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Many-zone effects in cuprate superconductors

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

1. Introduction

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

In this work a new approach to the SC problem is proposed (as a first step we will study the density of electron states (DES) in a crystal). Within the framework of our approach we do not suppose *a priori* that special pairing of electrons (with opposite spins and momenta as is traditionally supposed in the BCS method) takes place. However, electrons in the crystal have to satisfy the following natural conditions: (i) they move in the crystal under a periodic field generated by the lattice ions; (ii) the electrons interact with each other and the ions of the lattice by the Coulomb law, which means that colliding electrons may possess arbitrary momenta (k) and spins (s) allowed

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 new so-called coupled states can arise in the electron system which give rise to the lowering of the system energy and to the appearance of new features in the density of states. The appearance 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 the crystal. Similar types of excitations are well known in phonon and polariton spectra of crystals ([9, 10] and references therein). The essential difference is that the electrons have their own magnetic moment (spin), and therefore the coupled states in the electron system will also depend on the spins of the crystal electron bands generating these coupled states. It will be seen that the energies of some of the discussed coupled states precisely coincide with the values of the energy which are obtained for the 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) also contribute to the SC of crystals (see also [11, 12]). It should also be noted that 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 the electron system (for example, coupled states with a whole number ($S \neq 0$) of spins and located apart from the Fermi level can arise). The spin features ($S \neq 0$) agree with some results of recent work [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]

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

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

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

$$\Psi(x) = \sum_{k, \sigma, \nu} a_{k, \sigma}^{\nu} \varphi_{k, \sigma}^{\nu}(x) \quad (3)$$

where

$$\varphi_{k, \sigma}^{\nu}(x) = \varphi_k^{\nu}(x) \chi_{\sigma}(s) \quad [a_{k, \sigma}^{\nu}, a_{k', \sigma'}^{\nu'}]_{\pm} = \delta_{k, k'} \delta_{\sigma, \sigma'} \delta_{\nu, \nu'} \quad (4)$$

$\varphi_k^{\nu}(x)$ is the Bloch function of an electron in the ν th energy band of the crystal and $\chi_{\sigma}(s)$ describes the spin of this electron. The DES $\langle n(x) \rangle_0$ is expressed (equation (2)) by the Fourier components of the Green function $G(k, \omega)$; V_0 is the volume of the crystal.

The Hamiltonian describing the system of interacting electrons and phonons of the crystal after transformation by a unitary operator is written in the following form (it will be described in more detail elsewhere; see also [9, 10]):

$$\begin{aligned} H &= \sum_{k, \nu} \left(\varepsilon_k^{\nu} - \frac{1}{N} \sum_{s, q} \frac{|\chi_q^s|^2}{\Omega_{s, q}} \right) A_{k, \nu}^+ A_{k, \nu} \\ &+ \frac{1}{2N} \sum_{q, k, \nu, k', \nu'} \left(V_q - 2 \sum_s \frac{|\chi_q^s|^2}{\Omega_{s, q}} \right) \\ &\times A_{k, \nu}^+ A_{k', \nu'}^+ A_{k'+q, \nu'} A_{k-q, \nu} + \sum_{s, q} \Omega_{s, q} \beta_{s, q}^+ \beta_{s, q} \\ &- \frac{1}{N^{1/2}} \sum_{k, q, \nu} (\varepsilon_k^{\nu} - \varepsilon_{k-q}^{\nu}) A_{k, \nu}^+ A_{k-q, \nu} \sigma_q \end{aligned} \quad (5)$$

where $V_q = V_{-q}$, $\chi_q^{s*} = \chi_{-q}^s$ are the Fourier components of the Coulomb interaction of electrons with each other and their coupling constant with the lattice phonons respectively; ε_k^{ν} is the energy of the electron. The constants V_q and χ_q^s are both independent of the band and spin indices of electrons.

$$\begin{aligned} a_k^{\nu} &= [\exp S] A_{k, \nu} [\exp(-S)] \\ b_q^s &= [\exp S] \beta_{s, q} [\exp(-S)] \end{aligned} \quad (6)$$

where S is an anti-hermitian operator ($S^+ = -S$) and the σ_q operator is linear on the phonon operators $\beta_{s, q}$, $\beta_{s, q}^+$.

