Correlated phonons and the T_c-dependent dynamical phonon anomalies

T. Hakioğlu
Department of Physics, Bilkent University, TR-06533 Bilkent, Ankara, Turkey

H. Türeci
Department of Physics, Yale University, New Haven, Connecticut 06511

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Anomalously large low-temperature phonon anharmonicities can lead to static as well as dynamical changes in the low-temperature properties of the electron-phonon system. In this work, we focus our attention on the dynamically generated low-temperature correlations in an interacting electron-phonon system using a self-consistent dynamical approach in the intermediate coupling range. In the context of the model, the polaron correlations are produced by the charge-density fluctuations which are generated dynamically by the electron-phonon coupling. Conversely, the latter is influenced in the presence of the former. The purpose of this work is to examine the dynamics of this dual mechanism between the two using the illustrative Fröhlich model. In particular, the influence of the low-temperature phonon dynamics on the superconducting properties in the intermediate coupling range is investigated. The influence on the Holstein reduction factor as well as the enhancement in the zero-point fluctuations and in the electron-phonon coupling are calculated numerically. We also examine these effects in the presence of superconductivity. Within this model, the contribution of the electron-phonon interaction as one of the important elements in the mechanisms of superconductivity can reach values as high as 15–20 % of the characteristic scale of the lattice vibrational energy. The second motivation of this work is to understand the nature of the T_c-dependent temperature anomalies observed in the Debye-Waller factor, dynamical pair correlations, and average atomic vibrational energies for a number of high-temperature superconductors. In our approach we do not claim nor believe that the electron-phonon interaction is the primary mechanism leading to high-temperature superconductivity. Nevertheless, our calculations suggest that the dynamically induced low-temperature phonon correlation model can account for these anomalies and illustrates their possible common origin. Finally, the relevance of incorporating these low-temperature effects into more realistic models of high-temperature superconductivity including both the charge and spin degrees and other similar ideas existing in the literature are discussed. [S0163-1829(97)01541-5]

I. MOTIVATION AND PRELIMINARIES

Raman,[1,2] infrared,[3] neutron scattering,[4,5] and point-contact tunneling spectroscopy[6] experiments have consistently shown strong electron-phonon interaction in the Cu-O planes below T_c between certain selected phonon modes and charge carriers as a common feature of high-temperature superconductors (HTS). In particular the observed softening of the 340 cm^{-1} (41 meV) Raman active B_{1g} and the hardening of the 440 and 504 cm^{-1} (54.5 meV, 62.4 meV) Raman active A_{1g} modes of the YBCO compound[1,7] were described in terms of the strong electron-phonon coupling theory of Zeyher and Zwicknagl.[8] Their results also accord with the frequency shift and linewidth measurements of other $R\mathrm{Ba}_2\mathrm{Cu}_3\mathrm{O}_{7-x}$ (R=Er, Eu, Dy, Tm) compounds. However the strong-coupling scheme formulated as an extention of the Eliashberg formalism is insufficient particularly for explaining the important critical behavior observed in the dynamical structure factor $S(\mathbf{k},\omega)$ near T_c. Inelastic neutron-scattering experiments on $\mathrm{YBa}_2\mathrm{Cu}_3\mathrm{O}_{7-x}$ revealed strong short-range sensitivity of the momentum dependence of $S(\mathbf{k},\omega)$ within the region of few lattice spacing. Further, $S(\mathbf{k},\omega)$ experiences a significant enhancement in the vicinity of T_c by approximately 10% for certain z-polarized modes.[9,10] On the other hand, closely related to $S(\mathbf{k},\omega)$, the atomic pair distribution function measurements give evidence for anomalous temperature dependence of the correlated vibrations of the Cu and O atoms in the planes.[10,11] In contrast to the case of crystallographic measurements, the atomic pair distribution function and dynamical measurements have the advantage of clearly distinguishing between random impurities and correlated vibrations of specific atoms. The latter is reflected as consistent shifts in the peak positions of the pair distribution function.[4,10,11] Similar experiments were repeated more recently also for $\mathrm{La}_{1.85}\mathrm{Sr}_{0.15}\mathrm{CuO}_4$ and for some other HTS displaying a similar dynamical short-range behavior in the pair correlation function.[12] The coupling of the incoming polarized neutrons in the neutron-diffraction experiments to short-range spin fluctuations as a possible mechanism for such anomalies is ruled out since the wave vector is larger than 5 Å^{-1} where the magnetic response dies out. It has been suggested that the characterization of these local structures in terms of a dynamical model naturally indicates polaronic mechanisms.[13]

In the most general understanding, such effects imply the realization of a dynamical nonperturbative ground-state mixing electronic and vibrational degrees of freedom. As a result of strong electron-phonon interaction, the ground state of the system can accomodate quantum fluctuations in the phonon population even at very low temperatures.[13]

We start with the effective electron-electron coupling $V^{e-e}(\mathbf{k})$ in the presence of such low-temperature anomalies

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as expressed in the generalized McMillan approach by[14]

$$V^{e-e}(\mathbf{k}) = -\frac{1}{N}\sum_{\mathbf{k}'\mathbf{k}''s}^{\mathrm{FS}}\sum_{n}\frac{|\langle\psi_n|M(\mathbf{k}',\mathbf{k}'')|\psi_0\rangle|^2}{\hbar\Omega_{\mathbf{k}s}^{(n)}-\hbar\Omega_{\mathbf{k}s}^{(0)}}\,\delta_{\mathbf{k},\mathbf{k}'-\mathbf{k}''}, \tag{1}$$

where $\mathbf{k}',\mathbf{k}''$ are the momenta of the interacting electrons, $\hbar\Omega_{\mathbf{k}s}^{(n)}$ and $\hbar\Omega_{\mathbf{k}s}^{(0)}$ are respectively the nth vibrational energy eigenvalue and the $n=0$ ground-state energy of the exchanged nonperturbative phonon mode with momentum $\mathbf{k}$ and branch index s, $|\psi_n\rangle$ and $|\psi_0\rangle$ are the vibrational n particle eigenstates and the ground state corresponding to $\hbar\Omega_{\mathbf{k}s}^{(n)}$ and $\hbar\Omega_{\mathbf{k}s}^{(0)}$, respectively, and $M(\mathbf{k}',\mathbf{k}'')$ is the electron-phonon matrix element

$$M(\mathbf{k}',\mathbf{k}'')\,\delta_{\mathbf{k},\mathbf{k}'-\mathbf{k}''} = g_s(\mathbf{k})\langle\mathbf{k}'|c^{\dagger}_{\mathbf{k}''+\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}\mathbf{Q}_{\mathbf{k}}|\mathbf{k}''\rangle, \tag{2}$$

