d-wave superconductivity in a strongly correlated electron-phonon system

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The problem of phonon-mediated and phonon-free contributions to d-wave superconductivity in the twodimensional Hubbard model has been addressed. Strong local correlations $(U \rightarrow \infty \text{ limit})$ have been incorporated in the slave boson formulation. In order to consider electron-boson and electron-phonon coupling on equal footing, fluctuations of the auxiliary boson fields over their mean-field value have been introduced. The magnitude of effective pairing interactions derived with the help of a canonical transformation indicates that within the weak-coupling theory, phonon-mediated pairing plays a marginal role and can be dominated by a phonon-free pairing mechanism. On the other hand, in the strong-coupling limit (Eliashberg formulation), electron-phonon and electron-phonon-boson interactions can significantly enhance the superconducting transition temperature. It is also shown that Coulomb correlations together with the electron-phonon interaction can effectively stabilize a *d*-wave superconducting state.

I. INTRODUCTION

The problem of symmetry of the pairing state and related pairing mechanism of high-temperature superconductors is of current interest. With respect to the influence of phonons on the pairing mechanism, there are speculations that one may expect the presence of rather strong electron-phonon interactions in these systems.¹⁻⁴ As phonons are affected below the superconducting transition temperature^{5,6} and pronounced isotope effects are observed,⁷ one can assume that coupling of electrons to phonons gives at least partially rise to the formation of the superconducting state. On the other hand, strong Coulomb correlations can be considered as an intimate feature of quasiparticles in CuO₂ layers. Therefore, the possibility of a purely electronic pairing mechanism due to exchange of antiferromagnetic spin fluctuations has been discussed in detail.⁸⁻¹³ Since local correlations act in disfavor of on-site pairing, they can nevertheless induce $d_{x^2-y^2}$ wave pairing.^{8,11} For example, the gapless behavior observed in the case of $YBa_2Cu_3O_{7-x}$ (Ref. 14) can be interpreted in terms of d-wave $(d_{x^2-y^2})$ symmetry. However, in the case of $Nd_{2-r}Ca_rCuO_4$ (Ref. 15) a fit with a BCS s-wave density of states gives better results. This difference may perhaps be attributed to different pairing mechanisms in these two compounds but there is some evidence that a *d*-wave model may better account for most of the experimental data.¹⁶⁻¹⁹ One should bear in mind that experimental results are merely consistent with *d*-wave pairing, they can also be understood in terms of anisotropic s-wave pairing or mixture of s- and $d_{x^2-y^2}$ wave contributions. The interpretation of experiments which measure the momentum dependence of the gap $\Delta_{\mathbf{k}}$ on the Fermi surface [angular-resolved photoemission, $Bi_2Si_2CaCu_2O_{8-r}$ (Ref. 20)], are also not free from ambiguity. In particular, the sign reversal of the order parameter can be explained in terms of two-component s-wave pairing.²¹ We refer to Refs. 22-25 for further discussion on this subject.

A comprehensive treatment of phonon-induced and phonon-free contributions to superconductivity of strongly correlated systems is still missing. Generally, one faces a difficult problem of how to generalize the Eliashberg equations²⁶ in the presence of strong correlations.²⁷ A minimal model which accounts for strong correlations among quasiparticles in CuO_2 planes, is the two-dimensional (2D) Hubbard model²⁸ extended to include electron-phonon interactions. There are speculations that phonon-mediated superconductivity can survive in the presence of strong correlations;²⁹⁻³⁷ even an enhancement of the electronphonon coupling by Coulomb correlations may be possible.^{29,32,35,37} It is interesting to observe that well before the discovery of high-temperature superconductivity, Kim found that exchange interactions can enhance the electronphonon coupling.³⁸ This observation led to the suggestion that an exchange-enhanced electron-phonon interaction may be responsible for superconductivity in heavy fermion and high- T_c systems.³⁹ On the other hand, exchange interactions can considerably suppress the transport electron-phonon coupling function.³¹ So, in principle, there seems to be no contradiction of having large phonon-induced λ_{SC} value (1–2) giving rise to superconductivity and a much lower λ_{tr} value which determines the slope of electrical resistivity.

There is a rather widely accepted view that antiferromagnetic spin fluctuations, when sufficiently strong, increase T_c in the *d*-wave channel, whereas the electron-phonon interaction counteracts the *d*-wave pairing.⁴⁰ However, also the phonon-mediated attraction can be effective in the *d*-wave channel if the electron-phonon interaction is spatially nonlocal and Coulomb repulsion suppresses the superconductivity in the *s*-wave channel.^{34,36}

In this paper we will discuss the problem of phononinduced and phonon-free contributions to superconductivity in the frame of two-dimensional Hubbard model in the strong-coupling limit $(U \rightarrow \infty)$. As both contributions are present in the systems under consideration, any advanced theory should also take into account both of them. The problem which arises, is to consider phonon-mediated and correlation-mediated contributions on equal footing. In order to achieve this in the most simple manner, we treat strong local correlations in terms of auxiliary boson fields⁴¹ and introduce fluctuations over their mean-field values. This implies that the electron-boson interaction resembles the electron-phonon interaction, whereby the role of phonons is taken over by fluctuations of the boson fields. At the first stage, we eliminate the electron-boson and electron-phonon coupling with the help of a canonical transformation (weakcoupling limit) and derive effective intersite pairing interactions. The bare vertex of the boson-mediated interaction is proportional to the band energy which means that this contribution is by far the largest one. In order to get realistic values for the superconducting transition temperature T_c , one must evaluate vertex corrections and consider the strongcoupling limit, i.e., one has to solve the resulting Eliashberg equations. Results derived within the latter formulation demonstrate the dominating role of d-wave symmetry for small concentration of holes. They also show that the channels containing phonon contributions can significantly enhance T_c . These features support the view that phonon-mediated and phonon-free channels can cooperate in the formation of $d_{x^2-y^2}$ superconducting state in the frame of the single-band Hubbard model.

