Doping dependence of critical temperature for superconductivity induced by hole–phonon interaction

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A B S T R A C T

To understand the nature of the high-temperature superconductors (cuprates) we have taken into consideration the interaction terms, which possess the structure of the hole–phonon (HP) and hole–hole–phonon (HHP) type. It was shown that for the high value of the HHP potential in comparison to HP, the superconducting critical temperature (T_C) reaches the maximum value for the low concentration of holes, which fairly corresponds with the observed maximum of T_C for hole-doped cuprates. The analysis was performed within the framework of the Eliashberg approach.

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The high-temperature superconductivity can be observed in the compounds of copper and oxygen (so-called cuprates) [1,2]. The highest value of the critical temperature equal to 160 K was observed in $HgBa_2Ca_2Cu_3O_{8+y}$ compressed to 31 GPa [3]. However, Takeshita et al. suggest that the corrected value of T_C is 153 K for $p = 15$ GPa [4]. In the cuprates the critical temperature follows the nearly parabolic dependence on the hole concentration, with the maximum T_C at the low concentration of carriers [5]. This behaviour is clearly observed in: $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, $Bi_2Sr_2CaCu_2O_{8+y}$, and $TlSr_2CaCu_2O_{7+y}$ [6–8]. The existence of universal relation between the critical temperature and the hole concentration is related to the pairing mechanism, since the different combinations of constituent atoms scales only T_C. Unfortunately, to the present day the mechanism for the high-temperature superconductivity remains highly controversial [9–12]. A lot of proposals are based on the pure electronic models like the Hubbard or Emery Hamiltonian [5,13–15]. However, the experimental data show also the evidence for the electron–phonon interaction. For example, the isotope effect for the critical temperature in the underdoped region [16], and the phonon-related $I − V$ characteristic obtained in the tunnelling experiment [17]. Particularly interesting results are obtained by using the scanning tunnelling microscopy which allows direct observations of phonons [18]. One should also mention the low-energy kink in the quasiparticle spectrum mea-

sured by the ARPES method [19,20], and the ARPES isotope effect observed for the real part of the self-energy [21]. Although, the ARPES results for the isotope effect is strongly undermined in the paper [22]. Taking into account the above facts, it is interesting to study the hole dependence of critical temperature for the superconducting condensate induced by the hole–phonon coupling, where the Coulomb interaction affects destructively on the local Cooper pairs and is responsible for the induction of the d-wave order parameter [5,23]. In this paper, we have considered the effective Hamiltonian of the hole–phonon (HP) and hole–hole–phonon (HHP) type. The analysis has been performed within the framework of the Eliashberg scheme [24,25]. The general form of hole–phonon Hamiltonian is given by:

$$H = \sum_{\mathbf{k}\sigma} \overline{\varepsilon}_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \omega_0 \sum_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + v_1 \sum_{\mathbf{k}\mathbf{q}\sigma} a_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \left(b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}} \right)$$

$$+ \frac{v_2}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{l}\sigma} a_{\mathbf{k}-\mathbf{l}\sigma}^{\dagger} a_{\mathbf{k}\sigma} a_{\mathbf{k}'+\mathbf{l}+\mathbf{q}-\sigma}^{\dagger} a_{\mathbf{k}'-\sigma} \left(b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}} \right), \quad (1)$$

where: $\overline{\varepsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$, $\varepsilon_{\mathbf{k}}$ denotes the hole energy and μ is the chemical potential. In the case of the square lattice: $\varepsilon_{\mathbf{k}} = -t\gamma(\mathbf{k})$, where $\gamma(\mathbf{k}) = 2\left[\cos(k_x) + \cos(k_y)\right]$. The symbol t is the hopping integral. The hole creation operator with the momentum $\mathbf{k}$ and the spin σ is given by $a_{\mathbf{k}\sigma}^{\dagger}$. On the other hand, $b_{\mathbf{q}}^{\dagger}$ is the phonon creation operator, ω_0 represents the Einstein frequency. The paring potential for the hole–phonon and hole–hole–phonon interaction has been denoted by v_1 and v_2, respectively.

Table 1

The electronic parameters (spin-singlet) and the electron–ion coupling constants at the hydrogen-molecule equilibrium: $R_0 = 1.41968\ a_0$, where the symbol a_0 denotes the Bohr radius. The electron–ion coupling constants are given by: $g_x = dx/dR$, where $x \in \{\varepsilon, t, U, K, J, V\}$. The calculations were performed for the Wannier function of the form: $\Phi_j(\mathbf{r}) = A[\phi_j(\mathbf{r}) - B\phi_l(\mathbf{r})]$, where A and B are the normalization coefficients. $1s$ Slater-type orbital can be written as: $\phi_j(\mathbf{r}) = \sqrt{\alpha^3/\pi}\exp[-\alpha|\mathbf{r} - \mathbf{R}_j|]$, α is the inverse size of the orbital. The presented data are in agreement with the results obtained in [29–31]. Note that qualitatively similar results can be obtained also for the single Gaussian orbital per site [26].