where $\mathbf{Q}_{\mathbf{k}} = a_{\mathbf{k}s}+a^{\dagger}_{-\mathbf{k}s}$ with $a_{\mathbf{k}s}$ and $a^{\dagger}_{-\mathbf{k}s}$ corresponding to single mode phonon operators. The bare electron-phonon coupling constant is represented by $g_s(\mathbf{k})$ and the Fermi surface (FS) average of the scattering matrix $1/N\Sigma^{\mathrm{FS}}_{\mathbf{k}'}\langle\mathbf{k}'|c^{\dagger}_{\mathbf{k}'\sigma}c_{\mathbf{k}'+\mathbf{k}\sigma}|\mathbf{k}+\mathbf{k}'\rangle$ is proportional to average number of FS electrons per unit cell which we will consider to be on the order of unity for each spin degree of freedom. In the harmonic limit, $|\psi_0\rangle$, and $|\psi_n\rangle$ are given by the oscillator eigenstates $|0\rangle$ and $|n\rangle$, respectively, and $\Omega_{\mathbf{k}s}^{(n)}-\Omega_{\mathbf{k}s}^{(0)} = \omega_{\mathbf{k}s}n$. Using Eq. (2) in Eq. (1), it is easy to see that only $n=1$ term contributes in the harmonic limit; hence, Eq. (1) is reduced to its standard form $V^{e-e}(\mathbf{k}) = -|g_s(\mathbf{k})|^2/\hbar\omega_{\mathbf{k}s}$. In what follows, we will work in a single phonon branch and drop the branch index s. We will also simplify the notation for the frequently used $\Omega_{\mathbf{k}s}^{(0)}$ by $\Omega_{\mathbf{k}}$.

The purpose of this work is to examine the leading low-temperature contribution to the nonperturbative eigenstates $|\psi_n\rangle$ as well as $V^{e-e}(\mathbf{k})$ using the illustrative Fröhlich electron-phonon model in the intermediate range of the electron-phonon coupling constant. The method utilizes a self-consistent scheme in order to go beyond the standard polaronic approach by examining the coupling between the low-temperature fluctuations of the polaronic and vibrational degrees of freedom.

An example of a typical application of Eq. (1) is necessary for briefly illustrating its importance in the self-consistent frame of Sec. II. Recently we have shown[15] that, using a Fröhlich type interacting electron-*correlated phonon* model, the low-temperature correlated phonon ground state gives rise to an effective enhancement in the retarded electron-electron pairing attraction as [in the notation of Eqs. (1) and (2)]

$$V^{e-e}(\mathbf{k}) = -\frac{|g(\mathbf{k})|^2}{\hbar\Omega_{\mathbf{k}}}\left[\frac{\omega_{\mathbf{k}}+2\kappa_{\mathbf{k}}}{\Omega_{\mathbf{k}}}\right], \tag{3}$$

where $g(\mathbf{k})$, $\omega_{\mathbf{k}}$, and $\Omega_{\mathbf{k}}$ are as defined in Eq. (1), $\kappa_{\mathbf{k}}$ is an *order parameter* of the anomalous phonon pairing given by $\kappa_{\mathbf{k}} = \Omega_{\mathbf{k}}\langle a^{\dagger}_{-\mathbf{k}}a^{\dagger}_{\mathbf{k}}\rangle$ and $\Omega_{\mathbf{k}} = (\omega^2_{\mathbf{k}}-4\kappa^2_{\mathbf{k}})^{1/2}$ is the phonon eigenfrequency where $\omega_{\mathbf{k}}/\Omega_{\mathbf{k}} = \cosh(4\xi_{\mathbf{k}}) \geqslant 1$. Equation (3), which was derived in Ref. 15, is a specific case of Eq. (1) when the phonon pair correlations are appropriately taken into account in the vibrational eigenstates $|\psi_n\rangle$.

With the enhanced electron-phonon coupling, dynamical correlations can be created between the vibrational modes. The pair-correlated phonon ground state $|\psi_0\rangle$ is connected with the broadened harmonic oscillator ionic ground-state wave function[16] (super Gaussian). In the coordinate-$Q_{\mathbf{k}}$ representation this wave function corresponds to $\psi_0(Q_{\mathbf{k}}) = \langle Q_{\mathbf{k}}|S(\xi)|0\rangle$ where $S(\xi)$ is the pair-correlation operator described by

$$S(\xi) = \prod_{\mathbf{k}}\exp\{-\xi_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}} - a^{\dagger}_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}})\}, \tag{4}$$

where $S(\xi)$ transforms an arbitrary phonon operator $\mathcal{F}(a_{\mathbf{k}},a^{\dagger}_{\mathbf{k}})$ as

$$\mathcal{S}^{\dagger}(\{\xi\})\mathcal{F}(a_{\mathbf{k}},a^{\dagger}_{\mathbf{k}})\mathcal{S}(\{\xi\}) = \mathcal{F}(c_{\mathbf{k}}a_{\mathbf{k}}+s_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}},c_{\mathbf{k}}a^{\dagger}_{\mathbf{k}}+s_{\mathbf{k}}a_{-\mathbf{k}}). \tag{5}$$

Here, $\xi_{\mathbf{k}}$ is somewhat similar to an order parameter describing the strength of the pair correlations, $c_{\mathbf{k}} = \cosh 2\xi_{\mathbf{k}}$ and $s_{\mathbf{k}} = \sinh 2\xi_{\mathbf{k}}$ are given by $c_{\mathbf{k}} = 1/\sqrt{2}[(\omega_{\mathbf{k}}+\Omega_{\mathbf{k}})/\Omega_{\mathbf{k}}]^{1/2}$ and $s_{\mathbf{k}} = 1/\sqrt{2}[(\omega_{\mathbf{k}}-\Omega_{\mathbf{k}})/\Omega_{\mathbf{k}}]^{1/2}$. Here, in the notation of Eq. (1), $|\psi_0\rangle = S(\xi)|0\rangle_{\mathrm{ph}}$ describes the pair-correlated ground state which is annihilated by the operator $B_{\mathbf{k}} = c_{\mathbf{k}}a_{\mathbf{k}} - s_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}}$ with the correct normalization $[B_{\mathbf{k}},B^{\dagger}_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$, where $B^{\dagger}_{\mathbf{k}}$ is the creation operator of a single excitation and $|0\rangle_{\mathrm{ph}}$ is the phonon vacuum state. The n particle excited states $|\psi_n\rangle$ of the kth mode are described by $|\psi_n\rangle = (B^{\dagger}_{\mathbf{k}})^n/\sqrt{n!}\,S(\xi)|0\rangle_{\mathrm{ph}}$. The eigenvalues of $|\psi_n\rangle$ given thus are $\Omega^{(n)}_{\mathbf{k}} = \Omega_{\mathbf{k}}(n+1/2)$ (see Ref. 15). Using $|\psi_n\rangle$ in Eq. (1) and making use of the transformation in Eq. (5), it can be seen that, at low temperatures (i.e., $n=1$), Eq. (3) comprises the leading contribution in the summation of $V^{e-e}(\mathbf{k})$ in Eq. (1). The square bracket in Eq. (3) is identified as the enhancement factor of the zero-point fluctuations due to the pair correlations in the ground state $|\psi_0\rangle$. In order to illustrate this, we first write the ground-state wave function $|\psi_0\rangle$ in the coordinate representation, i.e., $\psi_0(Q_{\mathbf{k}}) \equiv \langle Q_{\mathbf{k}}|\psi_0\rangle$. Using Eq. (4), $\psi_0(Q_{\mathbf{k}})$ is verified by the broadened Gaussian,

