

Interlayer tunneling in a strongly correlated electron-phonon system

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We discuss the role of interlayer tunneling for superconducting properties of strongly correlated ($U \rightarrow \infty$ limit) two-layer Hubbard model coupled to phonons. Strong correlations are taken into account within the mean-field approximation for auxiliary boson fields. To consider phonon-mediated and interlayer tunneling contribution to superconductivity on equal footing we incorporate the tunneling term into the generalized Eliashberg equations. This leads to the modification of the phonon-induced pairing kernel and implies a pronounced enhancement of the superconducting transition temperature in the d -wave channel for moderate doping. In numerical calculations the two-dimensional band structure has been explicitly taken into account. The relevance of our results for high-temperature superconductors is briefly discussed. [S0163-1829(96)05737-2]

I. INTRODUCTION

The origin of pairing mechanism in high-temperature superconductors is still in debate and may be related to the actual symmetry of the superconducting order parameter.¹⁻⁶ To solve this nontrivial problem one has to reconsider intimate features of quasi-particles in CuO_2 layers. The proximity of an antiferromagnetic phase indicates that strong Coulomb correlations could contribute to a purely electronic pairing due to exchange of antiferromagnetic spin fluctuations.⁷⁻¹¹ On the other hand, phonons are affected below the superconducting transition temperature.¹²⁻¹⁵ The latter feature, combined with expected rather strong electron-phonon interactions,¹⁶⁻¹⁹ allows one to argue that coupling of electrons to phonons gives rise to the formation of the superconducting state. Therefore, the natural question which emerges is about the actual influence of strong correlations upon phonon-mediated pairing.²⁰⁻²⁵ In general one may expect that phonon-mediated superconductivity survives in the presence of strong correlations. Here, the main problem is how to consider correlations and electron-phonon coupling on equal footing. The solution of the generalized version of the Eliashberg equations indicates that mixed channels can significantly contribute to the enhancement of superconducting correlations.²⁵ In particular, the incorporation of strong correlations ($U \rightarrow \infty$ limit of the Hubbard model) in terms of auxiliary boson fields²⁶ shows that electron-phonon and electron-phonon-boson interactions can effectively cooperate in the stabilization of superconductivity in a d -wave state.²⁵

The layered structure of systems under consideration suggests that interlayer coupling should be taken into account in realistic description. The Josephson tunneling between adjacent CuO_2 planes can substantially contribute to the enhancement of the superconducting transition temperature.²⁷⁻²⁹ This enhancement is indifferent to the mechanism of intralayer pairing. Therefore, the interlayer tunneling can be considered as a possible source of correlations which amplify the conventional (in-plane) phonon-mediated pairing, usually considered on the BCS level. There is argumentation that this type of coupling originates from a single particle interlayer transfer.²⁷ The particular momentum dependence of the tunneling amplitude $T(\mathbf{k})$ seems to be of minor importance

when considering the symmetry of the superconducting state: the symmetry of the gap is completely determined by intralayer contributions to the pairing kernel.²⁸ However, an interesting feature is that originally introduced $T(\mathbf{k}) \sim (\cos k_x a - \cos k_y a)^4$ (Ref. 27) can lead to strongly temperature dependent gap anisotropy.³⁰

Our aim is to consider the role of interlayer tunneling in the strong coupling limit. This type of approach is based on the framework of Eliashberg equations³¹ and therefore more general than mean-field-like treatment. It means that we assume the electron-phonon interaction to be the in-plane pairing mechanism and incorporate the contribution of Josephson tunneling to the resulting Eliashberg equation for the superconducting transition temperature. Therefore, the interlayer tunneling and phonon mediated contributions to superconductivity can be considered on equal footing, within the strong coupling theory. This allows one to discuss larger values of the tunneling energy than dictated by the BCS type approach and describe the tunneling of electrons within bands which are renormalized by the intralayer pairing mechanism (electron-phonon interaction). Coupling to c -axis phonons can be considered as a possible source of the momentum conserving pair tunneling^{32,33} which contributes to the increase of $T(\mathbf{k})$.

