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MANY BAND EFFECTS IN CUPRATE SUPERCONDUCTORS

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The new theoretical approach is proposed for study the states responsible for superconductivity of crystals. Within the frameworks of worked out approach it is shown that in electron–phonon system a class of new so-called coupled states arises. Postulated in BCS method electron-pair states $k_1 + k_2 = 0$, $s + s' = 0$ are in natural manner included in this class. The model numerical calculations have shown that SC gap depends on number of bands crossing the Fermi level on the momenta $k_1 + k_2 = K \neq 0$ of interacting electrons and that the temperature dependence of SC gap for HTSC is more complicated (in agreement with the recent experimental data) then predicted in BCS approach.

1. Introduction

The explanation of high-T_c superconductivity of the crystals is now one of important problems in the condensed matter physics. It is confirmed by numerous papers and review articles[1–8] concerning of this aspect but the theoretical models describing this phenomena are in development up to now though this may be one of the most important questions. That is clearly seen for example from Refs. 5 and 7, works where the discussion about mechanisms of SC is the dominant problem of articles. We want to look at this problem once more and study in more detail some aspects of electron–phonon interactions. The theoretical study of superconductivity is based as a rule on the physical idea about pairing of electrons with the opposite spins ($s+s' = 0$) and momenta ($k + k' = 0$) [(Refs. 1, 2, and 5), the problem of electron pairing is postulated in all mechanisms)]. Using this postulate the possibility of arising of the coupled states in the electron (electron–phonon) system was investigated. These states are responsible for superconductivity in the mentioned system.

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In this work a new approach to the SC problem is proposed (as first step we will study the density of electron states in crystal). Within the frameworks of our approach we do not suppose *a priori* that special pairing of electrons (with opposite spins and momenta as it is traditionally supposed in BCS method) take place. However electrons in the crystal have to satisfy the following natural conditions:

(i) they are moving in the periodic crystal field generated by the lattice ions;
(ii) the electrons interact with each other and the ions of lattice by the Coulomb law; it means that colliding electrons may possess the arbitrary momenta (k) and spins (s) allowed for them by the corresponding electron zone (band) they belong to;
(iii) the structure and symmetry of electron bands are given by the crystal structure.

From our calculations it follows that in studied electrons system can arise new so called coupled states which give rise to lowering of system energy and to appearance of new features in the density of states. The arising of these states depends on the constants of electron–electron and electron–phonon interactions, on the structure of electron bands and on the temperature of crystal. The similar type of excitations are well known in phonon and polariton spectra of crystals (see Refs. 9 and 10 and references herein). The essential difference is that the electrons have an own magnetic moment (spin) therefore the coupled states in electron system will also depend on spins of crystal electron bands generating these coupled states. It will be seen the energy some of discussed coupled states precisely coincides with the value of energy which are obtained for superconducting gap using the traditional BCS pairing approach. However our results show that many other states (with nonzero momenta ($K = k + k' \neq 0$) and spins ($S = s + s' \neq 0$) of interacting electrons) give also contribution into SC of crystal (see also Refs. 11 and 12). It should be also noted the presence of several electron bands crossing the Fermi level (or closely located to the latter) gives rise to qualitatively new features in the density of states of electron system (for example the coupled states with whole number ($S \neq 0$) spins and located aside from Fermi level can arise). The spin features ($S \neq 0$) agrees with some results of recent work Pickett[13]).

2. Density of Current and Hamiltonian

In this article we present the general idea of our approach. The density of current can be written[14]

$$\langle j'(x,t)\rangle = \langle j(x)\rangle_0 - \frac{e^2}{mc}\langle n(x)\rangle_0 A(x,t) + \text{higher order} \tag{1}$$

$$\langle n(x)\rangle_0 = \langle \Psi^+(x)\Psi(x)\rangle_0$$
$$= \lim_{x'\to x, t'\to t-0} \{\delta(x-x') - i\langle -iT\Psi(x,t)\Psi^+(x',t')\}$$
$$= \frac{1}{V_0}\left[\sum_k 1 - i\sum_{k,\omega} G(k,\omega)\right], \tag{2}$$

where operators $\Psi(x)$ satisfy to Fermi commutation relations and are given by the expression

$$\Psi(x) = \sum_{k,\sigma,\nu} a^\nu_{k,\sigma}\varphi^\nu_{k,\sigma}(x), \tag{3}$$
$$\varphi^\nu_{k,\sigma}(x) = \varphi^\nu_k(x)\chi_\sigma(s),$$
$$\left[a^\nu_{k,\sigma}, a^{+\nu'}_{k',\sigma'}\right]_+ = \delta_{k,k'}\delta_{\sigma,\sigma'}\delta_{\nu,\nu'}, \tag{4}$$