$$\psi_0(Q_{\mathbf{k}}) = \sqrt{\frac{1}{\pi}\left(\frac{M\omega_{\mathbf{k}}}{\hbar}\right)e^{-2\xi_{\mathbf{k}}}}\exp\left\{-\left(\frac{M\omega_{\mathbf{k}}}{2\hbar}e^{-4\xi_{\mathbf{k}}}\right)Q^2_{\mathbf{k}}\right\}, \tag{6}$$

where the enhancement in the zero-point fluctuations is directly read from the width as $\langle(Q_{\mathbf{k}})^2\rangle = \exp(4\xi_{\mathbf{k}})\langle(Q_{\mathbf{k}})^2\rangle_0$. Here, $\langle(Q_{\mathbf{k}})^2\rangle_0 = \hbar/2M\omega_{\mathbf{k}}$ represents the average zero-point fluctuations of ions with mass M and the harmonic vibrational frequency $\omega_{\mathbf{k}}$ in the absence of anomalous pair correlations (i.e., $\xi_{\mathbf{k}} = 0$). In the pair-correlated ground state, the enhancement factor was derived to be[15,17]

$$e^{4\xi_{\mathbf{k}}} = (c_{\mathbf{k}}+s_{\mathbf{k}})^2 = \frac{1}{2}\left\{\left(\frac{\omega_{\mathbf{k}}+\Omega_{\mathbf{k}}}{\Omega_{\mathbf{k}}}\right)^{1/2}+\left(\frac{\omega_{\mathbf{k}}-\Omega_{\mathbf{k}}}{\Omega_{\mathbf{k}}}\right)^{1/2}\right\}^2 = \frac{\omega_{\mathbf{k}}+2\kappa_{\mathbf{k}}}{\Omega_{\mathbf{k}}}, \tag{7}$$

which is indeed the enhancement factor in the electron-electron pairing in Eq. (3). In the following, the dynamical aspects of the polaron ground state are examined in the Fröhlich model and shown that, an effective order parameter $\kappa_{\mathbf{k}}$

(or equivalently $\xi_{\mathbf{k}}$) can indeed be defined dynamically if one goes beyond the coherent polaron approximation in the intermediate coupling range. Certain hints have recently been pointed out by the supporters of the polaron school in particular by Ranninger and Thibblin, Das and Choudhury[13] as well as Alexandrov and Krebs[18] regarding the dynamical aspects of the low-temperature polaron models as possible origins of certain T_c dependent vibrational anomalies in high-temperature superconductors. We will explore more on this idea in Secs. II and III.

II. A DYNAMICAL POLARON MODEL AND THE GROUND-STATE CORRELATIONS

In order to investigate the T_c related phonon anomalies in Refs. 9, 10, 11, and 19, we consider the Fröhlich Hamiltonian

$$\mathcal{H}=\sum_{\mathbf{k},\sigma} \mathcal{E}_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} (a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} + 1/2) + \sum_{\mathbf{k},\mathbf{k}',\sigma} g(\mathbf{k}) c_{\mathbf{k}'\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{k}'\sigma} (a_{\mathbf{k}} + a^{\dagger}_{-\mathbf{k}}), \tag{8}$$

where $c^{\dagger}_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}$ create and annihilate electrons of momentum $\mathbf{k}$, spin σ and energy $\mathcal{E}_{\mathbf{k}}$, $a^{\dagger}_{\mathbf{k}}, a_{\mathbf{k}}$ create and annihilate phonons of frequency $\omega_{\mathbf{k}}$ as before. The formalism developed below is not based on the form and the symmetry of the coupling constant used. We will nevertheless use for the model interaction, the coupling of the high-frequency optical B_{1g} buckling phonon modes to planar electrons in the Cu-O planes of a typical HTS compound as

$$|g_b(\mathbf{k})|^2 = 4\lambda_b^2 (\sin^2 k_x/2 + \sin^2 k_y/2). \tag{9}$$

Using tight-binding effective single-band diagonalization, Song and Annett[20] have estimated the magnitudes of the coupling constant λ_b for the LSCO compound at the X point. Naturally for YBCO similar magnitudes are expected due to the common Cu-O planar bonding. However, we will keep λ_b as a phenomenological coupling constant in our model.

Applying on $\mathcal{H}$ the unitary Lang-Firsov transformation

$$\mathcal{U}=\exp\left\{ \sum_{\mathbf{k},\mathbf{k}',\sigma} \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}} c^{\dagger}_{\mathbf{k}+\mathbf{k}',\sigma} c_{\mathbf{k}',\sigma} (a_{\mathbf{k}} - a^{\dagger}_{-\mathbf{k}}) \right\}, \tag{10}$$

$\mathcal{H}$ is transformed into $\mathcal{H}'=\mathcal{U}\mathcal{H}\mathcal{U}^{\dagger}$ as

$$\mathcal{H}'=\sum_{\mathbf{k},\sigma} \tilde{\mathcal{E}}_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} (a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} + 1/2) - \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\sigma} \frac{|g(\mathbf{k})|^2}{\hbar\omega_{\mathbf{k}}} c^{\dagger}_{\mathbf{k}''+\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{k},\sigma'} c_{\mathbf{k}'',\sigma} c_{\mathbf{k}',\sigma'}, \tag{11}$$

In the strong-coupling limit and in the site representation, the first term in Eq. (11) is replaced by

$$\sum_{m,n} \epsilon_{\mathbf{m},\mathbf{n}} \sigma_{m,n} c^{\dagger}_m c_n, \tag{12}$$

where $\epsilon_{\mathbf{m},\mathbf{n}}$ is the translationally invariant hopping amplitude between the neigboring sites $\mathbf{m}$, $\mathbf{n}$ and the multiphonon operator is given by

$$\sigma_{\mathbf{m},\mathbf{n}}=\exp\left\{ \frac{1}{2N} \sum_{\mathbf{k}} \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}} (e^{i\mathbf{k}\cdot\mathbf{m}} - e^{i\mathbf{k}\cdot\mathbf{n}})(a_{\mathbf{k}} - a^{\dagger}_{-\mathbf{k}}) \right\}. \tag{13}$$

We will examine this term separately in Sec. II C.