II. ELIASHBERG-TYPE APPROACH TO INTERLAYER TUNNELING

We consider two identical planes coupled by Josephson tunneling term $T(\mathbf{k})$. The electron-phonon interaction is assumed to be source of intraplane pairing correlations. To formulate Eliashberg equations one has to introduce the Nambu representation which facilitates the derivation of an equation for the matrix self-energy. We define $\Psi_{ik}^+ = (f_{ik\uparrow}^+, f_{i-\mathbf{k}\downarrow}^+)$,³¹ where $i(=1,2)$ enumerates the planes. Our model Hamiltonian takes on the form

$$\begin{aligned}
 H = & \sum_{i=1}^2 \sum_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} \Psi_{ik}^+ \tau_3 \Psi_{ik} + \sum_{i=1}^2 \sum_{\mathbf{q}} \omega_{\mathbf{q}} B_{iq}^+ B_{iq} \\
 & + \sum_{i=1}^2 \sum_{\mathbf{k}, \mathbf{q}} \tilde{g}_{\mathbf{k}\mathbf{k}+\mathbf{q}} \Psi_{ik+\mathbf{q}}^+ \tau_3 \Psi_{ik} (B_{iq} + B_{i-\mathbf{q}}^+) - \sum_{\mathbf{k}} \tilde{T}(\mathbf{k}) \\
 & \times (\Psi_{1\mathbf{k}}^+ \tau_+ \Psi_{1\mathbf{k}} \Psi_{2\mathbf{k}}^+ \tau_- \Psi_{2\mathbf{k}} + \Psi_{2\mathbf{k}}^+ \tau_+ \Psi_{2\mathbf{k}} \Psi_{1\mathbf{k}}^+ \tau_- \Psi_{1\mathbf{k}}). \quad (1)
 \end{aligned}$$

$\tilde{\varepsilon}_{\mathbf{k}}$ denotes the band energy in which correlation effects can be incorporated within the mean-field approximation for auxiliary boson fields ($U \rightarrow \infty$ limit of the Hubbard model³⁴) (Refs. 21, 23–26): $\tilde{\varepsilon}_{\mathbf{k}} = r^2 \varepsilon_{\mathbf{k}} - \mu$. Here, $r^2 = 1 - n$ denotes the bandwidth narrowing factor, where n is the average number of electrons per site, $n = (1/N) \sum_{\mathbf{k}\sigma} \langle f_{i\mathbf{k}\sigma}^+ f_{i\mathbf{k}\sigma} \rangle$. μ stands for the effective chemical potential renormalized by the Lagrange multiplier which guarantees the exclusion of the double occupancy of the lattice sites.²⁶ For the two-dimensional lattice with the nearest-neighbor hopping t the bare band dispersion is $\varepsilon_{\mathbf{k}} = -t\gamma(\mathbf{k})$ where $\gamma(\mathbf{k}) = 2(\cos k_x a + \cos k_y a)$. In this paper we choose t as an energy unit. Similarly to Refs. 21 and 25 we consider only the covalent part of the electron-phonon interaction which implies that $\tilde{g}_{\mathbf{k}\mathbf{k}+\mathbf{q}} = r^2 g_{\mathbf{k}\mathbf{k}+\mathbf{q}}$ within the mean-field approximation for auxiliary boson fields. In our notation

$$\tau_{\pm} = \frac{1}{2} (\tau_1 \pm i\tau_2), \quad (2)$$

where τ_i ($i=0, \dots, 3$) are the Pauli matrices. The off-site character of interlayer tunneling causes that in a strongly correlated system $T(\mathbf{k})$ becomes renormalized by the bandwidth narrowing factor. In what follows we will not specify the momentum dependence of the effective tunneling energy $\tilde{T}(\mathbf{k})$; its actual form originates from the mechanism responsible for transportation of Cooper pairs between adjacent layers. Within the mean-field approximation for auxiliary boson fields $\tilde{T}(\mathbf{k}) = r^4 T(\mathbf{k})$.³³ The phonon contribution will be modeled by an Einstein oscillator of frequency ω_0 . As the planes are assumed to be identical it is sufficient to derive the Eliashberg equations for one of them. The matrix self-energy can be found from the Dyson equation³¹