$\varphi^\nu_k(x)$ is the Bloch function of electron in νth energy band of crystal and $\chi_\sigma(s)$ describes the spin of this electron. The density of electron states (DES) $\langle n(x)\rangle_0$ is expressed (2) by the Fourier components of Green function $G(k,\omega)$; V_0 is the volume of crystal

The Hamiltonian describing the system of interacting the electrons and phonons of crystal after transformation by unitary operator is written in the following form (more details will be described elsewhere, see also Refs. 9 and 10)

$$H = \sum_{k,\nu}\left(\varepsilon^\nu_k - \frac{1}{N}\sum_{s,q}\frac{|\chi^s_q|^2}{\Omega_{s,q}}\right)A^+_{k,\nu}A_{k,\nu}$$
$$+ \frac{1}{2N}\sum_{q,k,\nu,k',\nu'}\left(V_q - 2\sum_s\frac{|\chi^s_q|^2}{\Omega_{s,q}}\right)A^+_{k,\nu}A^+_{k',\nu'}A_{k'+q,\nu'}A_{k-q,\nu}$$
$$+ \sum_{s,q}\Omega_{s,q}\beta^+_{s,q}\beta_{s,q} - \frac{1}{\sqrt{N}}\sum_{k,q,\nu}(\varepsilon^\nu_k - \varepsilon^\nu_{k-q})A^+_{k,\nu}A_{k-q,\nu}\sigma_q, \tag{5}$$

where $V_q = V_{-q}$, $\chi^{*s}_q = \chi^s_{-q}$ are the Fourier components of Coulomb interaction of electrons between each other and their coupling constant with the lattice phonons respectively; ε^ν_k is the energy of electron. Both V_q and χ^s_q constants are independent on the band and on spin indices of electrons.

$$a^\nu_k = [\exp S]A_{k,\nu}[\exp(-S)];$$
$$b^s_q = [\exp S]\beta_{s,q}[\exp(-S)]; \tag{6}$$

where S is the anti-Hermitian operator ($S^+ = -S$) and σ_q operator is linear on phonons $\beta_{s,q}\beta^+_{s,q}$ operators.

In (5) we united two indexes so that $\nu = (\nu, \sigma)$, $\mu = (\mu, \sigma')$ are the complex indices which characterize the number of crystal band and spin of electron.

Unitary transformation gives rise to renormalization of electron energy (first term) and renormalization of Fourier component of Coulomb electron–electron interaction. In the latter case we can conclude if the crystal unit cell contains many atoms the effective Coulomb potential can became negative and large in value.

3. Two-Particle Green Function, Coupled States and Gap

To calculate the DES we have to study the Green function for case of striving for $t' \to t - 0$ in accordance with (2). For this situation arising two-particle Green function can be written as follows

$$G_2\left(\begin{matrix} k_2, \nu_2; k, \nu \\ k+q, \nu; k_2 - q, \nu_2 \end{matrix}; t - t'\right) = \left\langle -iTA_{k+q,\nu}(t)A_{k_2-q,\nu_2}(t)A^+_{k_2,\nu_2}(t')A^+_{k,\nu}(t')\right\rangle, \quad (t' \Rightarrow t - 0) \tag{7}$$

Such two-particle Green function satisfy the equation type Bethe-Salpeter (we do not split this function into two Gorkov type[15] one particle Green functions). The solution of mentioned equation following to Bogolubov–Tyablikov method[14,16] give rise to the next expression for Fourier component of two-particle Green function

$$G_2\left(\begin{matrix} k_2, \nu; k_1, \mu \\ k_1 + q, \mu; k_2 - q, \nu \end{matrix} \middle| \omega\right) \sim \frac{f(k_1, \mu; k_2, \nu; \omega) \sum_{\sigma,\sigma'} \varphi(\mu, \nu; \sigma, \sigma')}{1 - VK(k_1, \mu; k_2, \nu', \omega)}, \tag{8}$$

$$K(k_1, \mu; k_2, \nu; \omega) = \frac{1}{N} \sum_q \frac{1 - n^\mu_{k_1+q} - n^\nu_{k_2-q}}{\omega - \varepsilon_{k_1+q,\mu} - \varepsilon_{k_2-q,\nu}} \tag{9}$$

$$V = \tilde{V}_q = V_q - 2\sum_s \frac{|\chi^s_q|^2}{\Omega_{s,q}} \approx \text{const.},$$

where n^ν_k is the filling number of electrons, V is the effective Fourier component of electron–electron (e–e) interaction. If the constant of e–e interaction renormalized by e–ph interaction become negative ($V < 0$) the arising of new type of states (coupled states) in the electron system is possible. Equations (8) and (9) gives the spectral features in the region of two-particle states. Therefore let us study these expressions. It is seen from Eqs. (8) and (9) that if momenta of interacting electrons $k_1 = k_2 = 0$ or $k_2 = -k_1$ the denominator (8) is precisely reduced to well known expression describing the SC gap of crystal, but for other arbitrary meanings of momenta k_1 and k_2 of electrons the situation are significantly different. From Eqs. (8) and (9) it follows that besides states corresponding to traditional BCS pairing there are many new states occurring in Eq. (8) and giving the contribution into the SC gap, which therefore depends on the momenta of interacting electrons. That will be shown later. The numerator of Eq. (8) gives rise to new possibilities.