II. EFFECTIVE PAIRING INTERACTIONS IN THE WEAK-COUPLING LIMIT

We consider the 2D Hubbard model coupled to phonons. Strong correlations are incorporated in the auxiliary boson formulation⁴¹

$$H = -t \sum_{\langle i,j \rangle,\sigma} f_{i\sigma}^{+} f_{j\sigma} b_{j}^{+} b_{i} - \mu \sum_{i,\sigma} f_{i\sigma}^{+} f_{i\sigma}$$
$$+ \sum_{\langle i,j \rangle,l,\sigma} g_{ijl} f_{i\sigma}^{+} f_{j\sigma} b_{j}^{+} b_{i} (B_{l}^{+} + B_{l})$$
$$+ \lambda_{B} \sum_{i} \left(1 - b_{i}^{+} b_{i} - \sum_{\sigma} f_{i\sigma}^{+} f_{i\sigma} \right) + H_{\text{PH}}, \qquad (1)$$

where g_{ijl} is the Fourier transform of the momentumdependent electron-phonon interaction

$$g_{ijl} = \frac{1}{N^{3/2}} \sum_{\mathbf{k},\mathbf{q}} g_{\mathbf{k}\mathbf{k}+\mathbf{q}} e^{-i(\mathbf{k}+\mathbf{q})\cdot\mathbf{R}_i + \mathbf{k}\cdot\mathbf{R}_j + i\mathbf{q}\cdot\mathbf{R}_l}$$
(2)

and, similarly to Ref. 30, we consider only the covalent part of g_{ijl} , i.e., *i* and *j* are nearest-neighbor sites; *t* is the nearest-neighbor hopping integral leading to $\epsilon_{\mathbf{k}} = -t \gamma(\mathbf{k})$ with $\gamma(\mathbf{k}) = 2(\cos k_x a + \cos k_y a)$; μ stands for the chemical potential and λ_B is a Lagrange multiplier introduced to guarantee exclusion of double occupancy of the lattice sites. H_{PH} represents the phonon contribution which, for the sake of simplicity, will be modeled by an Einstein oscillator of frequency ω_0 . Within the mean-field approximation one replaces boson operators by classical numbers $b_i \rightarrow \langle b \rangle \equiv r$ which gives the bandwidth narrowing factor $\epsilon_{\mathbf{k}} \rightarrow r^2 \epsilon_{\mathbf{k}}$ with $r^2 = 1 - n$, where *n* is the average number of electrons per site, $n = (1/N) \sum_{\mathbf{k},\sigma} \langle f_{\mathbf{k}\sigma}^{\dagger} f_{\mathbf{k}\sigma} \rangle$. We define fluctuations of auxiliary boson fields over their mean-field value

$$\tilde{b}_i \equiv b_i - r. \tag{3}$$

Then the Hamiltonian (1) takes on the form

$$H = H_0 + H_1, \tag{4}$$

where

 $H_0 = H_{\rm MF} - t \sum_{\langle i,j \rangle,\sigma} f^+_{i\sigma} f_{j\sigma} \tilde{b}^+_j \tilde{b}^-_i - \lambda_B \sum_i \tilde{b}^+_i \tilde{b}^-_i + H_{\rm PH}, \quad (5)$

and

$$H_{1} = -rt \sum_{\langle i,j \rangle,\sigma} f_{i\sigma}^{+} f_{j\sigma} (\tilde{b}_{j}^{+} + \tilde{b}_{i})$$

+
$$\sum_{\langle i,j \rangle,l,\sigma} \hat{G}_{ijl} f_{i\sigma}^{+} f_{j\sigma} (B_{l}^{+} + B_{l}), \qquad (6)$$

$$\hat{G}_{ijl} = g_{ijl} [\tilde{b}_j^+ \tilde{b}_i + r(\tilde{b}_j^+ + \tilde{b}_i) + r^2].$$
(7)

The mean-field Hamiltonian $H_{\rm MF}$ is given by

$$H_{\rm MF} = -tr^2 \sum_{\langle i,j \rangle,\sigma} f^+_{i\sigma} f_{j\sigma} - (\mu + \lambda_B) \sum_{i,\sigma} f^+_{i\sigma} f_{i\sigma} - \lambda_B r^2 N + \lambda_B N.$$
(8)

In order to eliminate the H_1 term, we carry out the canonical transformation with the generating function given by $[H_0,S]=H_1$. Then $(1/2)[S,H_1]$ gives rise to the effective pairing interaction. The explicit presence of boson fields in H_1 will generate products of operators which have to be truncated. One also has to linearize the *t* term in Eq. (5) which brings about a dispersion for bosonic fluctuations.