The average effect of Eq. (10) is to maximally project the original Hamiltonian in Eq. (8) onto the *dynamically displaced* phonon ground state. At sufficiently weak couplings or in the nonitinerant (localized) small polaron limit the statically displaced ground state is a good approximation since it approximates, in these coupling ranges, the well defined quasiparticle states of the polaronic system.[13] In addition to a simple shift from the vacuum to a coherent state which is parametrized by the mean occupation per spin per mode as $\overline{n_{\mathbf{k}}} = \langle \Sigma_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}+\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \rangle$, the ground state shifted by Eq. (10) can also accomodate fluctuations in the charge density around this mean value of which strength is determined by the electron-phonon coupling. In the conventional polaron theory, in the strong-coupling limit, the Hamiltonian (11) with (13) is conventionally used to describe the polaron-polaron attraction and polaronic band narrowing. In the small polaron problem, as a consequence of the large Holstein reduction in the bandwidth, the fluctuations in the charge density are strongly suppressed, and, to a good approximation Eq. (10) can be replaced by its purely *coherent* component[21] as

$$\mathcal{U}_c=\exp\left\{ \sum_{\mathbf{k}} \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}} 2\overline{n_{\mathbf{k}}} (a_{\mathbf{k}} - a^{\dagger}_{\mathbf{k}}) \right\}, \tag{14}$$

which amounts to replacing the electron density $\rho_{\mathbf{k}} = \Sigma_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ by its mean value $2\overline{n_{\mathbf{k}}}$. Here the factor of 2 represents the sum over the spins. In the large range of coupling strengths, between what we might call the small and the strong-coupling limits, the coherent shift induced by Eq. (14) renders to be a poor approximation to the polaronic ground state and the fluctuations of the charge density around its mean value should be considered in a self-consistent frame. This effect has been largely ignored in the past, nevertheless, in the intermediate-coupling range where the polarons are neither strongly localized nor weakly interacting, the fluctuations in the charge density are not negligible and can induce anomalies in the phonon subsystem such as the temperature-dependent enhancement in the Debye-Waller factor as well as in the average vibrational energy $\langle P^2 \rangle_T / 2M$ which is closely linked with the ion momentum fluctuations. In particular, when these fluctuations are driven by superconducting pairs, T_c dependent temperature anomalies are expected to appear (see Sec. III). In principle, the nature of the true ground state can be extracted by examining the induced correlations within the electron-phonon system. Similar retardation effects have also been noticed earlier, for instance, by Ranninger and Thibblin as well as Das and Choudhury.[13] In the former they examined the anomalies in detail in the context of a polaron model with finite number of sites. In the latter the importance of two-phonon correlations have also been stressed.

A. The nature of the polaron ground state

We will now consider the action of Eq. (8) on a particular state $|\Phi_0\rangle \equiv |0\rangle_{ph}\otimes|\psi\rangle_e$. The transformation in Eq. (10) shifts $|\Phi_0\rangle$ to a polaronic dynamical state $|\psi\rangle_p = \mathcal{U}|\Phi_0\rangle$ where the lowest order anomaly appears in the phonon pair correlations

$$_p\langle(a_{\mathbf{k}}-\langle a_{\mathbf{k}}\rangle)(a_{-\mathbf{k}}-\langle a_{-\mathbf{k}}\rangle)\rangle_p = {}_p\langle a_{\mathbf{k}}a_{-\mathbf{k}}\rangle_p - {}_p\langle a_{\mathbf{k}}\rangle\langle a_{-\mathbf{k}}\rangle_p, \tag{15}$$

where $|\ \rangle_p$ indicates $|\psi\rangle_p$. The coherent shift $_p\langle a_{\mathbf{k}}\rangle_p$ is described in the same spirit as in Ref. 21 by

$$_p\langle a_{\mathbf{k}}\rangle_p = \langle\Phi_0|\mathcal{U}^\dagger a_{\mathbf{k}}\mathcal{U}|\Phi_0\rangle = \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}2\overline{n_{\mathbf{k}}}. \tag{16}$$

Equation (15) can be equivalently written, by directly subtracting the coherent part $\mathcal{U}_c$ of the polaron wave function as given by Eq. (14), as $\langle\Phi_0|[\mathcal{U}^\dagger\mathcal{U}_c]a_{\mathbf{k}}a_{-\mathbf{k}}[\mathcal{U}_c^\dagger\mathcal{U}]|\Phi_0\rangle$ where the *reduced* Lang-Firsov transformation is given by

$$\mathcal{U}_c^\dagger\mathcal{U} \equiv \mathcal{U}\mathcal{U}_c^\dagger = \exp\left\{\sum_{\mathbf{k}} \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\delta\rho_{\mathbf{k}}(a_{\mathbf{k}}-a_{-\mathbf{k}}^\dagger)\right\}, \tag{17}$$

with $\delta\rho_{\mathbf{k}} = \Sigma_{\mathbf{k}'\sigma}c_{\mathbf{k}+\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}'\sigma} - 2\overline{n_{\mathbf{k}}}$ describing the charge-density fluctuation operator. The coherent part comprises the zeroth order contribution in the dynamical polaron ground state. The reduced Lang-Firsov transformation is necessary to explore beyond the standard polaron model; since, it is a projection operator on the dynamical polaron wave function $|\psi\rangle_p$ which extracts the proper subspace (where the anomalous pair correlations are to be sought) orthogonal to the zeroth order coherent part.

We seek for the lowest order pair correlations in this orthogonal subspace. The result is given by the density-density correlations as

$$\langle\Phi_0|\mathcal{U}^\dagger\mathcal{U}_c(a_{\mathbf{k}}-\langle a_{\mathbf{k}}\rangle)(a_{-\mathbf{k}}-\langle a_{-\mathbf{k}}\rangle)\mathcal{U}\mathcal{U}_c^\dagger|\Phi_0\rangle = \left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^2\langle\Phi_0|\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}|\Phi_0\rangle. \tag{18}$$

As we calculate higher anomalous pair correlations the nature of the dynamical polaronic state is revealed. For instance, for the nth order anomalous pairing one finds

$$\langle\Phi_0|\mathcal{U}^\dagger\mathcal{U}_c\{(a_{\mathbf{k}}-\langle a_{\mathbf{k}}\rangle)(a_{-\mathbf{k}}-\langle a_{-\mathbf{k}}\rangle)\}^n\mathcal{U}\mathcal{U}_c^\dagger|\Phi_0\rangle = \left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^n\langle\Phi_0|\{\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}\}^n|\Phi_0\rangle. \tag{19}$$

In the following we extract the optimal leading contribution to the ground-state pair correlations using an effective pairing operator.