$$\hat{\Sigma}_{1\mathbf{k}}(i\omega_l) = \hat{G}_{01\mathbf{k}}^{-1}(i\omega_l) - \hat{G}_{1\mathbf{k}}^{-1}(i\omega_l), \quad (3)$$

where

$$\hat{G}_{01\mathbf{k}}^{-1}(i\omega_l) = i\omega_l \tau_0 - \tilde{\varepsilon}_{\mathbf{k}} \tau_3, \quad (4)$$

and $\hat{G}_{1\mathbf{k}}(i\omega_l)$ stands for the Matsubara Green's function

$$\hat{G}_{1\mathbf{k}}(i\omega_l) = \langle \langle \Psi_{1\mathbf{k}} | \Psi_{1\mathbf{k}}^+ \rangle \rangle. \quad (5)$$

ω_l is the Matsubara frequency $\omega_l = (\pi/\beta)(2l+1)$; $\beta = (kT)^{-1}$. Usually one chooses $\hat{\Sigma}_{1\mathbf{k}}$ in the form

$$\hat{\Sigma}_{1\mathbf{k}}(i\omega_l) = [1 - Z_{1\mathbf{k}}(i\omega_l)] i\omega_l \tau_0 + \phi_{1\mathbf{k}}(i\omega_l) \tau_1 \quad (6)$$

which is valid when the energy shift ($\sim \tau_3$) is a small quantity and can be neglected.^{31,23,25} $\phi_{1\mathbf{k}}$ is the momentum-dependent order parameter. In the strongly correlated case only intersite (nearest neighbor) pairing is important. This leads to

$$\phi_{1\mathbf{k}}(i\omega_l) = \gamma(\mathbf{k}) \phi_{1\gamma}(i\omega_l) + \eta(\mathbf{k}) \phi_{1\eta}(i\omega_l), \quad (7)$$

where $\eta(\mathbf{k}) = 2(\cos k_x a - \cos k_y a)$ and $\phi_{1\gamma}(\phi_{1\eta})$ corresponds to the extended s -wave (d -wave) amplitude of the singlet pairing state.^{23,25}

The general solution of the Eliashberg equations originating from the model Hamiltonian (1) is a very difficult task, in particular if momentum dependence of the superconducting order parameter and details of the two-dimensional band structure are to be taken into account. Therefore, we will consider the limiting case of $T = T_c$. One can assume that the momentum dependence of formfactors in the order parameter $[\gamma(\mathbf{k}), \eta(\mathbf{k})]$ and the band energy $[\sim \gamma(\mathbf{k})]$ is of major importance and neglect the momentum index of the renormalization factor, $Z_{i\mathbf{k}}(i\omega_l) = Z_i(i\omega_l)$. Then, at $T = T_c$, different types of symmetry separate.^{23,25} This feature is impervious to the details of the interlayer part of the pairing kernel.^{28,30} As we are interested in the relative significance of phonon and interlayer contributions to the formation of a superconducting state, the momentum dependence of $\tilde{T}_{\mathbf{k}}$ will be neglected from now on. There are the following contributions to the self-energy.

(i) The electron-phonon contribution:

$$\hat{\Sigma}_{1\mathbf{k}}^{PH} = \sum_{\mathbf{q}} \tilde{g}_{\mathbf{k}-\mathbf{q}\mathbf{k}} \tilde{g}_{\mathbf{k}\mathbf{k}-\mathbf{q}} \tau_3 \langle \langle \Psi_{1\mathbf{k}-\mathbf{q}} (B_{1\mathbf{q}} + B_{1-\mathbf{q}}^+) | \Psi_{1\mathbf{k}-\mathbf{q}}^+ \rangle \rangle \times (B_{1-\mathbf{q}} + B_{1\mathbf{q}}^+) \tau_3, \quad (8)$$

which has already been investigated to some extent and the results of Refs. 23–25 can be adapted to the present case.