Within the mean-field approximation the dispersion for fermions $(\epsilon_{\mathbf{k}} \rightarrow r^2 \epsilon_{\mathbf{k}})$ originates from the replacement: $b_i^+ b_j \rightarrow \langle b_i^+ \rangle \langle b_j \rangle \equiv r^2$. In order to evaluate in the same way the dispersion for bosonic fluctuations we have to calculate $\Sigma_{\sigma} \langle f_{i\sigma}^+ f_{j\sigma} \rangle_{i\neq j} \simeq 2 \langle f_{i\sigma}^+ \rangle \langle f_{j\sigma} \rangle \equiv f^2$. To do this we make use of the Caron-Pratt approximation⁴² for $H_{\rm MF}$. It has been proved that the Caron-Pratt approximation gives rise to the best single-site effective Hamiltonian for the Hubbard model.⁴³ Within this approximation each atom is not coupled to any other but can exchange electrons with a particle reservoir which plays the role of its environment. This corresponds to the following decoupling for the *t* term in $H_{\rm MF}$:

$$H_{\rm MF} \simeq -tr^2 \sum_{i,\sigma} \left(\langle f_{i\sigma}^+ \rangle f_{i\sigma} + \langle f_{i\sigma} \rangle f_{i\sigma}^+ \right) - (\mu + \lambda_B) \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma} + \text{const.}$$
(9)

Then, the straightforward calculation leads to $f^2 = n(1-n)$ which means that we can quantitatively distinguish between metallic $(f^2 \neq 0)$ and insulating $(f^2 \rightarrow 0)$ phase of the system. The resulting dispersion relation for the fluctuating boson field is given by

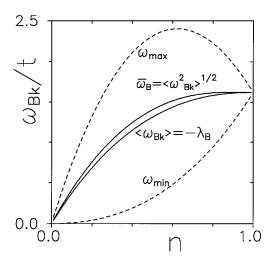


FIG. 1. Dispersion relation for fluctuating boson fields defined in Eq. (10) versus occupation number; $\langle \cdots \rangle$ stands for the average over the Brillouin zone.

$$\omega_{B\mathbf{k}} = -f^2 t \, \gamma(\mathbf{k}) - \lambda_B \,. \tag{10}$$

It is shown in Fig. 1 as a function of the occupation number. f^2 can be very well modeled by a function which accounts for the periodicity of the 2D lattice³⁷

$$f^{2} = \frac{1}{8} \frac{1}{N} \sum_{\mathbf{k}} \langle f_{\mathbf{k}\sigma}^{+} f_{\mathbf{k}\sigma} \rangle [\gamma^{2}(\mathbf{k}) - \eta^{2}(\mathbf{k})], \qquad (11)$$

where $\eta(\mathbf{k}) = 2(\cos k_x a - \cos k_y a)$.

In the momentum representation the generating function *S* is of the form

$$S = S^{\rm PH} + S^{\rm SB} + S^{\rm PHSB} \tag{12}$$

where

$$S^{\rm PH} = \sum_{\mathbf{k}\mathbf{q}\sigma} f^+_{\mathbf{k}+\mathbf{q}\sigma} f_{\mathbf{k}\sigma} [u(\mathbf{k},\mathbf{q})B_{\mathbf{q}} + v(\mathbf{k},\mathbf{q})B^+_{-\mathbf{q}}], \quad (13)$$

$$S^{\rm SB} = \frac{r}{\sqrt{N}} \sum_{\mathbf{k}\mathbf{q}\sigma} f^+_{\mathbf{k}+\mathbf{q}\sigma} f_{\mathbf{k}\sigma} [t(\mathbf{k},\mathbf{q})b_{\mathbf{q}} + z(\mathbf{k},\mathbf{q})b^+_{-\mathbf{q}}], \quad (14)$$

$$S^{\text{PHSB}} = \frac{r}{\sqrt{N}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\sigma} f^{+}_{\mathbf{k}\sigma} f_{\mathbf{k}'\sigma} [x_1(\mathbf{k}, \mathbf{k}', \mathbf{q}) b_{\mathbf{k}-\mathbf{k}'-\mathbf{q}} B_{\mathbf{q}} + x_2(\mathbf{k}, \mathbf{k}', \mathbf{q}) b_{\mathbf{k}-\mathbf{k}'-\mathbf{q}} B^{+}_{-\mathbf{q}} + x_3(\mathbf{k}, \mathbf{k}', \mathbf{q}) b_{\mathbf{k}'-\mathbf{k}+\mathbf{q}} B_{\mathbf{q}} + x_4(\mathbf{k}, \mathbf{k}', \mathbf{q}) b_{\mathbf{k}'-\mathbf{k}+\mathbf{q}} B^{+}_{-\mathbf{q}}].$$
(15)

The corresponding coefficients u, v, ... have to be determined from the condition $[H_0S] = H_1$. The contribution coming from the first term in Eq. (7) is negligibly small because \tilde{b}_i^+ and $\tilde{b}_i^+ \tilde{b}_i$ vanish when averaged over the mean-field ground state.

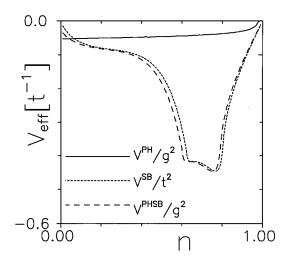


FIG. 2. Effective pairing interactions defined in Eqs. (14)–(16) versus occupation number; $\omega_0=0.1t$.

In the case of large local repulsion $(U \rightarrow \infty)$ only intersite Cooper pairs will survive and the nearest-neighbor pairing interaction originating from $(1/2)[S,H_1]$ will be of the form

$$(H_{\rm SC})_{\rm nn} = \frac{1}{2} V_{\rm eff} \sum_{\langle i,j\rangle,\sigma,\sigma'} f^+_{i\sigma} f^+_{j\sigma'} f_{i\sigma'} f_{j\sigma}.$$
(16)