Extracting the strength of the ground-state pair correlations

To extract the component of the polaronic dynamical wave function acting on pairs of correlated phonons, we first introduce a unitary effective pairing generator as in Eq. (4) by

$$\mathcal{S}(\{\xi\}) = \prod_{\mathbf{k}}\exp\{-\xi_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}}-a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger)\}, \tag{20}$$

and look for the optimal solution of $\xi_{\mathbf{k}}$ self-consistently with the condition that no pair correlations are present in the back transformed state $\mathcal{S}^\dagger(\{\xi\})\mathcal{U}_c^\dagger\mathcal{U}|\Phi_0\rangle$. This amounts to

$$\mathcal{C}_2 \equiv \langle\Phi_0|\mathcal{U}^\dagger\mathcal{U}_c\mathcal{S}(\{\xi\})\{(a_{\mathbf{k}}-\langle a_{\mathbf{k}}\rangle)\times(a_{-\mathbf{k}}-\langle a_{-\mathbf{k}}\rangle)\}\mathcal{S}^\dagger(\{\xi\})\mathcal{U}_c^\dagger\mathcal{U}|\Phi_0\rangle, \tag{21}$$

where $\mathcal{C}_2=0$ yields the condition on $\xi_{\mathbf{k}}$. The action of the effective pairing operator $\mathcal{S}(\{\xi\})$ on the single phonon operators is defined in Eq. (5). Using this property, Eq. (21) yields the self-consistency condition for $\xi_{\mathbf{k}}$ as

$$c_{\mathbf{k}}s_{\mathbf{k}} = e^{4\xi_{\mathbf{k}}}\left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^2\langle\Phi_0|\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}|\Phi_0\rangle, \tag{22}$$

where $c_{\mathbf{k}}=\cosh 2\xi_{\mathbf{k}}$, $s_{\mathbf{k}}=\sinh 2\xi_{\mathbf{k}}$ are as defined before. The solution of Eq. (22) for $\xi_{\mathbf{k}}$ is given by

$$e^{4\xi_{\mathbf{k}}} = \left[1-4\left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^2\langle\Phi_0|\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}|\Phi_0\rangle\right]^{-1/2}. \tag{23}$$

It can be proven that this choice of $\xi_{\mathbf{k}}$ in Eq. (23) also incorporates the next-leading contribution to four-phonon correlations until the six-phonon-correlation terms become important. In order to show this, we examine the four-phonon correlations by

$$\mathcal{C}_4 = \langle\Phi_0|\mathcal{U}^\dagger\mathcal{U}_c\mathcal{S}(\{\xi\})\{(a_{\mathbf{k}}-\langle a_{\mathbf{k}}\rangle)\times(a_{-\mathbf{k}}-\langle a_{-\mathbf{k}}\rangle)\}^2\mathcal{S}^\dagger(\{\xi\})\mathcal{U}_c^\dagger\mathcal{U}|\Phi_0\rangle. \tag{24}$$

Following a tedious calculation similar to Eqs. (22)–(24), Eq. (24) yields

$$\mathcal{C}_4 = 2\mathcal{C}_2^2 - \left\{\left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^2\langle\Phi_0|\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}|\Phi_0\rangle\right\}^3, \tag{25}$$

where we considered a Gaussian type density-density correlations. With Eq. (23) satisfied, the last term in Eq. (25) becomes equivalent to $1/4\{1-\exp(-8\xi_{\mathbf{k}})\}^3$. It is not possible to account for this term without examining the next-to-leading-order contributions to pair correlations. However, it is guaranteed that wherever the solution of Eq. (23) yields a real and positive $\xi_{\mathbf{k}}$, the strength of the second term in Eq. (25) does not exceed 1% of the strength of the anomalous two-phonon correlations given by Eq. (18), which renders Eq. (20) to be a good approximation for representing the two- and four-phonon anomalous pair correlations. The result that four-phonon correlations are accurately represented in terms of combinations of two-phonon correlations in Eq. (25) also indicates that Eq. (20) is an accurate effective generator of the anomalous phonon correlations at low temperatures determined by $\xi_{\mathbf{k}}$ in Eq. (23).

The two-phonon correlations existing in the dynamical polaron state have been examined in various other approaches in the past. For instance, Hang studied the properties of the electron-phonon ground state by introducing a variational parameter for pair correlations in the presence of strong electron-phonon interaction.[22] The properties of the superconducting state in the presence of such correlations have been examined when they are driven externally.[15] Phonon softening and deviations from the conventional isotope effect have also been studied in systems such as borocarbides and boronitrides where, additionally, strong electron correlations are also believed to be present (see the second reference in Ref. 15). The analogy with the squeezed states in quantum optics[16] has also been elaborated by Hu and Nori.[23]

B. Zero-point fluctuations

As pointed out in Sec. I, an essential feature of the phonon pair correlations, whether they are driven externally or dynamically, is the enhancement of the zero-point fluctuations in the vibrational amplitudes. In the context of Sec. II A, this effect is dynamical, and, the zero-point fluctuations are explicitly given by

$$_p\langle\psi|(Q_{\mathbf{k}}-\langle Q_{\mathbf{k}}\rangle)^2|\psi\rangle_p=\langle(Q_{\mathbf{k}}-\langle Q_{\mathbf{k}}\rangle)^2\rangle_0\exp\{4\xi_{\mathbf{k}}\}, \tag{26}$$

where the enhancement factor $\exp\{4\xi_{\mathbf{k}}\}$ is introduced in Eq. (23). On the right-hand side of Eq. (26), $\langle\ \rangle_0$ describes the amplitude of the zero-point fluctuations in the harmonic limit.

The fluctuation in the kth component of ion momentum $P_{\mathbf{k}}=i(a_{\mathbf{k}}-a^{\dagger}_{-\mathbf{k}})$ is given by

$$_p\langle\psi|(P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2|\psi\rangle_p=\langle(P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2\rangle_0\exp\{-4\xi_{\mathbf{k}}\}. \tag{27}$$

In the calculations of Eqs. (26) and (27) we also need $_p\langle a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}\rangle_p$. These terms are evaluated in a similar method which leads to Eq. (18).

We will examine in the following the temperature behavior and the T_c dependent anomalies in Eqs. (26) and (27) when the fluctuations in the charge density are driven, in particular, by superconducting pairs.

C. The electron-electron interaction

With the $\xi_{\mathbf{k}}$ as found in Eq. (23), we utilize Eq. (1) to formulate $V^{e-e}(\mathbf{k})$ in the presence of pair correlations as

$$V^{e-e}(\mathbf{k})=-\sum_{n=1}^{\infty}\frac{|\langle\psi_n|(a_{\mathbf{k}}+a^{\dagger}_{-\mathbf{k}})|\psi_0\rangle|^2}{\hbar\Omega_{\mathbf{k}}n}, \tag{28}$$

with $|\psi_n\rangle=(B^{\dagger}_{\mathbf{k}})^n/\sqrt{n!}\mathcal{S}(\xi)|0\rangle_{\rm ph}$, $|\psi_0\rangle=\mathcal{S}(\xi)|0\rangle_{\rm ph}$, and $S(\xi)$ effectively representing the phonon pair correlations in $\mathcal{U}_c^{\dagger}\mathcal{U}|\Phi_0\rangle$ as found in the previous part. Using the transformation (5) it is possible to see that only $n=1$ term has a nonzero contribution to the matrix element yielding

$$V^{e-e}(\mathbf{k})=-\frac{g(\mathbf{k})^2}{\hbar\omega_{\mathbf{k}}}\cosh(4\xi_{\mathbf{k}})e^{4\xi_{\mathbf{k}}}, \tag{29}$$

where $\xi_{\mathbf{k}}$ is given again by Eq. (23). The $\omega_{\mathbf{k}}/\Omega_{\mathbf{k}}=\cosh(4\xi_{\mathbf{k}})$ describes the nonperturbative phonon frequency renormalization as described in Sec. I and $\exp\{4\xi_{\mathbf{k}}\}$ is the enhancement factor in the zero-point fluctuations as in Eq. (26).

