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Phonon and magnon mediated d-wave superconductivity in cuprates

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We use the Eliashberg formalism for calculating T_c in the $2D$ t-J model supplemented by an interaction with fully-symmetric apex-oxygen vibrations. It is shown that in this model holes form an anomalous $2D$ Fermi liquid with a Fermi surface which is also two-dimensional in a certain range of hole concentrations x. This Fermi surface is a part of a large nearly flat region around the boundaries of the magnetic Brillouin zone. Extended saddle points, analogous to those observed in angle-resolved photoemission spectra, form the main part of this region. It produces a pronounced maximum in the density of states near the Fermi level. However, in spite of this favorable condition for superconductivity, created by the hole-magnon interaction, we found this interaction alone to be unable to yield high T_c. Only together with a moderate hole-phonon interaction does it lead to d-wave superconductivity at temperatures and hole concentrations observed in cuprates. High T_c are connected with a large density of states in the nearly flat region, a conformity of the two interactions for the $d_{x^2-y^2}$ symmetry, and a high phonon frequency Ω. The obtained dependences of T_c on x and on Ω are in close agreement with observations in cuprates.

It is known from experiments on neutron scattering [1] that antiferromagnetic fluctuations are retained in cuprate perovskites at large levels of doping, including the superconducting state. Together with a small isotope effect [2] this gives grounds for believing that these fluctuations play an essential role in the superconducting pairing. On the other hand, there is a number of experimental facts indicating a pronounced electron-phonon interaction in these crystals (see, e.g., [2–4]). These experimental facts have prompted us to investigate a model of cuprates with the superconducting pairing provided by both magnons and phonons. To describe the CuO_2 plane we use the $2D$ t-J model supplemented by fully-symmetric apex-oxygen vibrations, which in accord with the tunneling and Raman spectroscopy data [4], interact most strongly with holes. The consideration is based on the spin-wave approximation [5], which has been able to describe [6] the destruction of the long-range antiferromagnetic order at the observed small hole concentrations x [1] and hole energy bands containing extended saddle points similar to those observed in angle-resolved photoemission spectra [7].

In this approximation the Hamiltonian of the considered model reads [5]

$$H = \sqrt{2} \sum_{\mathbf{k}\mathbf{k}'\sigma} \left(g_{\mathbf{k}\mathbf{k}'} h^+_{\mathbf{k}\sigma} h_{\mathbf{k}-\mathbf{k}',-\sigma} b_{\mathbf{k}'\sigma} + \mathrm{H.c.} \right) + \sum_{\mathbf{k}\sigma} \omega^0_{\mathbf{k}} b^+_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} - \frac{4\varepsilon}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\sigma} \gamma_{\mathbf{q}} h^+_{\mathbf{k}-\mathbf{q},\sigma} h_{\mathbf{k}\sigma} h^+_{\mathbf{k}'+\mathbf{q},-\sigma} h_{\mathbf{k}',-\sigma} +$$

$$+ \sqrt{2/N} \sum_{\mathbf{k}\mathbf{k}'\sigma} h^+_{\mathbf{k}\sigma} h_{\mathbf{k}'\sigma} \left(\sqrt{S_1\Omega}\, Q_{\mathbf{k}-\mathbf{k}',\sigma} + 4\gamma_{\mathbf{k}-\mathbf{k}'} \sqrt{S_2\Omega}\, Q_{\mathbf{k}-\mathbf{k}',-\sigma} \right) + \Omega \sum_{\mathbf{k}\sigma} \beta^+_{\mathbf{k}\sigma} \beta_{\mathbf{k}\sigma}, \qquad (1)$$

where $h^+_{\mathbf{k}\sigma}$ is the creation operator of a hole with the $2D$ wave vector $\mathbf{k}$ in one of the classical Néel states; $\sigma = \pm 1$ labels two sublattices with spins up or down in this state, summations over $\mathbf{k}$ are limited to the magnetic Brillouin zone; $b^+_{\mathbf{k}}$ is the creation operator of a magnon with the unperturbed frequency $\omega^0_{\mathbf{k}} = 2J(1 - \gamma^2_{\mathbf{k}})^{1/2}$, where J is the superexchange constant; $\gamma_{\mathbf{k}} = \frac{1}{2}[\cos k_x + \cos k_y]$. The interaction constant $g_{\mathbf{k}\mathbf{k}'} = -4t(\gamma_{\mathbf{k}-\mathbf{k}'} u_{\mathbf{k}'} + \gamma_{\mathbf{k}} v_{\mathbf{k}'})/N^{1/2}$ comprises the hopping constant t, the number of sites N, $u_{\mathbf{k}} = \mathrm{ch}\, \alpha_{\mathbf{k}}$, $v_{\mathbf{k}} = \mathrm{sh}\, \alpha_{\mathbf{k}}$, and $\alpha_{\mathbf{k}} = \frac{1}{4} \ln [(1 + \gamma_{\mathbf{k}})/(1 - \gamma_{\mathbf{k}})]$. The third term in Eq. (1) describes the static attraction of holes on neighboring sites due to the bond-breaking mechanism [8] with the binding energy ε. In Eq. (1), we took into account the deformation-potential type of the hole-phonon interaction [4] and neglected a weak dispersion of relevant phonons with the frequency Ω, created by the operator $\beta^{+}_{\mathbf{k}\sigma}$. Since a doped hole spreads over four oxygen sites of a plaquette and two neighboring plaquettes contain a common oxygen site, a shift of an apex oxygen produces a comparable influence on site states of the nearest plaquette and the neighboring plaquettes. The Stokes shifts S_1 and S_2 characterize these interactions, $Q_{\mathbf{k}\sigma} = \beta_{\mathbf{k}\sigma} + \beta^{+}_{-\mathbf{k}\sigma}$.