(ii) The interlayer tunneling contribution: Here we distinguish between three types of terms. The most important are terms linear in \tilde{T} because they are directly related to the intralayer Cooper pairs. This shows up in the off-diagonal elements in $\hat{\Sigma}_{1\mathbf{k}}^T$:

$$\hat{\Sigma}_{1\mathbf{k}}^T = \begin{pmatrix} 0 & -\tilde{T} \langle f_{2-\mathbf{k}\downarrow} f_{2\mathbf{k}\uparrow} \rangle \\ -\tilde{T} \langle f_{2\mathbf{k}\uparrow}^+ f_{2-\mathbf{k}\downarrow}^+ \rangle & 0 \end{pmatrix}. \quad (9)$$

Note that when evaluating $\hat{\Sigma}_{1\mathbf{k}}^T$ the self-energy effects should be self-consistently taken into account. Second order contributions of the form

$$\tilde{T}^2 \tau_+ \langle \langle \Psi_{1\mathbf{k}} f_{2-\mathbf{k}\downarrow} f_{2\mathbf{k}\uparrow} | \Psi_{1\mathbf{k}}^+ f_{2-\mathbf{k}\downarrow} f_{2\mathbf{k}\uparrow} \rangle \rangle \tau_+ \quad (10)$$

are negligible at $T = T_c$ and the remaining terms like

$$\tilde{T}^2 \tau_+ \langle \langle \Psi_{1\mathbf{k}} f_{2-\mathbf{k}\downarrow} f_{2\mathbf{k}\uparrow} | \Psi_{1\mathbf{k}}^+ f_{2\mathbf{k}\uparrow}^+ f_{2-\mathbf{k}\downarrow}^+ \rangle \rangle \tau_- \quad (11)$$

do not contain off-diagonal elements and contribute only to the renormalization factor Z_1 . The two-dimensional-like properties of copper-oxides superconductors suggest that intralayer correlations are by far larger than interlayer correlations. One can consider the tunneling potential \tilde{T} as a small quantity when compared with the bandwidth and intraplane electron-phonon coupling. This allows one to neglect the \tilde{T}^2 part of Z_1 (see the values of \tilde{T} considered in the numerical analysis) and assume that Eq. (9) represents the most important contribution of interlayer tunneling to the kernels within strong-coupling theory:

$$\hat{\Sigma}_{1\mathbf{k}}(i\omega_l) = \hat{\Sigma}_{1\mathbf{k}}^{PH}(i\omega_l) + \hat{\Sigma}_{1\mathbf{k}}^T. \quad (12)$$

After some algebra one can incorporate $\hat{\Sigma}_{1\mathbf{k}}^T$ into the Dyson equation (3)

$$[\hat{\Sigma}_{1\mathbf{k}}^T]_{ab} = \tilde{T}(\delta_{ab} - 1) \frac{1}{\beta} \sum_n [\hat{G}_{2\mathbf{k}}(i\omega_n)]_{ab}, \quad (13)$$

where ab enumerate matrix elements. This allows one to commence the construction of the Eliashberg equations for the superconducting transition temperature. As the strong local repulsion acts in disfavor of on-site pairing, the natural assumption is that the dominating contribution to superconductivity originates from the nearest neighbor Cooper pairs. Due to the identity of planes $Z_i(i\omega_n) = Z(i\omega_n)$, $\phi_{1\mathbf{k}}(i\omega_n) = \phi_{\mathbf{k}}(i\omega_n)$ and the resulting Eliashberg equations take on the form

$$Z(i\omega_l) = 1 + \frac{1}{\beta\omega_l} \sum_n \frac{\lambda\nu^2}{(l-n)^2 + \nu^2} \frac{1}{N} \times \sum_{\mathbf{k}} Z(i\omega_n)\omega_n d_{\mathbf{k}}(i\omega_n), \quad (14)$$

$$\phi_a(i\omega_l) = \frac{1}{\beta} \sum_n \left(\frac{\lambda_\gamma\nu^2}{(l-n)^2 + \nu^2} + \tilde{T} \right) \frac{1}{4N} \sum_{\mathbf{k}} a^2(\mathbf{k}) d_{\mathbf{k}}(i\omega_n) \times \phi_a(i\omega_n). \quad (15)$$