ε (Ry)	t (Ry)	U (Ry)	K (Ry)	J (Ry)	V (Ry)
-1.7495	-0.7377	1.6613	0.9620	0.0220	-0.0119
g_ε (Ry/a_0)	g_t (Ry/a_0)	g_U (Ry/a_0)	g_K (Ry/a_0)	g_J (Ry/a_0)	g_V (Ry/a_0)
0.0017	0.6090	-0.1263	-0.2363	-0.0075	-0.0004

Below, we justify qualitatively the assumed form of the operator (1). Let us consider the dimer Hamiltonian, which includes all two-site interactions [26]:

$$H_{dim} = \varepsilon \sum_{j=1,\sigma}^{2} c_{j\sigma}^{\dagger} c_{j\sigma} + t \sum_{jl=1, j\neq l, \sigma}^{2} c_{j\sigma}^{\dagger} c_{l\sigma} \qquad (2)$$

$$+ U \sum_{j=1}^{2} c_{j\uparrow}^{\dagger} c_{j\uparrow} c_{j\downarrow}^{\dagger} c_{j\downarrow} + \frac{1}{2}\left(K - \frac{J}{2}\right) \sum_{jl=1, j\neq l, \sigma, \sigma'}^{2} c_{j\sigma}^{\dagger} c_{j\sigma} c_{l\sigma'}^{\dagger} c_{l\sigma'}$$

$$- 2J\mathbf{S}_1\mathbf{S}_2 + J \sum_{jl=1, j\neq l}^{2} c_{j\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} c_{l\downarrow} c_{l\uparrow}$$

$$+ V \sum_{\sigma} \left(\sum_{j=1}^{2} c_{j\sigma}^{\dagger} c_{j\sigma}\right) \left(\sum_{jl=1, j\neq l}^{2} c_{j-\sigma}^{\dagger} c_{l-\sigma}\right),$$

where $c_{j\sigma}^{\dagger}$ is the electron creation operator. The spin operator is given by $\mathbf{S}_j$. The parameters of the Hamiltonian are defined by the following integrals:

$$\varepsilon = \int d^3\mathbf{r}\Phi_1(\mathbf{r})\left[-\nabla^2 - \frac{2}{|\mathbf{r} - \mathbf{R}|}\right]\Phi_1(\mathbf{r}), \qquad (3)$$

$$t = \int d^3\mathbf{r}\Phi_1(\mathbf{r})\left[-\nabla^2 - \frac{2}{|\mathbf{r} - \mathbf{R}|}\right]\Phi_2(\mathbf{r}),$$

$$U = \int\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Phi_1^2(\mathbf{r}_1)\frac{2}{|\mathbf{r}_1 - \mathbf{r}_2|}\Phi_1^2(\mathbf{r}_2),$$

$$K = \int\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Phi_1(\mathbf{r}_1)\Phi_2(\mathbf{r}_1)\frac{2}{|\mathbf{r}_1 - \mathbf{r}_2|}\Phi_1(\mathbf{r}_2)\Phi_2(\mathbf{r}_2),$$

$$J = \int\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Phi_1^2(\mathbf{r}_1)\frac{2}{|\mathbf{r}_1 - \mathbf{r}_2|}\Phi_2^2(\mathbf{r}_2),$$

$$V = \int\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Phi_1^2(\mathbf{r}_1)\frac{2}{|\mathbf{r}_1 - \mathbf{r}_2|}\Phi_1(\mathbf{r}_2)\Phi_2(\mathbf{r}_2),$$

where the symbol $\Phi_j(\mathbf{r})$ is the Wannier function.

Minimizing the total energy of the system (the energy of the electron system plus the energy of the ion core repulsion: $E_{ic} \sim 1/R$, where R is the distance between the cores), it can be shown that besides the on-site Coulomb repulsion also the inter-site Coulomb interaction (K) has to be taken into account. What is more important, the interaction of the electron–phonon has to be additionally included. The exemplary results obtained for the hydrogen molecule are collected in Table 1. Note that in the case of cuprates, also the on-site and the inter-site Coulomb repulsion plays the most significant role [5,15,27,28].