Self-energy equations of the Gor'kov-Eliashberg theory were derived in the Born approximation. We neglected comparatively small changes in the phonon spectrum, caused by the hole-phonon interaction [4]. The hole and magnon spectral functions were calculated self-consistently from the self-energy equations on a 20×20 lattice for given x and temperature T. In these calculations the following set of parameters was used:

$$J = 0.2t\,, \quad \varepsilon = 0.5J\,, \quad S = \sqrt{S_1 S_2} = 0.8t\,. \qquad (2)$$

The first two relations were estimated with the use of parameters of La_2CuO_4 [9] (which are expected to be approximately valid also for related p type cuprates because they refer to well-isolated CuO_2 planes) and the procedure [5] reducing the extended Hubbard Hamiltonian to the t-J Hamiltonian. From these estimations $t \approx 0.5$ eV, S was selected to obtain T_c in the range observed in cuprates. This value corresponds to a moderate coupling constant $\lambda \sim S/B$ where $B \approx 3t - 5t$ is the hole bandwidth [6]. The phonon frequency Ω was selected from the range $0.1t - 0.15t$ the lower and upper boundaries of which approximately correspond to the La and Bi2212 compounds [4].

The energy spectrum of the considered system is significantly changed upon variation of x [6]. At $x \approx 0.05$ narrow spin-polaron bands with bandwidths of the order of J are transformed into a much wider band with the bandwidth B. Its shape is a distorted version of the band $E_{\mathbf{k}} = 2t[\cos k_x + \cos k_y]$. Such two-cosine band would be generated by the kinetic energy term of the t-J Hamiltonian at complete absence of correlations. Thus, this transformation indicates a considerable weakening of correlations at comparatively small x. These changes in the hole energy spectrum are conditioned by the changes in the magnon spectrum connected with the destruction of the long-range antiferromagnetic order at $x \approx 0.02$ [6]. In the rigorous antiferromagnetic order the hole transport is impossible without creation and destruction of magnons (see Eq. (1)). As a consequence, hole bandwidths are of the order of the magnon bandwidth. The destruction of the long-range order opens the way for holes to move without magnons, which allows the kinetic energy term to reveal itself in the energy spectrum.

However, pronounced correlations are retained and reveal themselves in the short-range antiferromagnetic order [1,6] and in a considerable distortion of the band shape in comparison with the two-cosine band [10]. The most essential feature of this distortion is a large nearly flat region, a plateau, around the boundaries of the magnetic Brillouin zone. The plateau is positioned in the vicinity of the Fermi level and exists in the entire range $0.05 \lesssim x \lesssim 0.3$. The plateau is comprised mainly of four large areas around $\mathbf{k} = (\pm\pi, 0)$, $(0, \pm\pi)$ which are analogous in shape and position to the extended saddle points observed in angle-resolved photoemission spectra in a number of cuprates [7].

The plateau in closest proximity to the Fermi level suggests the possible existence of *a flat region of the energy band just on this level.* It would mean that the *holes form an anomalous 2D Fermi liquid with a Fermi surface that is also two-dimensional.* This does occur in our calculations [10], at least in the range $0.17 \lesssim x \lesssim 0.26$. Our calculated Fermi surfaces are close to those observed in a number of cuprates [7]. We believe that insufficient accuracy hindered the identification of the experimental Fermi surfaces as $2D$ objects.

The plateau produces a pronounced maximum in the DOS, $\rho(\omega)$, shown in Fig. 1. The Fermi level $\omega = 0$ remains near this maximum throughout the entire relevant range of x. Thus, the hole-magnon interaction creates very favorable conditions for superconductivity. However, in spite of this fact, we found this

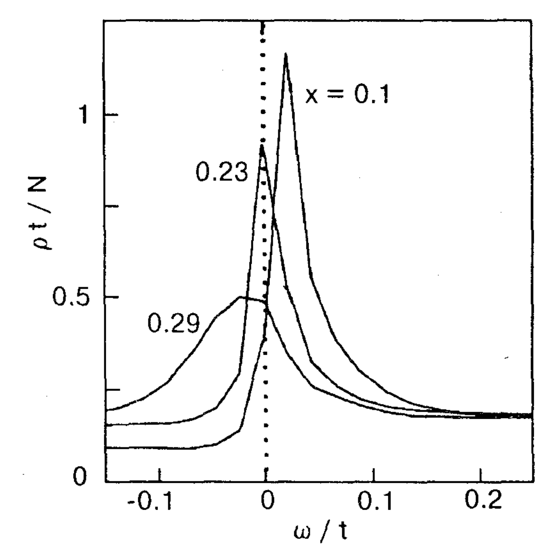

Fig. 1. DOS near the Fermi level for different values of x.