Here $f(k_1, \mu; k_2, \nu', \omega)$ is the function depending on the frequency (ω) and momenta k_1 and k_2 of interacting electrons; the second function $\varphi(\mu, \nu', \sigma, \sigma')$ is expressed by numbers of delta-functions $\delta_{i,j}$ and define the spin forbidden rules for coupled state (responsible for superconductivity effects)

$$\varphi(\mu, \nu', \sigma, \sigma') = \delta_{\sigma\sigma}\delta_{\sigma'\sigma'} - \delta_{\mu\nu}\delta_{\sigma\sigma'}\delta_{\sigma\sigma'}\,, \tag{10}$$

where σ, σ' are spins of first (σ) and second (σ') electrons respectively; μ, ν show the number of the electron band. The next particular cases are possible:

(1) $\mu = \nu$.

(i) if spins of electrons are equal to each other ($\sigma = \sigma'$) then $\varphi(\mu, \mu; \sigma, \sigma') = 0$;

(ii) if spins of both electrons are nonequal ($\sigma \neq \sigma'$) the second term in the right hand side of (10) (which is proportional to $\delta_{\sigma,\sigma'}$) disappear and therefore $\varphi(\mu, \mu; \sigma, \sigma') \neq 0$. It means that only states with the oppositely directed spins (namely singlet states $\sigma + \sigma' = 0$ in this simplest case) can contribute into coupled states of electron system.

(2) $\mu \neq \nu'$. This case corresponds to more complex structure of crystal zones (in particular that takes place for layer Bi-based type of crystal[17,18]). The second term in the right hand part of Eq. (10) (which is proportional to $\delta_{\mu\nu}$) disappears and therefore $\varphi(\mu, \nu', \sigma, \sigma') \neq 0$ for all values of spins. It means that all possible spin states (for example $\sigma + \sigma' = 0,\ \pm 1$, etc.) are admitted.

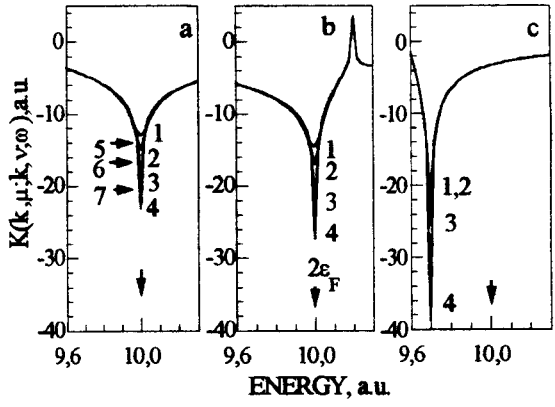
The energy position of coupled states are given by zero of denominator of (8) and depends on function $K(k_1, \mu; k_2, \nu'; \omega)$ and constant V (9). Let us study the particular case supposing $k_1 = k_2 = k_0 + k$ and $\varepsilon_{k_0,\mu} = \varepsilon_\mu$ corresponds to extremum of zone. Then expanding the energy by momentum $k \pm q$ in series up to terms of second order we can obtain

$$\varepsilon_{k\pm q,\mu} = \varepsilon_\mu + \frac{(k \pm q)^2}{2m_\mu} = \varepsilon_f + \Delta_\mu + \frac{(k \pm q)^2}{2m_\mu}\,, \tag{11}$$

where m_μ is the effective mass of electron in the μth ($\mu = 1, 2$), energy band of crystal; Δ_μ is a parameter which points out the position of the μ-band extremum relative to Fermi level. It may be negative and positive and the effective mass the same. (The anisotropy of crystal can be simply taken into account by anisotropy of the effective mass in Eq. (11)). At the traditional approximation ($\mu = 1$) the function $K(k, \mu; k, \mu; \omega)$ and the SC gap are described the well known standard expressions[12] but exact numerical calculation of function $K(k, \mu; k, \mu; \omega)$ give rise to new features especially if several electron bands ($\mu \neq 1$) are included into consideration. It is due to that the analytical analysis is not taking into account many features which are contained in the function $K(k, \mu; k, \nu'; \omega)$ because of the influence of momenta and temperature through the electron filling number. It should be also noted that for some type of SC crystals the minimum of electron band is

located much lower (0.7–0.8 eV for $Ba_2Sr_2CaCu_2O_8$)[17,18] of the Fermi level energy. Therefore we study namely similar situation because the mentioned crystal have a high T_c temperature.