The resulting effective pairing potential, V_{eff} , consists of contributions from electron-phonon (PH), electron-boson (SB), and electron-phonon-boson (PHSB) interactions

$$V_{\rm eff} = V^{\rm PH} + V^{\rm SB} + V^{\rm PHSB} \tag{17}$$

with

$$V^{\rm PH} = r^4 \; \frac{\omega_0 g^2}{2N} \sum_{\mathbf{k}, \mathbf{p}} \; \frac{\gamma(\mathbf{p}) \, \gamma(\mathbf{k})}{(\tilde{\boldsymbol{\epsilon}}_{\mathbf{p}} - \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}})^2 - \omega_0^2}, \tag{18}$$

$$V^{\rm SB} = r^2 \frac{t^2}{2N^2} \sum_{\mathbf{k},\mathbf{p}} \frac{\gamma^2(\mathbf{k})}{\tilde{\epsilon}_{\mathbf{p}} - \tilde{\epsilon}_{\mathbf{k}} - \omega_{B\mathbf{p}-\mathbf{k}}},\tag{19}$$

$$V^{\rm PHSB} = r^2 \frac{g^2}{2N^2} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} \frac{\gamma^2(\mathbf{k})}{\tilde{\epsilon}_{\mathbf{p}} - \tilde{\epsilon}_{\mathbf{k}} - \omega_0 - \omega_{B\mathbf{q}}}, \qquad (20)$$

and $\tilde{\epsilon}_{\mathbf{k}} = r^2 \epsilon_{\mathbf{k}} - \mu - \lambda_B$. In the numerical evaluation we have used $g_{\mathbf{k}\mathbf{k}+\mathbf{q}} \simeq \gamma(\mathbf{k})g_{\mathbf{q}}$ (Ref. 37) and have replaced $g_{\mathbf{q}}$ by some average, momentum-independent quantity g.

Figure 2 shows the behavior of the different contributions to V_{eff} as functions of the occupation number. It is obvious that V^{SB} is by far the largest contribution. Also the PHSB contribution is larger than the PH one. In order to facilitate the numerical work we have neglected the momentum dependence of $\omega_{B\mathbf{k}}$ ($\omega_{B\mathbf{k}} \rightarrow \bar{\omega}_B$ in Fig. 1). But this simplification does not lead to any essential changes in the values of the V's. Therefore, within the weak-coupling theory, phononmediated pairing interactions play a minor role and may be dominated by phonon-free interactions which originate in our case from fluctuations of the auxiliary boson field over its mean-field value. This observation is in agreement with out previous results obtained for the $U \rightarrow \infty$ limit of the 2D Hubbard model,⁴⁴ where we have used a decoupling scheme for Hubbard operators.

With respect to symmetry considerations we note that the evaluated interactions are of the same magnitude (and of attractive character) for *d*-wave and extended *s*-wave pairing. Due to the strong enhancement of V_{eff} for small concentrations of holes, *d*-wave symmetry will dominate in the region, where nesting effects eliminate extended *s*-wave contributions to the pairing state.³⁷ Note also that we have got repulsive effective interaction for the *p*-wave channel. This feature is consistent with the seeming experimental evidence that *p*-wave pairing can be ruled out.⁴⁵

The above discussion shows that in order to get a more realistic picture of the relative significance of phononmediated and phonon-free superconductivity one has to go beyond the mean-field-slave-boson approximation. Also one has to use the strong-coupling Eliashberg formulation²⁶ which allows one to consider the electron-phonon, electron-boson, and electron-phonon-boson interactions on an equal footing. One should bear in mind that vertex corrections, not considered here, may be of some importance. However, this is a difficult problem^{30,35,46} which needs a separate study and for the sake of simplicity we will consider only bare interactions in this paper.

III. ELIASHBERG-TYPE APPROACH TO DEAL WITH THE FLUCTUATING BOSON FIELDS

In order to construct the Eliashberg equations, one usually introduces the Nambu representation,²⁶ $\Psi_i^+ = (f_{i\uparrow}^+ f_{i\downarrow})$, and rewrites the Hamiltonian (4) in terms of the Ψ operators. This leads to

$$H = -tr^{2} \sum_{\langle i,j \rangle} \Psi_{i}^{+} \tau_{3} \Psi_{j} - (\mu + \lambda_{B}) \sum_{i} \Psi_{i}^{+} \tau_{3} \Psi_{i}$$
$$-tf^{2} \sum_{\langle i,j \rangle} \tilde{b}_{j}^{+} \tilde{b}_{i} - \lambda_{B} \sum_{i} \tilde{b}_{i}^{+} \tilde{b}_{i} - rt \sum_{\langle i,j \rangle} [\Psi_{i}^{+} \tau_{3}^{1} \Psi_{j} (\tilde{b}_{j}^{+} + \tilde{b}_{i}) + \Psi_{i}^{+} \tau_{3}^{2} \Psi_{j} (\tilde{b}_{j} + \tilde{b}_{i}^{+})] + \sum_{\langle i,j \rangle, l} \hat{G}_{ijl} \Psi_{i}^{+} \tau_{3} \Psi_{j} (B_{l} + B_{l}^{+}) + H_{\text{PH}}, \qquad (21)$$

where

$$\tau_3^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$
, $\tau_3^2 = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$,

and τ_i (i=1...4) are the Pauli matrices. The exclusion of double occupancy imposes a restriction on the components of the Matsubara Green's function $\langle \langle \Psi_n | \Psi_m^+ \rangle \rangle$ and the matrix self-energy. Only intersite contributions enter the nondiagonal elements of $\langle \langle \Psi_n | \Psi_m^+ \rangle \rangle$ which corresponds to non-local pairing in the $U \rightarrow \infty$ limit.^{33,36,37} The matrix self-energy can be found from²⁶

$$\hat{\Sigma}_{\mathbf{k}}(i\omega_l) = \hat{G}_{0\mathbf{k}}^{-1}(i\omega_l) - \hat{G}_{\mathbf{k}}^{-1}(i\omega_l), \qquad (22)$$

where

$$\hat{G}_{0\mathbf{k}}(i\omega_l) = (i\omega_l\tau_0 - \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}}\tau_3)^{-1}, \qquad (23)$$

and $\hat{G}_k(i\omega_l)$ stands for the Fourier transform of the Matsubara Green's function

$$\langle \langle \Psi_n | \Psi_m^+ \rangle \rangle_{i\omega_l} = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{e}^{-i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \hat{G}_{\mathbf{k}}(i\omega_l).$$
 (24)