D. The Holstein reduction factor in the presence of pair correlations

We now examine the influence of the phonon pair correlations on the operator $\sigma_{m,n}$ in Eq. (13). Since both $a_{\mathbf{k}}$ and $a^{\dagger}_{-\mathbf{k}}$ are shifted as given by Eq. (16), the coherent part of $|\psi\rangle_p$ has no influence on $\sigma_{m,n}$. The leading pair correlations transform $_p\langle\psi|\sigma_{m,n}|\psi\rangle_p$ into

$$_p\langle\psi|\sigma_{m,n}|\psi\rangle_p=\langle\Phi_0|\exp\left\{\frac{1}{2N}\sum_{\mathbf{k}}\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}(e^{i\mathbf{k}\cdot m}-e^{i\mathbf{k}\cdot n})\right.$$
$$\left.\times\exp\{-2\xi_{\mathbf{k}}\}(a_{\mathbf{k}}-a^{\dagger}_{-\mathbf{k}})\right\}|\Phi_0\rangle, \tag{30}$$

which is similar to Eq. (13) except in the appearance of the factor $\exp\{-2\xi_{\mathbf{k}}\}$ in the exponent. The $\sigma_{m,n}$ has an exponential dependence on the momentum operator $P_{\mathbf{k}}=i(a_{\mathbf{k}}-a^{\dagger}_{-\mathbf{k}})$. The suppression factor $\exp\{-2\xi_{\mathbf{k}s}\}$ is naturally connected with the suppression in the momentum fluctuations as examined in Sec. II B. Thus, for increasing strength of the electron-phonon coupling, the fluctuations of the multiphonon operator from its average are increasingly suppressed. Using the $|\Phi_0\rangle$ in Sec. II A, Eq. (30) further yields

$$\langle\psi_p|\sigma_{m,n}|\psi_p\rangle=\exp\left\{-\frac{1}{2N}\sum_{\mathbf{k}}\left(\frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}}\right)^2[1-\cos(\mathbf{k}\cdot\mathbf{a})]\right.$$
$$\left.\times(2N_{\mathbf{k}}+1)\exp(-4\xi_{\mathbf{k}})\right\}, \tag{31}$$

where $\mathbf{a}=\mathbf{m}-\mathbf{n}$ is the unit lattice vector and $N_{\mathbf{k}}=[\exp(\beta\Omega_{\mathbf{k}})+1]^{-1}$. Equation (31) is the renormalized Holstein reduction factor in the presence of the term $\exp\{-4\xi_{\mathbf{k}}\}$. The fluctuations induced by the phonon pair correlations partially suppress the band narrowing induced by the coherent part of the ground state. This effect will be examined in Sec. III once the self-consistent solution for the pair correlations is obtained.

The existence of the $\exp\{-4\xi_{\mathbf{k}s}\}$ term was also noticed earlier, for instance, by Hang[22] and some other authors. It will be shown in Sec. IV that the Debye Waller factor is also renormalized by pair correlations connected with an enhancement in the zero-point fluctuations of the ion vibrational amplitudes. Both quantum effects are manifestations of Eqs. (26) and (27).

Using Eq. (30) and calculating the action of the phonon operators on $|\Phi_0\rangle$, the $\tilde{\epsilon}_{\mathbf{k}}$ in first term in Eq. (11) is now replaced by (in the momentum representation)

$$\tilde{\epsilon}_{\mathbf{k}}=\epsilon_{\mathbf{k}}\exp\left\{-\frac{1}{2N}\sum_{\mathbf{k}s}\left(\frac{g_s(\mathbf{k})}{\hbar\omega_{\mathbf{k}s}}\right)^2[1-\cos(\mathbf{k}\cdot\mathbf{a})]\right.$$
$$\left.\times(2N_{\mathbf{k}}+1)\exp(-4\xi_{\mathbf{k}s})\right\}. \tag{32}$$

III. THE SUPERCONDUCTING SOLUTION

The dynamical model developed above is formulated in a general frame which can be specifically examined by choosing $|\Phi_0\rangle$ from those configurations which the Fröhlich model supports at low temperatures. The essence of the approach in the Sec. II A lies in the fact that ultimate care must be taken in order to separate the polaronic and vibrational degrees of freedom. The transformation in Eq. (10) performs this separation in the Hamiltonian. The expense one has to pay is that the correlations are now projected onto the dynamical polaronic wave function, and, an effective model which claims to separate these two degrees of freedom has to incorporate them in a self-consistent frame.

We have previously shown[15] that externally driven phonon correlations enhance the average superconducting gap Δ and increase the dimensionless parameter $2\Delta/T_c$ beyond the weak coupling limit 3.53. In this section we will reexplore this effect within the self-consistent model developed in Sec. II as well as suggest an explanation for other vibrational anomalies observed particularly in certain high-temperature superconductors. Let us now consider a specific electronic ground state $|\psi\rangle_e$ which represents superconducting pairs on the Fermi surface by

$$|\psi\rangle_e=\prod_{\mathbf{k}\sigma} \exp\{U_{\mathbf{k}}+V_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{-\mathbf{k}-\sigma}\}|\mathrm{FS}\rangle. \tag{33}$$

The complete self-consistent picture requires the calculation of density-density correlations to be used in Eq. (23). An explicit calculation following Eq. (33) yields

$$\begin{aligned}\langle\Phi_0|\delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}}|\Phi_0\rangle&=\langle\psi_e|\rho_{\mathbf{k}}\rho_{-\mathbf{k}}|\psi_e\rangle-2\overline{n_{\mathbf{k}}^2}\\&=2\frac{1}{N}\sum_{\mathbf{k}'} U_{\mathbf{k}'}V_{\mathbf{k}'}U_{\mathbf{k}'+\mathbf{k}}V_{\mathbf{k}'+\mathbf{k}},\end{aligned} \tag{34}$$

where the factor of 2 appears again as a result of the spin degeneracy. Here $U_{\mathbf{k}}$ and $V_{\mathbf{k}}$ are given in their conventional form,

$$U_{\mathbf{k}}^2=\frac{1}{2}\left[1+\frac{\tilde{\epsilon}_{\mathbf{k}}}{E_{\mathbf{k}}}\right],\quad V_{\mathbf{k}}^2=\frac{1}{2}\left[1-\frac{\tilde{\epsilon}_{\mathbf{k}}}{E_{\mathbf{k}}}\right], \tag{35}$$

where the renormalized single particle excitation energy $E_{\mathbf{k}}$ and the superconducting gap function $\Delta_{\mathbf{k}}=1/N\Sigma_{\mathbf{k}'}V^{e-e}(\mathbf{k}-\mathbf{k}')\langle\psi_e|c^{\dagger}_{\mathbf{k}'\sigma}c^{\dagger}_{-\mathbf{k}'-\sigma}|\psi_e\rangle$ are given by