To explain the notation: In Eq. (15) $a = \gamma(\eta)$ differentiate between types of symmetry of the superconducting state. We have denoted

$$d_{\mathbf{k}}(i\omega_n) = [Z(i\omega_n)\omega_n^2 + \varepsilon_{\mathbf{k}}^2]^{-1}, \quad (16)$$

and, following Kresin's procedure,³⁵ introduced some average phonon frequency $\langle\Omega\rangle$

$$\nu = \frac{\langle\Omega\rangle}{2\pi kT_c} \quad (17)$$

which will be identified with the frequency of an Einstein oscillator ω_0 . The electron-phonon coupling function is defined by

$$\lambda_{(\gamma)} = r^4 \lambda_{(\gamma)}^0, \quad (18)$$

where $\lambda_{(\gamma)}^0$ is derived with the help of Fermi-surface averaged Eliashberg function:

$$\lambda^0 = 2 \int_0^\infty \frac{d\Omega}{\Omega} \left\langle -\frac{1}{\pi} g_{\mathbf{k}\mathbf{p}} g_{\mathbf{p}\mathbf{k}} \text{Im} D_{\mathbf{k}-\mathbf{p}}(\Omega + i0^+) \right\rangle_{\mathbf{k},\mathbf{p}}, \quad (19)$$

$$\lambda_\gamma^0 = 2 \int_0^\infty \frac{d\Omega}{\Omega} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{4} \gamma(\mathbf{q}) \left\langle -\frac{1}{\pi} g_{\mathbf{k}\mathbf{k}-\mathbf{q}} g_{\mathbf{k}-\mathbf{q}\mathbf{k}} \text{Im} D_{\mathbf{q}} \times (\Omega + i0^+) \right\rangle_{\mathbf{k}}, \quad (20)$$

with $D_{\mathbf{q}}$ being the phonon propagator. An important point is that these simplifications do not influence the way in which interlayer tunneling enters the Eliashberg equations. It is nontrivial that beyond the weak-coupling limit the \tilde{T} term gives an additional contribution to the phonon-induced ker-

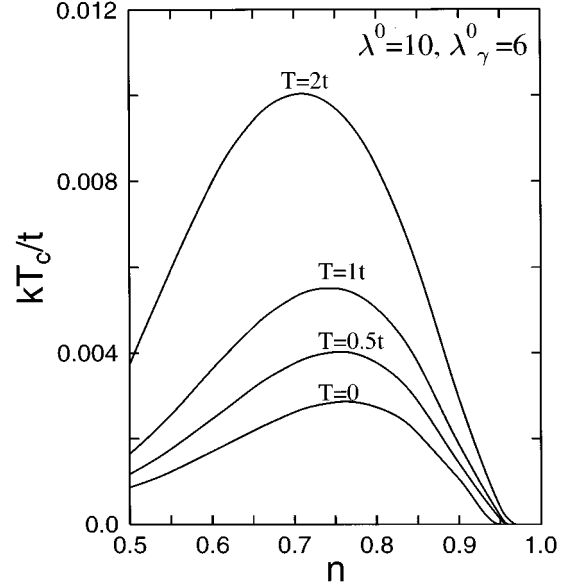


FIG. 1. Superconducting transition temperature for d -wave symmetry as a function of the occupation number for different values of the bare tunneling parameter T . λ^0 and λ_γ^0 are the unrenormalized electron-phonon coupling functions. The quantities of actual physical meaning originate from the renormalization by the factor of $r^4 = (1-n)^2$.

nel in an equation for the superconducting transition temperature [Eq. (15)]. As this is a frequency independent shift which does not contribute to the renormalization factor Z , one can expect the pronounced enhancement of T_c .

