delta^*_{ij\sigma}c_{i-\sigma}c_{j\sigma}\right\} - \sum_{i\sigma}\tilde{\mu}_\sigma n_{i\sigma}, \tag{8}$$

where $\tilde{\mu}_\sigma = \tilde{\mu} - \sigma J(0)\langle S^z\rangle$, $\tilde{\mu} = \mu + \xi$, $\langle S^z\rangle$ is a mean electron spin and $\sigma = \pm 1$. The gap functions are expressed via exchange parameters:

$$\begin{aligned}\Delta_{ij\sigma} &= -J_{ij}\langle c_{i-\sigma}c_{j\sigma}\rangle,\\ \Delta^*_{ij\sigma} &= -J_{ij}\langle c^+_{i\sigma}c^+_{j-\sigma}\rangle.\end{aligned} \tag{9}$$

In a wave space the Hamiltonian (8) takes the form

$$\widehat{H}_{0f} = \sum_{\mathbf{k}\sigma}\{\Delta_{\mathbf{k}\sigma}c^+_{\mathbf{k}\sigma}c^+_{-\mathbf{k}-\sigma} + \Delta^*_{\mathbf{k}\sigma}c_{-\mathbf{k}-\sigma}c_{\mathbf{k}\sigma}\} - \sum_{\mathbf{k}\sigma}\tilde{\mu}_\sigma n_{\mathbf{k}\sigma}, \tag{10}$$

where the gap functions $\Delta_{\mathbf{k}\sigma}$ can be presented as

$$\Delta_{\mathbf{k}\sigma} = -\frac{1}{N}\sum_{\mathbf{q}} J(\mathbf{q}+\mathbf{k})\langle c_{-\mathbf{q}-\sigma}c_{\mathbf{q}\sigma}\rangle, \tag{11}$$

and $\Delta^*_{\mathbf{k}\sigma}$ is conjugate function $\Delta_{\mathbf{k}\sigma}$. One can point out that in Eqs. (9) and (11) the operators of creation and destruction are not transformed by operator Y_i from (7). The Bogolyubov's u–v transform

$$\begin{aligned}c_{\mathbf{k}\sigma} &= u^*_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} + v_{\mathbf{k}\sigma}\alpha^+_{-\mathbf{k}-\sigma},\\ c^+_{\mathbf{k}\sigma} &= u_{\mathbf{k}\sigma}\alpha^+_{\mathbf{k}\sigma} + v^*_{\mathbf{k}\sigma}\alpha_{-\mathbf{k}-\sigma},\end{aligned} \tag{12}$$

to new operators $\alpha_{\mathbf{k}\sigma}$ and $\alpha^+_{-\mathbf{k}-\sigma}$ allows to diagonalize $\widehat{H}_{0f}$ with the next conditions

$$u_{\mathbf{k}\sigma} = u_{-\mathbf{k}-\sigma}, \quad v_{\mathbf{k}\sigma} = -v_{-\mathbf{k}-\sigma}, \quad |u_{\mathbf{k}\sigma}|^2 + |v_{\mathbf{k}\sigma}|^2 = 1. \tag{13}$$

Then we have

$$\widehat{H}_{0f} = \sum_{\mathbf{k}\sigma}\widetilde{E}_{\mathbf{k}\sigma}\alpha^+_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma}, \tag{14}$$

where

$$\widetilde{E}_{\mathbf{k}\sigma} = -\tilde{\mu}\sqrt{1+\left(\frac{\Delta_{\mathbf{k}}}{\tilde{\mu}}\right)^2}. \tag{15}$$

In what follows we will consider a paramagnetic state when $\langle S^z\rangle = 0$. Then one can put

$$\tilde{\mu}_\sigma = \tilde{\mu}, \quad |\Delta_{\mathbf{k}\sigma}| = |\Delta_{-\mathbf{k}-\sigma}| = \Delta_{\mathbf{k}}. \tag{16}$$

So far it has been obtained that the BCS Hamiltonian (14) coincides with similar Hamiltonian of Baskaran–Zou–Anderson [3]. Unfortunately, the authors of work [3] do not separate perturbation $\widehat{V}$ from (1). Instead of this they narrow band multiplying the hopping integral t by factor x to be equal to hole concentration. It does not allow to find the rigorous statement relatively an appearance of the superconductivity since the band energy at $x\approx 0$ has finite quantity. That's why we will expand Eq. (14) in terms of the small parameter up to third order:

$$\widetilde{E}_{\mathbf{k}} = -\tilde{\mu}\left\{1 + \frac{1}{2}\frac{\Delta^2_{\mathbf{k}}}{\tilde{\mu}^2} - \frac{1}{8}\frac{\Delta^4_{\mathbf{k}}}{\tilde{\mu}^4} + \frac{3}{48}\frac{\Delta^6_{\mathbf{k}}}{\tilde{\mu}^6} - \cdots\right\}. \tag{17}$$