The Hamiltonian (2) supplemented by the term of the electron–phonon interaction (H_{e-ph}) is very difficult to analyze. The paper [26] shows that for the single Gaussian orbital per site, it can be brought to the effective electronic (polaronic) Hamiltonian by using the generalized Lang–Firsov (displaced-oscillator) transformation [32,33]. Hence, we obtain: $H_{dim} + H_{e-ph} \rightarrow H_{dim}(\varepsilon^\star, t^\star, U^\star, K^\star, J^\star, V^\star) + E_{ph}$, where the star denotes the effective parameters, and E_{ph} is the energy of the phonons in the ground-state. It turns out that the mostly significant parameters are $t^\star$, $U^\star$ and $K^\star$. In the paper [26], it has been found that in the courses of the functions $t^\star(R)$, $U^\star(R)$, and $K^\star(R)$ appear the characteristic jumps. For example, if the electron–phonon coupling equals 470 meV, the Einstein frequency is equal to 100 meV, and $t^\star \simeq 250$ meV (the order of the values characteristic for the high-temperature superconducting state), the jumps are observed for $R \simeq 3$ Å. So rapid changes of the considered functions are the cause of the existence of the high values of the effective coupling constants of the electron–phonon and the electron–electron–phonon type: $g_{t^\star} = dt^\star/dR$, $g_{U^\star} = dU^\star/dR$, and $g_{K^\star} = dK^\star/dR$, while $|g_{U^\star}| - |g_{K^\star}|$ is at least the one order greater than that $g_{t^\star}$. Thus, the most significant terms of the hole–phonon interaction (in the momentum representation) have the same form as the operator (1).

Note that the motivation of hole–phonon Hamiltonian presented above should be treated only as the guide, which enables the construction of the minimum effective model for the superconducting state in cuprates. The biggest drawback of our reasoning is connected with the atomic parameters. In the real solid, one should take into account the change in these parameters caused by the polarizability of the lattice and screening effects. For example, the atomic U value of the $3d$ orbitals of Cu is on the order of 20 eV. In the solid this value is reduced to ~ 8 eV. Hence, the question arises whether the HHP term survives in the real material? We can not precisely answer this question because of the enormous mathematical difficulties. However, the experimental results suggesting the interaction between the Cooper pairs in the cuprates, causing the admixture of quartets to the condensate [34]. Note that the existence of the effective four-fermion interaction follows naturally from the HHP term. It suffices to use the canonical Fröhlich transformations, what has been discussed in [35]. Let us note also that similar structure like the Hamiltonian (1) have the operators analyzed in the papers [36–43], where the selected properties of the high-temperature superconducting state were reconstructed.

The thermodynamic properties of the system, in the framework of the Eliashberg approach, are determined by the matrix Green function [25]:

$$G_{\mathbf{k}}(i\omega_n) = \begin{pmatrix} \langle\langle a_{\mathbf{k}\uparrow}|a_{\mathbf{k}\uparrow}^{\dagger}\rangle\rangle_{i\omega_n} & \langle\langle a_{\mathbf{k}\uparrow}|a_{-\mathbf{k}\downarrow}\rangle\rangle_{i\omega_n} \\ \langle\langle a_{-\mathbf{k}\downarrow}^{\dagger}|a_{\mathbf{k}\uparrow}^{\dagger}\rangle\rangle_{i\omega_n} & \langle\langle a_{-\mathbf{k}\downarrow}^{\dagger}|a_{-\mathbf{k}\downarrow}\rangle\rangle_{i\omega_n} \end{pmatrix}, \qquad (4)$$

where: $i = \sqrt{-1}$, and $\omega_n = (\pi/\beta)(2n - 1)$. The inverse temperature is given by: $\beta = 1/k_B T$ (k_B is the Boltzmann constant). The Green function fulfils the Dyson equation [44,45]: $G_{\mathbf{k}}^{-1}(i\omega_n) = G_{0\mathbf{k}}^{-1}(i\omega_n) - M_{\mathbf{k}}(i\omega_n)$. The symbol $G_{0\mathbf{k}}(i\omega_n)$ represents the propagator of non-interacting holes: $G_{0\mathbf{k}}(i\omega_n) = (i\omega_n\tau_0 - \bar{\varepsilon}_{\mathbf{k}}\tau_3)^{-1}$; τ_j are the Pauli matrices. The open form of the matrix self-energy ($M_{\mathbf{k}}(i\omega_n)$) is extensive:

$$M_{\mathbf{k}}^{(A)}(i\omega_n) \simeq -(v_1 + v_2\langle n\rangle)^2\frac{1}{\beta}\sum_{\omega_m}\sum_{\mathbf{q}} << a_{\mathbf{k}-\mathbf{q}\uparrow}|a_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} >>_{i\omega_m}$$

$$\times << \left(b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}}\right)|\left(b_{\mathbf{q}}^{\dagger} + b_{-\mathbf{q}}\right) >>_{i(\omega_n - \omega_m)}, \qquad (5)$$

$$M_{\mathbf{k}}^{(B)}(i\omega_n) \qquad (6)$$

$$\simeq \left(v_1^2 + 2v_1 v_2\langle n\rangle\right)\frac{1}{\beta}\sum_{\omega_m}\sum_{\mathbf{q}} << a_{\mathbf{k}-\mathbf{q}\uparrow}|a_{-\mathbf{k}+\mathbf{q}\downarrow} >>_{i\omega_m}$$