The results of some numerical calculations are given in Figs. 1–3. The effect of temperature is seen in Figs. 1(a)–(c) where T-dependences of $K(k,\mu;k,\nu',\omega)$ functions for different cases of electron bands structure (EBS) are presented. It follows from Fig. 1(c) that presence of several electron bands generates the $K(k,\mu;k,\nu';\omega)$ function having the minimum located aside from $2\varepsilon_F$ energy level. The arrows 5–7 in Fig. 1(a) corresponds to different values of constant $1/V$ ($V<0$), (see captions to figures). The intersection, if it occurs, the curves 1–4 with the extension of arrows give the energy of coupled states because obtained solutions correspond to zero of denominator (8).

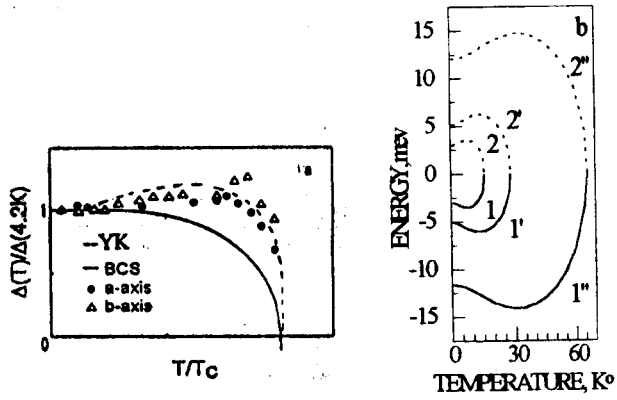


(a) (b) (c)

Fig. 1. (a) The effect of temperature on the $K(k,\mu;k,\nu;\omega)$ function ($E=k^2/2m=0$) for different structures of energy zones: (a) $\Delta_1=-1$, $m_1^*=1$; (b) $\Delta_2=0.2$, $m_2^*=-2$; and (c) $\Delta_1=-1$, $m_1^*=1$, $\Delta_2=0.2$, $m_2^*=-2$; curve 4, $T=2$ K; curve 3, $T=10$ K; curve 2, $T=50$ K; curve 1, $T=100$ K; arrows 5–7 corresponds to different of values $1/V$ (arrow 5, $V=-0.07$; arrow 6, $V=0.06$; arrow 7, $V=-0.05$). All energetic values are taken as arbitrary values, i.e. $V=V/M$, where M is scale factor ($M=1$ eV, for convenience; $m_i^*=m_i/m$, m is free electron mass).

Therefore the coupled states obtained all crossing of extension of the arrows 5–7 with the mentioned function will be also located good far from $2\varepsilon_F$ energy level. As a result T-dependence of SC state may became more complicated than for only one electron band. In Figs. 1(a)–(c) the curves $4\to 1$ describe the change of $K(k,\mu;k,\nu',\omega)$ function with increase of temperature. Therefore for fixed value of constant V (arrow 7 for example) the coupled states arise at low temperature (curve 4) but disappear at more high temperatures (curves 3–1). The temperature dependences of coupled states energies (for case of band given in Fig. 1(a) are pictured in Fig. 2(b) by curves 1, 1′ and 1″ (solid lines) corresponding to different

values of parameter V. The obtained dependences are not similar to standard BCS ones. For illustration the experimental dependences of SC gap obtained in work[19] for crystal $Ba_2Sr_2CaCu_2O_8$ are presented in Fig. 2(a) together with the theoretical curves of BCS type and our calculation. It is clearly seen that our calculation predicting the maximum in the T-dependence of SC gap gives the curve which is more close to the experimental results.



(a) (b)

Fig. 2. The temperature dependences of SC gap: (a) experiment (•, Δ) and theory [(—) BCS (- - -) our calculation) (b) calculated dependences of SC gap for different values of parameters effective e–e interaction V (the structure of electron bands and meaning of V as taken in Fig. 1(a).

Our calculations also show that SC gap depends on momenta (k) of interacting electrons. But coupled states arise if $k \leq k_{\text{lim}}$ takes place where k_{lim} depends on V. It is obviously that k-factor must be contained in the experimental T-dependence of SC gap and so that may be one of reasons of difference between the curve YK (Fig. 2(a)) calculated by us for $k = 0$ and experimental results.

In conclusion, the new theoretical approach is proposed for studying the coupled states responsible for superconductivity in crystal without using the idea of electron pairing. The proposed approach is shown that SC coupled states can be created by pairs of Coulomb interacting electrons with nonzero full momenta and spins ($k_1 + k_2 \neq 0$, $s + s' \neq 0$). The model numerical calculations have shown that dependence of SC gap (energy of coupled states) on temperature is different from BCS type and depends on the momenta of interacting electrons.

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