III. NUMERICAL RESULTS

To solve Eqs. (14) and (15) numerically one has to evaluate $\lambda_{(\gamma)}$ which is a difficult task. In order to get the first insight into the significance of the tunneling term, we will use λ^0 and λ_γ^0 as parameters.^{23,25} However, one should bear in mind that due to the averaging over the Fermi surface these are occupation number dependent quantities.³⁶ This feature can be, to some extent, smeared out by the presence of the renormalization factor in Eq. (18). To get realistic values of the transition temperatures we have examined Eqs. (14) and (15) for values of $\lambda_{(\gamma)}^0$ between 4 and 10. This corresponds to the variation of the electron-phonon coupling function $\lambda_{(\gamma)}$ [Eq. (18)] between 1 and 2.5 for $n=0.5$ and 0 for $n \rightarrow 1$, which is roughly the region of physical interest. To see the impact of the tunneling term we have varied T/t between 0 and 2. The latter value corresponds to $\tilde{T} \approx 0.125t$ at $n \approx 0.75$ (where T_c achieves its maximal value) which also is of reasonable order of magnitude.

Figure 1 shows the occupation number dependence of the superconducting transition temperature for different values of bare tunneling parameter T . With respect to the averaged phonon frequency we have assumed $\langle\Omega\rangle = 0.1t$ throughout this paper.²³⁻²⁵ It is remarkable that already for $T=t$ ($\tilde{T} \approx 0.0625t$) one can observe that maximal value of T_c , T_c^{max} , increases by the factor of 2. Note that these results correspond to d -wave symmetry; extended s -wave superconductivity does not set in at the physically interesting region of doping.²³⁻²⁵

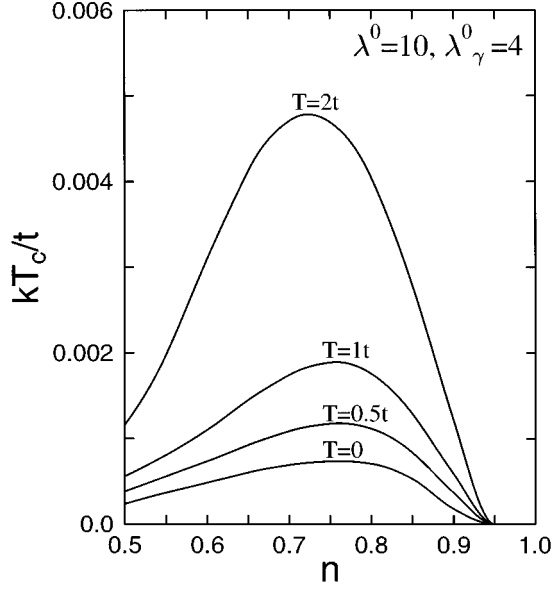


FIG. 2. The same as in Fig. 1 but for smaller value of the superconducting coupling function λ_γ^0 .

The relative magnitude of λ^0 and λ_γ^0 depends on the details of the electron-phonon matrix elements. Therefore, for smaller values of the unrenormalized superconducting coupling λ_γ^0 even more drastic effects are expected when the tunneling term is plugged in, as shown in Fig. 2. Figure 3 shows the superconducting transition temperature at optimal doping as a function of the bare tunneling parameter for different values of λ_γ^0 . The changes in λ^0 affect T_c less than changes in λ_γ^0 , as shown in Fig. 4. This is due to the fact that λ^0 determines directly only the magnitude of the renormal-

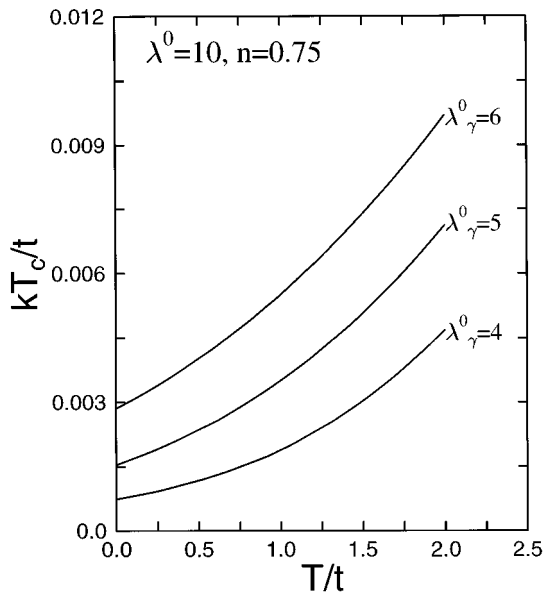


FIG. 3. Superconducting transition temperature for d -wave symmetry at the optimal doping as a function of the bare tunneling parameter for different values of the unrenormalized superconducting coupling function λ_γ^0 .