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

The unitary transformation gives rise to renormalization of the electron energy (first term) and renormalization of the Fourier component of the Coulomb electron–electron interaction. In the latter case we can conclude that if the crystal unit cell contains many atoms the effective Coulomb potential can become 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 the case with approximation $t' \rightarrow t - 0$ in accordance with equation (2). When this situation arises the two-particle Green function can be written as follows:

$$G_2 \langle_{k_1+q, \nu; k_2-q, \nu_2}^{k_2, \nu_2; k_1, \nu_1}; t-t' \rangle = | \langle -iT A_{k_1+q, \nu_1}(t) A_{k_2-q, \nu_2}(t) \times A_{k_2, \nu_2}^+(t') A_{k_1, \nu_1}^+(t') \rangle | \quad t' \rightarrow t - 0. \quad (7)$$

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

$$G_2 \langle_{k_1+q, \mu; k_2-q, \nu}^{k_2, \nu; k_1, \mu} | \omega \rangle \sim \frac{f(k_1, \mu; k_2, \nu; \omega) \sum_{\sigma, \sigma'} \varphi(\mu, \nu; \sigma, \sigma')}{1 - VK(k_1, \mu; k_2, \nu; \omega)} \quad (8)$$

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

$$V = \tilde{V}_q = V_q - 2 \sum_s \frac{|\chi_q^s|^2}{\Omega_{s, q}} \approx \text{constant} \quad (9)$$

n_k^{ν} is the filling number of electrons; V is the effective Fourier component of the electron–electron (e–e) interaction. If the constant of the e–e interaction renormalized by the electron–phonon interaction becomes negative ($V > 0$) the appearance of new types of states (coupled states) in the electron system is possible. Equations (8) and (9) give the spectral features in the region of two-particle states. Therefore, let us study these expressions. It is seen from equations (8) and (9) that if the momenta of interacting electrons satisfy $k_1 = k_2 = 0$ or $k_2 = -k_1$ the denominator in the right-hand side of equation (8) is precisely reduced to the well-known expression describing the SC gap of a crystal, but for other arbitrary momenta k_1 and k_2 of the electrons the situation is significantly different. From equations (8) and (9) it follows that in addition to states corresponding to traditional BCS pairing there are many new states occurring in equation (8) and contributions to the SC gap which, hence, depends on the momenta of the interacting electrons. This will be shown below. The numerator of the right-hand side of equation (8) gives rise to new possibilities. Here $f(k_1, \mu; k_2, \nu; \omega)$ is some 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 in terms of functions $\delta_{i, j}$ and defines the spin-forbidden rules for the coupled state (responsible for superconductivity effects):

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

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

(i) $\mu = \nu$. (1) If the spins of the electrons are equal to each other ($\sigma = \sigma'$) then $\varphi(\mu, \mu; \sigma, \sigma') = 0$. (2) If the spins of both electrons are different ($\sigma \neq \sigma'$) the second term in the right-hand part of equation (10) (which is proportional to $\delta_{\sigma, \sigma'}$) disappears and therefore $\varphi(\mu, \mu; \sigma, \sigma') \neq 0$. This means that only states with oppositely directed spins (namely singlet states $\sigma + \sigma' = 0$ in this simplest case) can contribute to the coupled states of the electron system.

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

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

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

where m_μ is the effective mass of an electron in the μ th ($\mu = 1, 2, \dots$) energy band of the crystal. Δ_μ is a parameter which indicates the position of the extremum of μ band relative to the Fermi level. It may be negative or positive and the effective mass the same. (The anisotropy of the crystal can be simply taken into account by the anisotropy of the effective mass in equation (11).) In the traditional approximation ($\mu = 1$) the function $K(k, \mu; k, \mu; \omega)$ and the SC gap are described by the well-known standard expressions [12] but exact numerical calculation of function $K(k, \mu; k, \mu; \omega)$ gives rise to new features especially if several electron bands ($\mu \neq 1$) are taken into consideration. This is because the analytical analysis does not take 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 also be noted that for some types of SC crystals the minimum of the electron band is located much lower (for $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ [17, 18]) than the Fermi level energy. As an example two cases of Bi-based crystals are presented in figure 1.