 ω_l is the Matsubara frequency, $\omega_l = (2l+1)\pi/\beta$, $\beta = (kT)^{-1}$. The usual ansatz for $\hat{\Sigma}_k$ is of the form²⁶

$$\hat{\Sigma}_{\mathbf{k}}(i\omega_l) = [1 - Z_{\mathbf{k}}(i\omega_l)]i\omega_l\tau_0 + \phi_{\mathbf{k}}(i\omega_l)\tau_1 + \chi_{\mathbf{k}}(i\omega_l)\tau_3,$$
(25)

which in the case of intersite (nearest-neighbor) pairing leads to the momentum-dependent order parameter $\phi_{\mathbf{k}}$

$$\phi_{\mathbf{k}}(i\omega_l) = \gamma(\mathbf{k})\phi_{\gamma}(i\omega_l) + \eta(\mathbf{k})\phi_{\eta}(i\omega_l), \qquad (26)$$

where ϕ_{γ} (ϕ_{η}) corresponds to the extended *s*-wave (*d*-wave) component of the singlet pairing state.

There are the following leading contributions to the matrix self-energy:

(i) the electron-phonon contribution:

$$\hat{\Sigma}_{\mathbf{k}}^{\text{PH}} = \frac{r^4}{N} \sum_{mn} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \\ \times \sum_{j(\neq n), i(\neq m), l, h} \tau_3 g_{njl} g_{imh} \langle \langle \Psi_j \Phi_l | \Psi_i^+ \Phi_h \rangle \rangle \tau_3,$$
(27)

with $\Phi_l = B_l + B_l^+$, (ii) the electron-boson contribution:

$$\begin{split} \hat{\Sigma}_{\mathbf{k}}^{\mathrm{SB}} &= \frac{1}{N} \sum_{mn} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \\ & \times \sum_{\langle j \rangle_n \langle i \rangle_m} t^2 r^2 \langle \langle [\tau_3^1(\tilde{b}_n + \tilde{b}_j^+) + \tau_3^2(\tilde{b}_n^+ \\ &+ \tilde{b}_j)] \Psi_j | \Psi_i^+ [(\tilde{b}_i \tilde{b}_m^+) \tau_3^1 + (\tilde{b}_i^+ + \tilde{b}_m) \tau_3^2] \rangle \rangle, \end{split}$$
(28)

(iii) the electron-boson-phonon contribution:

$$\hat{\Sigma}_{\mathbf{k}}^{\text{PHSB}} = \frac{1}{N} \sum_{mn} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \sum_{j(\neq n), i(\neq m), l, h} \tau_3 r^2 g_{njl} g_{imh}$$

$$\times \langle \langle [\tau_3^1(\tilde{b}_n + \tilde{b}_j^+) + \tau_3^2(\tilde{b}_n^+ \tilde{b}_j)] \Psi_j \Phi_l | \Phi_h \Psi_i^+ [(\tilde{b}_i + \tilde{b}_m^+) \tau_3^1 + (\tilde{b}_i^+ + \tilde{b}_m^-) \tau_3^2] \rangle \rangle.$$
(29)

It can be shown that χ_k is a small quantity and can be neglected.³⁶ At $T = T_c$, different types of symmetry separate and one gets the system of Eliashberg equations

$$Z(i\omega_l) = 1 + \frac{1}{\pi(2l+1)} \sum_n \left[r^2 \Lambda^{\text{PH}}(l-n) + r^2 \Lambda^{\text{SB}}(l-n) + \frac{1}{\beta} \sum_m \Lambda^{\text{PHSB}}(l-n-m) \right] \frac{1}{N}$$
$$\times \sum_{\mathbf{p}} Z(i\omega_n) \omega_n d_{\mathbf{p}}(i\omega_n), \qquad (30)$$

$$\phi_{a}(i\omega_{l}) = \frac{1}{4\beta} \sum_{n} \left[r^{2} \Lambda_{\gamma}^{\text{PH}}(l-n) + r^{2} \Lambda_{\gamma}^{\text{SB}}(l-n) + \frac{1}{\beta} \sum_{m} \Lambda_{\gamma}^{\text{PHSB}}(l-n-m) \right] \frac{1}{N} \times \sum_{\mathbf{p}} a^{2}(\mathbf{p}) \phi_{a}(i\omega_{n}) d_{\mathbf{p}}(i\omega_{n}), \qquad (31)$$

where Z_k has been replaced by some average, momentumindependent quantity. We have used the following notation:

$$\Lambda^{\rm PH}_{(\gamma)}(m) = \lambda_{(\gamma)} \nu^2 [m^2 + \nu^2]^{-1}, \qquad (32)$$

$$\Lambda_{(\gamma)}^{\text{PHSB}}(m) = 2\,\bar{\omega}_B \left[\omega_m^2 + \bar{\omega}_B^2\right]^{-1} \Lambda_{(\gamma)}^{\text{PH}}(m), \qquad (33)$$

$$\Lambda^{\rm SB}(m) = 8t^2 \bar{\omega}_B [\omega_m^2 + \bar{\omega}_B^2]^{-1}, \qquad (34)$$

$$\Lambda_{\gamma}^{\rm SB}(m) = 2t^2 \frac{1}{N} \sum_{\mathbf{k}} \omega_{B\mathbf{k}} \gamma(\mathbf{k}) [\omega_m^2 + \omega_{B\mathbf{k}}^2]^{-1}, \quad (35)$$

and

$$d_{\mathbf{k}}(i\omega_n) = [(Z(i\omega_n)\omega_n)^2 + \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}}^2]^{-1}.$$
 (36)