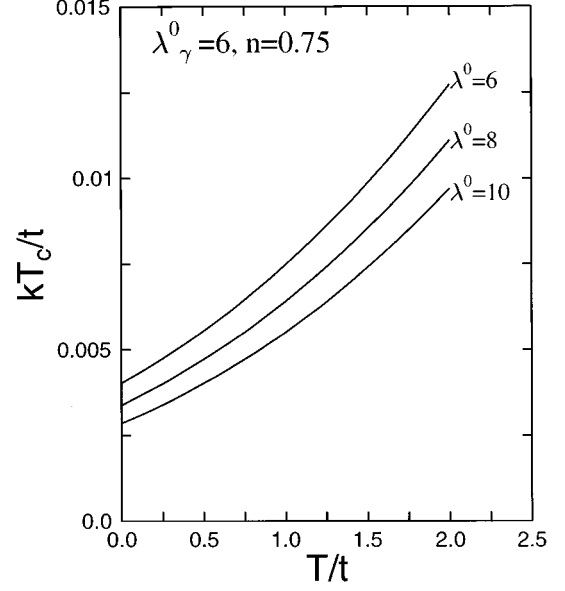


FIG. 4. The same as in Fig. 3 but for different values of the unrenormalized coupling function λ^0 .

ization factor $Z(i\omega_n)$. Therefore, small corrections to Z contained in the neglected \tilde{T}^2 terms are not of any importance when considering superconducting properties.

IV. CONCLUDING REMARKS

We have considered the role of interlayer Josephson tunneling for superconductivity within the two-dimensional, strongly correlated electron-phonon system described by the Hubbard model ($U \rightarrow \infty$ limit) coupled to phonons. To account for strong correlations we have applied the mean-field approximation for auxiliary boson fields. The tunneling term has been incorporated into the structure of generalized Eliashberg equations. Such a formulation allows one to discuss the possible role of the interlayer transportation of Cooper pairs beyond the weak-coupling theory. In contradistinction to the electron-phonon mechanism, modification of the renormalization factor Z due to the tunneling of Cooper pairs is small ($\sim \tilde{T}^2$) when compared with the contribution to the pairing kernel ($\sim \tilde{T}$). The tunneling term modifies the phonon-induced pairing kernel by the frequency independent contribution which leads to the pronounced enhancement of the superconducting transition temperature. Details of the two-dimensional band structure have explicitly been taken into account. Similarly to the weak-coupling case,²⁸ the symmetry of the superconducting order parameter is determined by the intralayer pairing. Numerical analysis of the Eliashberg equations shows that interlayer tunneling can substantially stabilize a d -wave superconducting state. This feature remains in agreement with recent findings for layered copper oxides.^{37–40} In the present paper we stick to the picture developed in our previous works.^{23–25} Phonon-induced superconductivity can survive in a strongly correlated system where correlations are responsible for the dressing of carriers. In particular, d -wave superconductivity can originate from “dressed” electron-phonon interaction. This view finds

corroboration in Ref. 39 where the possibility of phonon-induced d -wave superconductivity in the presence of short-range antiferromagnetic correlations has seriously been considered.

We have neglected momentum dependence of the tunneling energy $\tilde{T}(\mathbf{k})$. The separate question refers to the relative significance of different possible tunneling mechanisms. The interlayer degrees of freedom can play an important role in high- T_c superconductors.^{41,42} The c -axis phonon mediated

interlayer coupling^{32,33} may significantly enhance tunneling effects.⁴³ This problem is presently under investigation.

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