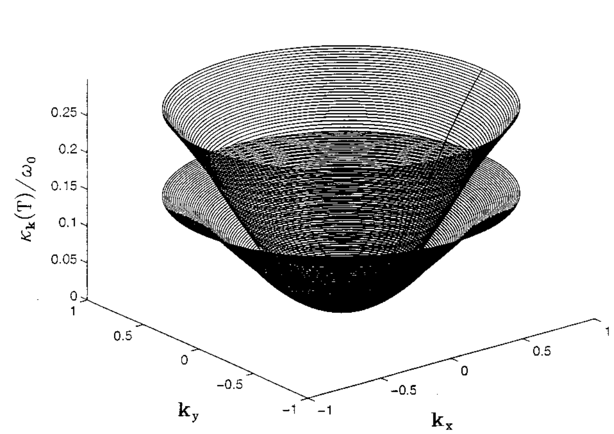

FIG. 1. The typical momentum dependence of the low-temperature anomalous phonon correlations $\kappa_{\mathbf{k}}(T)$ at two arbitrary temperatures and for $\lambda_{e-e}=0.85$. Here $\kappa_{\mathbf{k}}(T)/\omega_0=1/2\tanh(4\xi_{\mathbf{k}})$ is chosen as defined below Eq. (3) rather than $\xi_{\mathbf{k}}$ because the former explicitly corresponds to the pair correlations $\langle a^{\dagger}_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}}\rangle$ (see Ref. 15). The momentum dependence of $\Delta_{\mathbf{k}}(T)$ is uniform and is not shown here.

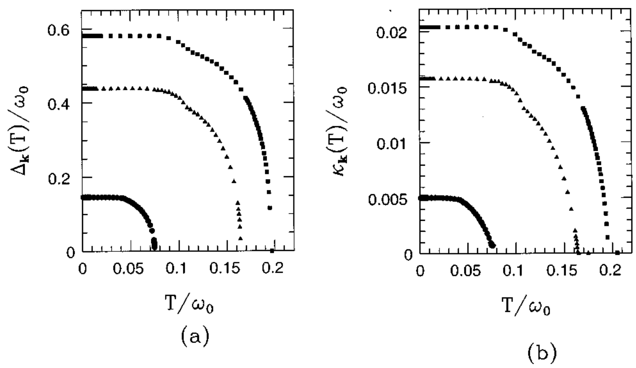

FIG. 2. Temperature dependence of the (a) superconducting gap $\Delta_{\mathbf{k}}(T)$, and (b) $\kappa_{\mathbf{k}}(T)/\omega_0$ at $\mathbf{k}=(1/4, 1/4)$ and for particular values of λ_{e-e} [$(\triangle)\Rightarrow\lambda_{e-e}=0.85$; $(\square)\Rightarrow\lambda_{e-e}=0.75$; $(\bullet)\Rightarrow\lambda_{e-e}=0.54$].

$$E_{\mathbf{k}}=\sqrt{\tilde{\epsilon}_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2},$$

and

$$\Delta_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{k}'} V^{e-e}(\mathbf{k}-\mathbf{k}')\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\frac{\beta E_{\mathbf{k}'}}{2}. \tag{36}$$

Equation (36) together with Eqs. (35), (34), (32), (29), and (23) form the basis of a closed and coupled set of equations to be solved numerically in two dimensions for the dispersionless harmonic phonon frequency $\omega_{\mathbf{k}}=\omega_0$. The self-consistent nature of this extended approach, where renormalizations are handled dynamically in the phonon subsystem, is a distinguishing feature of it from the standard BCS formalism.

A typical momentum dependent low-temperature solution of anomalous phonon pairing is given in Fig. 1. The solution naturally acquires the symmetry of the coupling constant. The solutions for $\Delta_{\mathbf{k}}$ and the pair correlations are shown in Figs. 2(a) and 2(b), respectively, in a larger temperature range for the effective dimensionless bare electron-electron coupling $\lambda_{e-e}=0.54$, 0.75, 0.85. In the calculations, the bare coupling is extracted from the $\xi_{\mathbf{k}}=0$ solution in Eq. (29) where $\lambda_{e-e}=\rho(0)\langle g(\mathbf{k})^2\rangle/\omega_0$ with $\rho(0)$ representing the electron density of states on the Fermi surface.

In the solution of the superconducting gap, the enhancement is up to 25% in both $\Delta_{\mathbf{k}}(0)$ and T_c for small λ_{e-e} (i.e., $\lambda_{e-e}=0.54$). For larger λ_{e-e}, the increase in T_c is slower, whereas, $\Delta_{\mathbf{k}}(0)$ is enhanced up to 30%. In Table I below, the dimensionless $2\Delta(0)/T_c$ ratio is also shown for the same λ_{e-e} values.

In Fig. 3 the influence of the pair correlations on the Holstein reduction factor in Eq. (31) is examined as a function of

TABLE I. The variation of the dimensionless $2\Delta/T_c$ ratio above the standard BCS value 3.53 for different values of λ_{e-e}.

λ_{e-e}	$2\Delta/T_c$
0.85	5.94
0.75	5.36
0.54	4.61

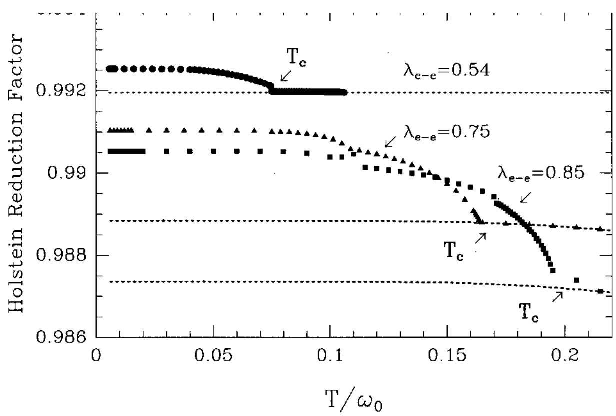

FIG. 3. The influence of pair correlations on the Holstein reduction factor as a function temperature and for particular values of λ_{e-e} [(□)⇒$\lambda_{e-e}=0.85$; (△)⇒$\lambda_{e-e}=0.75$; (●)⇒$\lambda_{e-e}=0.54$].