Figure 1(a) shows the band structure obtained by Sterne and Wang [17, 19] for the high- T_c $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ compound which is very similar to calculations of Hyberstein and Mattheiss [20], Krakauer and Pickett [18] and Freeman *et al* [21]. The new feature of this compound is the presence of two bismuth p-electron bands which dip below E_F by about 0.7 eV around the K point. A shallow band of mixed Bi and Cu-O₂ character which barely crosses E_F and a more dispersive band which has almost pure bismuth character crossing E_F are seen, indicating that

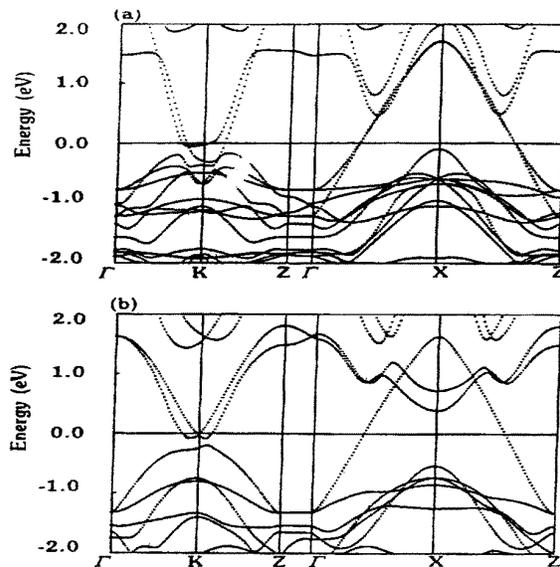


Figure 1. Energy band structures around the Fermi energy for (a) the high-temperature superconductor $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ and (b) the low-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CuO}_6$ from [19].

bismuth oxide layers are metallic. It should also be noted that the Krakauer-Pickett calculations showed that mixed Bi-CuO bands can arise and extend near 0.1–0.5 eV higher than E_F .

For comparison the band structure of the low- T_c $\text{Bi}_2\text{Sr}_2\text{CuO}_6$ compound is shown in figure 1(b). The principal difference between the band structures of crystals can be observed around the K point. The two Bi p bands barely cross and extend less than 0.1 eV below E_F , compared with 0.7 eV in the case of the higher- T_c compound in figure 1(a). This difference in the location of extremal bands relative to ε_f (parameter Δ_μ in equation (11)) is very important for the value of T_c and for small Δ_μ the coupled states and SC effect may be absent as was shown in [12].

Therefore we will study theoretically the situation close to the $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ crystal because it has a high T_c .

The results of some numerical calculations are given in figures 2 and 3. The effect of temperature is seen in figure 2 where the T dependences of $K(k, \mu; k, \nu; \omega)$ functions for different electron band structures are presented. It follows from figure 2(c) that the presence of several electron bands generates a $K(k, \mu; k, \nu; \omega)$ function having the minimum located apart from the $2\varepsilon_f$ energy level. The arrows 5–7 in figure 1(a) correspond to different values of the constant $1/V$ ($V < 0$) (see caption to figure). The intersection, if it occurs, of curves 1–4 with the extensions of the arrows gives the energy of coupled states because the solutions obtained correspond to the zeros of the denominator in the right-hand side of equation (8).

Therefore the coupled states obtained from the crossing of the extensions of the arrows 5–7 with the function K in figure 2(c) will also be located a substantial distance from the $2\varepsilon_f$ energy level. As result the T dependence of the SC state (SC gap) may become more complicated than for only