Following Kresin's procedure,⁴⁷ we introduce some average phonon frequency $\langle \Omega \rangle$

$$\nu = \frac{\langle \Omega \rangle}{2\pi kT_c} \tag{37}$$

which, similarly to the previous section, corresponds to the frequency of an Einstein oscillator ω_0 . The electron-phonon coupling functions $\lambda_{(\gamma)}$ are defined by

$$\lambda_{(\gamma)} = 2 \int_0^\infty d\Omega \; \frac{\alpha^2 F_{(\gamma)}(\Omega)}{\Omega},\tag{38}$$

where $\alpha^2 F_{(\gamma)}(\Omega)$ stands for the Fermi-surface averaged Eliashberg function

$$\alpha^{2}F(\Omega) = \left\langle -\frac{r^{2}}{\pi} g_{\mathbf{pk}}g_{\mathbf{kp}} \operatorname{Im}D_{\mathbf{k}-\mathbf{p}}(\Omega+i\delta) \right\rangle_{\mathbf{k},\mathbf{p}}, \quad (39)$$

$$\alpha^{2} F_{\gamma}(\Omega) = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{4} \gamma(\mathbf{q}) \\ \times \left\langle -\frac{r^{2}}{\pi} g_{\mathbf{k}\mathbf{k}-\mathbf{q}} g_{\mathbf{k}-\mathbf{q}\mathbf{k}} \operatorname{Im} D_{\mathbf{q}}(\Omega+i\delta) \right\rangle_{\mathbf{k}},$$
(40)

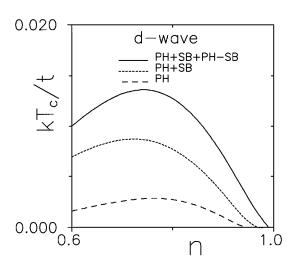


FIG. 3. Superconducting transition temperature for the different phonon-boson channels as a function of the occupation number; $\lambda_{\gamma} \lambda = 0.6$, $\lambda(T_c^{max}) = 2$.

with $D_q(\Omega)$ being the phonon propagator. The $a(\mathbf{k})$'s are formfactors determined by the symmetry of the order parameter, $a = \gamma$ (extended *s*-wave) or η (*d*-wave). Note that we have taken into account details of the two-dimensional band structure. This shows up in the explicit presence of $\tilde{\epsilon}_{\mathbf{k}}$ in (30) and (31).

The *ab initio* evaluation of $\lambda_{(\gamma)}$ is a difficult task, especially if one would like to take into account the renormalization of $D_{\mathbf{k}}(\Omega)$ originating from the electron (boson)-phonon interaction. In particular, softening of the phonon mode can lead to a pronounced enhancement of $\lambda_{(\gamma)}$ for small concentrations of holes. Therefore, in order to get the first insight into the relative significance of the different kernels, we will use λ and λ_{γ} as parameters.

To get satisfactory convergence when solving the resulting system of equations for T_c we had to sum over 50 Matsubara frequencies. Figure 3 shows the occupation number dependence of the superconducting transition temperature corresponding to *d*-wave symmetry. Note that the Eliashberg function $\alpha^2 F_{(\gamma)}(\Omega)$ contains the bandwidth narrowing factor r^2 which reflects the destructive role of correlations for superconductivity at small concentration of holes. We have used $\langle \Omega \rangle = 0.1t$, $\lambda_{\gamma} \lambda = 0.6$, and $\lambda(T_c^{\text{max}}) = 2$. The maximal value of T_c , T_c^{max} , corresponds to $n \approx 0.75$. Therefore, λ varies between $\simeq 4$ and 0 for physically interesting region of n between ≈ 0.5 and 1. Despite the rather large value of the electron-phonon coupling function, phonons alone play a minor role in the formation of the superconducting state. The situation changes when the remaining interactions are also taken into account. In particular the mixed PHSB contribution plays an important role in the enhancement of T_c . Figure 4 shows how extended s-wave superconductivity sets in at larger doping values. These results only serve as a guideline since the use of the mean-field value of λ_B in the boson propagators in Λ^{SB} and Λ^{PHSB} is a rather crude procedure for small values of *n* because thermal excitations of low-energy bosons overestimate the role of contributions in which fluctuating boson fields are involved. Figure 5 shows that even for smaller values of the electron-phonon coupling function $(\lambda_{\lambda} = 0.3)$, the inclusion of the PH channel can significantly

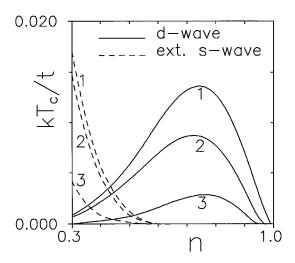


FIG. 4. Superconducting transition temperature for *d*-wave and extended *s*-wave symmetry as a function of the occupation number. Curves 1–3 refer to the PH+SB+PHSB, PH+SB and PH channel, respectively; $\lambda_{\gamma} \lambda = 0.6$, $\lambda(T_c^{\text{max}}) = 2$.

enhance T_c compared to its value arising from the boson fluctuations alone. The inclusion of the mixed PHSB contribution leads to further enhancement of T_c . We observe that the ratio T_c/T_c^{max} shows some kind of universal behavior as a function of the occupation number: it weakly depends on the ratio λ_{γ}/λ as shown in Fig. 6, where curves for $\lambda_{\gamma}/\lambda=0.6$ and 0.3 correspond to $\lambda(T_c^{\text{max}})=2$ and the curve for $\lambda_{\gamma}/\lambda=0.5$ corresponds to $\lambda(T_c^{\text{max}})=1.2$.