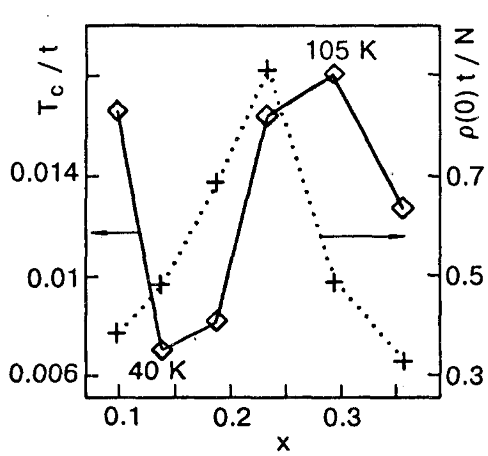

Fig. 2. T_c vs. x^2 shown by ◇ for the $d_{x^2-y^2}$ even frequency gap, parameters (2), and $\Omega = 0.15t$. T_c is recalculated in K for $t = 0.5$ eV. The dependence of $\rho(0)$ on x is shown by +. Connecting lines are for guiding the eye only.

interaction alone to be unable to yield high T_c (singlet order parameters belonging to all one-dimensional representations of the point group of the CuO_2 plane were tested) [10]. The absence of the superconducting transition is due to a negligibly small interaction constant g for magnon-mediated transfer of a hole from one portion of the Fermi surface to another which is connected with the spin flip accompanying magnon absorption and generation processes [see Eq. (1)]. The situation is not changed by incorporating the static attraction between holes [the third term in Eq. (1)] which is too small to produce a perceptible contribution to pairing.

Cardinal changes occur when the hole-phonon interaction is included in hole pairing. For the $d_{x^2-y^2}$ gap moderate interaction (2) already leads to a superconducting transition at high temperatures, as shown in Fig. 2 [10]. One of the reasons for the occurrence of high temperatures is the possibility for the hole-phonon interaction to exploit the plateau region near the Fermi surface where the maximum of DOS originates. We note here that our values of the DOS at the Fermi level $\rho(0) \approx 1$ state/eV Cu spin (also shown in Fig. 2) are close to the experimental estimations made in Bi compounds [11]. The second reason is the particular form of the hole-phonon interaction, Eq. (1), which, due to the structure factor $\gamma_{\mathbf{k}-\mathbf{k}'}$ is ideally suitable for increasing a $d_{x^2-y^2}$ eigenvalue. For this symmetry there is no mutual cancellation of contributions and the eigenvalue is approximately equal to the sum of eigenvalues produced separately by hole-magnon and hole-phonon interactions. For the parameters (2) and $T = T_c$ both interactions give comparable contributions to the eigenvalue at all considered x. For other considered symmetries the situation is markedly different: due to a competing character of the two interactions in these cases eigenvalues grow only slightly. The third reason for an efficiency of the hole-phonon interaction in the hole pairing is high frequency Ω of relevant phonons, which exceeds significantly phonon frequencies of conventional superconductors. With decreasing Ω from $0.15t$ to $0.1t$, in the range $x \gtrsim 0.15$ the highest T_c drops from $0.018t \approx 105$ K to $0.013t \approx 70$ K. An analogous correlation between the highest T_c and the frequency of full-symmetric apex-oxygen vibrations in different cuprates was pointed out in Ref. 4.

For $x \gtrsim 0.15$ the obtained dependence of T_c on x is close in shape to that observed in cuprates [11]. As is seen in Fig. 2, T_c in the considered system is not directly connected with $\rho(0)$, in contrast to the weak-coupling case. There is a marked dip of T_c near $x = 0.14$ in this Figure. An analogous dip was observed in the Ba and Sr doped La_2CuO_4 [11]. In Fig. 2 T_c starts to grow with decreasing x from $x \approx 0.14$. It peaks at $x \approx 0.04$ and vanishes with a further fall of x. This behavior is connected with the fact that for decreasing x quasiparticle maxima of the hole Green's function become sharper and more intensive. However, we have neglected the long-range Coulomb repulsion, the influence of which is most significant for small x. The maximum of T_c near $x = 0.04$ will be substantially decreased or even completely suppressed by this repulsion. Another reason for a depression of T_c in this region is phase fluctuations [12], which are out of scope of the mean-field Eliashberg theory.

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