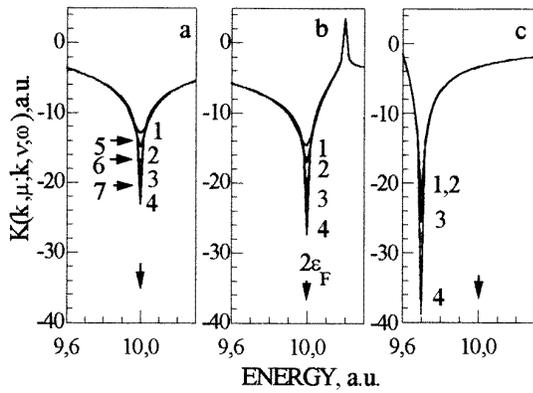


Figure 2. The effect of temperature on the $K(k, \mu; k, \nu; \omega)$ function ($E = k^2/2m = 0$) for different structures of the energy zones: (a) $\Delta_1 = -1$, $m_1^* = 1$; (b) $\Delta_2 = 0.2$, $m_2^* = -2$; (c) $\Delta_1 = -1$, $m_1^* = 1$, $\Delta_2 = 0.2$, $m_2^* = -2$; curves 4, $T = 2$ K;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

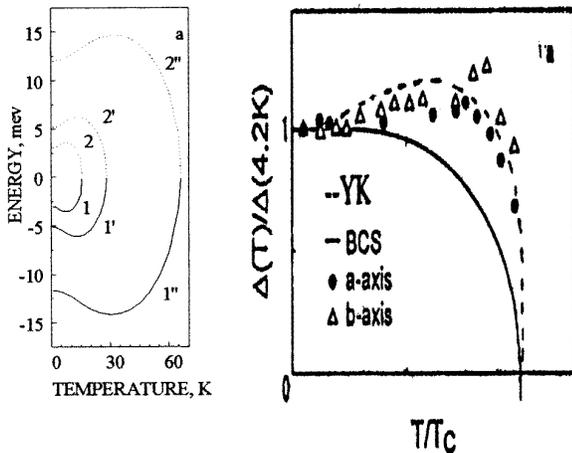


Figure 3. The temperature dependences of the SC gap: (a) calculated dependences of the SC gap for different values of the effective e–e interaction parameter V (the structure of the electron bands and meaning of V as in figure 2(a)); (b) experiment (\bullet , Δ) and theory (—, BCS; our calculation).

one electron band. In figure 1 the curves 4 \rightarrow 1 describe the change of the $K(k, \mu; k, \nu; \omega)$ function with increase of temperature. Therefore, for a fixed value of the constant V (arrow 7, for example) the coupled states arise at low temperature (curve 4) but disappear at higher temperatures (curves 3–1). The temperature dependence of the coupled state energies (for the case of the band given in figure 1(a)) is shown in figure 3(b) by curves 1, 1' and 1'' (full lines) corresponding to different values of the parameter V . The obtained dependences are not similar to standard BCS ones. For illustration the experimental dependences of the SC gap obtained in [22] for $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ crystal are presented in figure 3(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 the SC gap gives the curve which is closer to the experimental results.

In our approach we take into account that all electron bands (the numerical calculations show that only bands located near the Fermi level are important) contribute to the coupled states. Therefore the energy of the coupled states depends on change with temperature of the filling number n_k and on the DES, i.e. on the dispersion of the electron band. The latter means that the resulting T dependence of the SC gap may be more complicated, especially for the presence of several bands near the Fermi level.

Moreover, the presence of some electron bands crossing the Fermi level generates a very complex density function of two-electron states (responsible for the appearance of coupled states) and as a result a singularity in the density of two-electron states (saddle point type) may arise within the band (far from the Fermi level energy) which can dominate the description of the SC properties of the crystal. This is demonstrated in figure 2(c).

Our calculations also show that the SC gap depends on the momenta (k) of the interacting electrons. However, coupled states arise if $k \leq k_{lim}$ where k_{lim} depends on V . It is obvious that the k factor must be contained in the experimental T dependence of the SC gap and so that may be one of the reasons for the difference between the curve YK (figure 3(a)) calculated by us for $k = 0$ and experimental results.

4. Conclusion

In conclusion, a new theoretical approach is proposed for the study of the coupled states responsible for superconductivity in crystals without using the idea of electron pairing. In the proposed approach it is shown that SC coupled states arise naturally as poles of the two-particle Green function and are created as a result of the effective Coulomb interaction of electrons with nonzero full momenta and spins ($k_1 + k_2 \neq 0$, $s + s' \neq 0$) in the general case. The model numerical calculations have shown that the dependence of the SC gap (energy of coupled states) on temperature is different from the BCS type and depends on the momenta of interacting electrons.

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