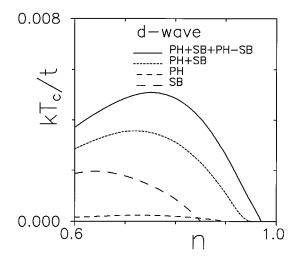


FIG. 5. Superconducting transition temperature for the different phonon-boson channels as a function of the occupation number; $\lambda_{\gamma} \lambda = 0.3$, $\lambda(T_c^{max}) = 2$.

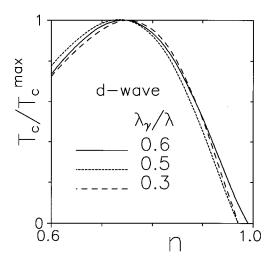


FIG. 6. T_c/T_c^{max} versus occupation number. Curves for $\lambda_{\gamma}\lambda=0.6$ and 0.3 correspond to $\lambda(T_c^{\text{max}})=2$, the curve for $\lambda_{\gamma}\lambda=0.5$ corresponds to $\lambda(T_c^{\text{max}})=1.2$.

IV. CONCLUDING REMARKS

We have considered phonon-induced and phonon-free superconductivity in a strongly correlated electron system represented by the 2D Hubbard model in the $U\rightarrow\infty$ limit coupled to phonons. Strong correlations have been accounted for by auxiliary boson formulation. In order to consider correlation and phonon-mediated contributions on equal footing, we have introduced fluctuations of auxiliary boson fields over their mean-field value. This causes the leading terms to resemble the electron-phonon interaction kernel with phonons replaced by boson fluctuations.

This particular form of interaction originates from the linear character of correlations over the mean-field value Eq. (3)]. A similar type of interaction arises when considering the motion of a hole in the quantum antiferromagnetic Heisenberg model within linear spin-wave theory.⁴⁸ Here, magnons take over the role of phonons. The phonon-free superconductivity in strongly correlated Hubbard model (or t-J model) originates from many-body effects (exchange of antiferromagnetic spin fluctuations, for instance,⁸⁻¹³) represented by unusual commutation rules of Hubbard operators $X_i^{0\sigma}$. The Hubbard operators are related to the boson fields by $X_i^{0\sigma} = b_i^+ f_{i\sigma}^{4}$.⁴¹ The many-body effects responsible for the exchangelike origin of superconducting pairing are drastically reduced within the mean-field approximation for the boson fields. However, they are partially restored when introducing fluctuations over the mean-field value, $X_i^{0\sigma} = (r + \tilde{b}_i^+) f_{i\sigma}$. Therefore, the terms linear in \tilde{b} 's can be interpreted as a source of exchange-mediated superconducting pairing.

There are three contributions to the superconducting pairing state: electron-phonon (PH), electron-boson (SB), and mixed electron-phonon-boson (PHSB) interactions. A simple canonical transformation leads to a large value for the pairing interaction in the SB channel showing that in the weakcoupling limit phonons play a marginal role as compared to the phonon-free contributions. Therefore, in order to get more insight into the actual situation, we have discussed the relative significance of different channels within the Eliashberg scheme. Details of the two-dimensional band structure have explicitly been taken into account. Our results support the view that *d*-wave superconductivity may survive in strongly correlated systems for small and moderate concentrations of holes. Even if only low T_c values are possible in the PH channel, the inclusion of this channel can substantially enhance T_c . The mixed PHSB channel also plays a non-negligible role in the formation of the superconducting state. These results are consistent with the general scenario that both electron-electron and electron-phonon effects can cooperate in the formation of the *d*-wave superconducting state in strongly correlated systems.

However, one should bear in mind that the treatment presented here is far from being complete. For example, we have not incorporated vertex corrections. Also we have simulated with the 2D Hubbard model a single CuO_2 layer in high- T_c superconductors. Interlayer effects must be taken into account in a more realistic description. It is well known that the coupling between electrons in adjacent layers can give rise to higher T_c values,^{49,50} and in particular the enhancement of the electron-phonon interaction by interlayer tunneling can substantially contribute to the formation of the superconducting state.⁵¹

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- ¹R. E. Cohen, W. E. Pickett, L. L. Boyer, and H. Krakauer, Phys. Rev. Lett. **60**, 817 (1988).
- ²R. Zeyher and G. Zwicknagl, Z. Phys. B 78, 175 (1990); R. Zeyher, *ibid.* 80, 187 (1990).
- ³S. Barisić, K. Kupcić, and I. Batistić, Int. J. Mod. Phys. B 3, 2051 (1993).
- ⁴H. Krakauer, W. E. Pickett, and R. E. Cohen, Phys. Rev. B 47, 1002 (1993).
- ⁵M. C. Krantz, C. Tomsen, H. Mattausch, and M. Cardona, Phys. Rev. B **50**, 1165 (1994).
- ⁶A. P. Litvinchuk et al., Phys. Rev. B 50, 1171 (1994).
- ⁷J. P. Franck *et al.*, Phys. Rev. Lett. **71**, 283 (1993).
- ⁸P. Monthoux, A. Balatsky, and D. Pines, Phys. Rev. B **46**, 14 803 (1992).
- ⁹D. Thelen, D. Pines, and Jian Ping Lu, Phys. Rev. B 47, 9151 (1993).
- ¹⁰K. Maki and H. Won, Phys. Rev. Lett. 72, 1758 (1994).
- ¹¹N. Bulut, D. J. Scalapino, and S. R. White, J. Supercond. 7, 572 (1994).
- ¹²P. Monthoux and D. Pines, Phys. Rev. B 49, 4261 (1994).
- ¹³ P. Monthoux and D. J. Scalapino, Phys. Rev. Lett. **72**, 1874 (1994); For a recent overview, see A. P. Kampf, Phys. Rep. **249**, 219 (1994); D. J. Scalapino, *ibid*. **250**, 329 (1995).
- ¹⁴J. M. Valles *et al.*, Phys. Rev. B **44**, 11 986 (1991).
- ¹⁵A. G. Sun *et al.*, Phys. Rev. Lett. **72**, 2267 (1994).
- ¹⁶T. P. Deveraux et al., Phys. Rev. Lett. 72, 396 (1994).
- ¹⁷D. A. Wollman, D. J. Van Harlingen, J. Giapintzakis, and D. M. Ginsberg, Phys. Rev. Lett. **74**, 797 (1995).
- ¹⁸S. M. Quinlan and D. J. Scalapino, Phys. Rev. B 51, 497 (1995).
- ¹⁹T. Dahm and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995).
- ²⁰Z. Y. Shen *et al.*, Phys. Rev. Lett. **70**, 1553 (1993).
- ²¹A. A. Golubov and I. I. Mazin, Physica C **243**, 153 (1995); A. I. Liechtenstein, I. I. Mazin, and O. K. Andersen, Phys. Rev. Lett. **74**, 2303 (1995).
- ²²V. Z. Kresin and S. A. Wolf, J. Supercond. 7, 531 (1994).
- ²³R. C. Dynes, Solid State Commun. **92**, 53 (1994).
- ²⁴J. R. Schrieffer, Solid State Commun. **92**, 129 (1994).
- ²⁵See contributions to the Proceedings of the International Conference, Materials and Mechanisms of Superconductivity, Grenoble, France, 1994 [Physica C 235–240 (1994)].
- ²⁶For a general discussion of the Eliashberg equations [originally formulated by G. M. Eliashberg, Sov. Phys. JETP **11**, 696

(1960)], we refer to P. B. Allen and B. Mitrović, *Solid State Physics: Advances in Research and Applications* (Academic, New York, 1982), Vol. 37, p. 1.

- ²⁷Chan Minh-Tien and N. M. Plakida, Mod. Phys. Lett. B 6, 1309 (1992); Physica C 206, 90 (1993).
- ²⁸J. Hubbard, Proc. R. Soc. London Ser. A **376**, 238 (1963).
- ²⁹J. Zieliński, M. Matlak, and P. Entel, Phys. Lett. A **165**, 285 (1992); J. Zieliński and M. Matlak, Phys. Lett. A **172**, 467 (1993).
- ³⁰Ju H. Kim and Z. Tesanović, Phys. Rev. Lett. **71**, 4218 (1993).
- ³¹M. L. Kulić and R. Zeyher, Phys. Rev. B **49**, 4395 (1994); R. Zeyher, J. Supercond. **7**, 537 (1994).
- ³²G. M. Eliashberg, J. Supercond. 7, 525 (1994).
- ³³J. Zieliński, M. Mierzejewski, P. Entel, and R. Grabowski, J. Supercond. 8, 135 (1995).
- ³⁴ J. Song and J. F. Annett, Phys. Rev. B **51**, 3840 (1995).
- ³⁵J. D. Lee, K. Kang, and B. I. Min, Phys. Rev. B **51**, 3850 (1995).
- ³⁶M. Mierzejewski, J. Zieliński, and P. Entel, J. Supercond. (to be published).
- ³⁷M. Mierzejewski and J. Zieliński, Phys. Rev. B **52**, 3079 (1995).
- ³⁸D. J. Kim, Phys. Rev. B **17**, 468 (1978); For an overview, see also Phys. Rep. **171**, 129 (1988).
- ³⁹D. J. Kim, Jpn. J. Appl. Phys. 26, L741 (1987).
- ⁴⁰H. Rietschel, J. Low Temp. Phys. **95**, 293 (1994).
- ⁴¹G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986);
 P. Coleman, Phys. Rev. B **35**, 5072 (1987); D. M. Newns and R. Read, Adv. Phys. **36**, 799 (1987).
- ⁴²L. G. Caron and G. W. Pratt, J. Appl, Phys. **39**, 485 (1868); Rev. Mod. Phys. **40**, 802 (1968).
- ⁴³J. Monecke, Phys. Status Solidi B 51, K81 (1972).
- ⁴⁴ M. Mierzejewski, J. Zieliński, and P. Entel, Physica C 235–240, 2143 (1994).
- ⁴⁵C. P. Slichter, J. Phys. Chem. Solids **54**, 1439 (1993).
- ⁴⁶M. Grabowski and L. J. Sham, Phys. Rev. B **29**, 6132 (1984).
- ⁴⁷ V. Z. Kresin, H. Gutfreund, and W. A. Little, Solid State Commun. **51**, 339 (1984); V. Z. Kresin, Phys. Lett. A **122**, 434 (1987).
- ⁴⁸S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
- ⁴⁹Z. Tesanović, Phys. Rev. B **36**, 2364 (1987).
- ⁵⁰B. D. Yu, H. Kim, and J. Ihm, Phys. Rev. B 45, 8007 (1992).
- ⁵¹S. Chakravarty, A. Sudbo, P. W. Anderson, and S. Strong, Science 261, 337 (1993).