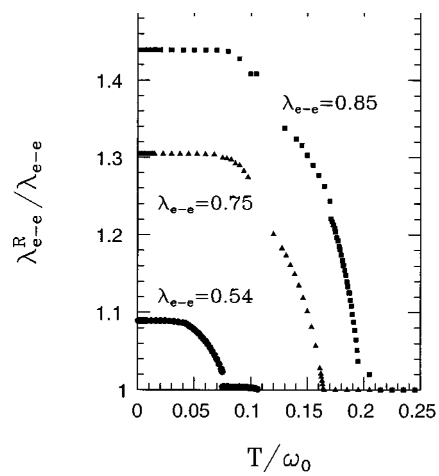

FIG. 4. The relative enhancement of the renormalized and Fermi-surface-averaged coupling constant λ^R_{e-e} to the bare coupling λ_{e-e} as a function temperature and for particular values of the bare coupling λ_{e-e} [(□)⇒$\lambda_{e-e}=0.85$; (△)⇒$\lambda_{e-e}=0.75$; (●)⇒$\lambda_{e-e}=0.54$].

temperature corresponding to the same values of the bare coupling as in Fig. 2. The dashed lines correspond to the $\xi=0$ *forced solution* which is included for the sake of comparison (note that the forced solution is totally unphysical in this approach). As the coupling constant increases, the increasing effect of the band narrowing is opposed by an increasing suppression due to the pair correlations below T_c. The suppression on the Holstein reduction factor thus observed is maximal at the zero temperature and is on the order of 0.1–0.2% on the absolute scale (e.g., as compared to unity). Below T_c, and relative to the forced $\xi=0$ solution, the pair correlations suppress the Holstein reduction by as large as 35% for $\lambda_{e-e}=0.75$, and, nearly 20% for $\lambda_{e-e}=0.85$. In the absolute scale, the overall influence of the Holstein reduction factor does not exceed 1% for the range of the coupling constants examined. Near $\lambda_{e-e}\simeq 0.5$ and below both the Holstein reduction factor and its suppression due to pair correlations become unobservably small. In our approach the multiphonon operator in Eq. (13) is replaced by its average over the dynamical polaronic state. In the small polaron problem the fluctuations in the multiphonon operator gives rise to a *residual* interaction. Alexandrov and Capellmann[24] recently examined this interaction in the strong-coupling limit $1<\lambda_{e-e}$. The multiphonon operator is unitary and bounded within the unit interval. For such operators, the fluctuations around the average are also bounded by the same interval disregarding the particular statistical distribution it is applied to. This implies that within the examined range of coupling constants the strength of fluctuations in $\sigma_{m,n}$ cannot exceed more than one percent of the Holstein reduction which simply corresponds to the distance between the average value of the multiphonon operator and unity. As the Holstein reduction is increased by increasing coupling constant, there is more room for $\sigma_{m,n}$ to fluctuate which has to be properly taken into account in the strong-coupling limit. The relatively weak Holstein reduction observed in our calculations also does not play a crucial role in the anomalous temperature dependence of the pair correlations.

In Fig. 4, the enhancement of the renormalized coupling constant $\lambda^R_{e-e}=\langle V^{e-e}(\mathbf{k})\rangle\rho(0)$ relative to the bare coupling λ_{e-e} (both are averaged over the FS) is also shown as a function of temperature.

IV. DYNAMICAL STRUCTURE FACTOR

The main motivation of this self-consistent approach is the observation of the temperature-dependent critical anomaly of the dynamical structure factor $S(\mathbf{k},\omega)$ in the vicinity of T_c for YBCO and LSCO based compounds using inelastic neutron scattering.[10,11] Similar anomalies have also been observed for the Tl(2212) compound[11,12] in the dynamical pair distribution function measurements.

Here fluctuation in the pair distribution is crucial to examine for understanding the observed temperature anomalies. This quantity is the Fourier transform of the static structure factor $S(\mathbf{k})$ given by

$$\delta g(\mathbf{r})=\int_{-\infty}^{\infty}\frac{d\mathbf{k}}{(2\pi)^2}\,e^{-i\mathbf{k}\cdot\mathbf{r}}[1-S(\mathbf{k})], \tag{37}$$

where $S(\mathbf{k})=\int d\omega S(\mathbf{k},\omega)$ and

$$S(\mathbf{k},\omega)=\int dt e^{-i\omega t}\frac{1}{N}\sum_{m,n} e^{-i\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})}\langle e^{-i\mathbf{k}\cdot\mathbf{u}_m(t)}e^{i\mathbf{k}\cdot\mathbf{u}_n(0)}\rangle, \tag{38}$$

where $\mathbf{u}_m(t)$ is the time-dependent displacement vector of the ion at site $\mathbf{m}$. In Eq. (37), the anomalous temperature dependence of $\delta g(\mathbf{r})$ is given by that of the structure factor. Hence, to examine the dynamical structure factor, one has to follow the standard prescription to calculate $S(\mathbf{k},\omega)$ exclusively in the presence of pair correlations. A routine calculation similar to the one carried out in Sec. II C yields

$$S(\mathbf{k})=\frac{1}{N}\sum_{m,n}\exp\left\{-\frac{1}{N}\sum_{\mathbf{k}'}\frac{\hbar}{M\omega_{\mathbf{k}'}}|\mathbf{k}\cdot\mathbf{e}_{\mathbf{k}'}|^2\exp(4\xi_{\mathbf{k}'})\times(2N_{\mathbf{k}'}+1)[1-\cos[\mathbf{k}'\cdot(\mathbf{m}-\mathbf{n})]]\right\}. \tag{39}$$

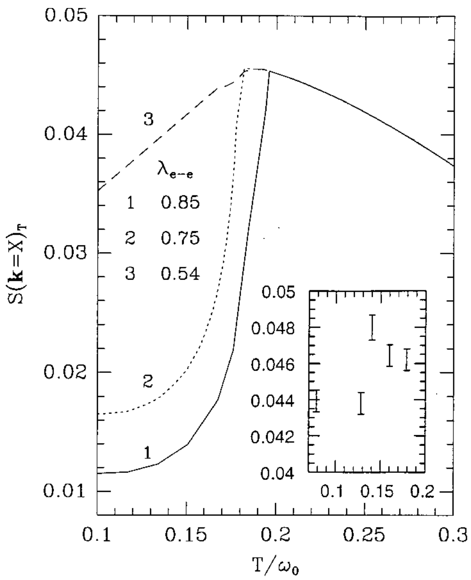

FIG. 5. Temperature dependence of the structure factor as calculated in Eq. (39) in the vicinity of T_c. In the inlet, the data describes a typical T_c anomaly of $S(\mathbf{k},\omega)$ from Ref. 10.

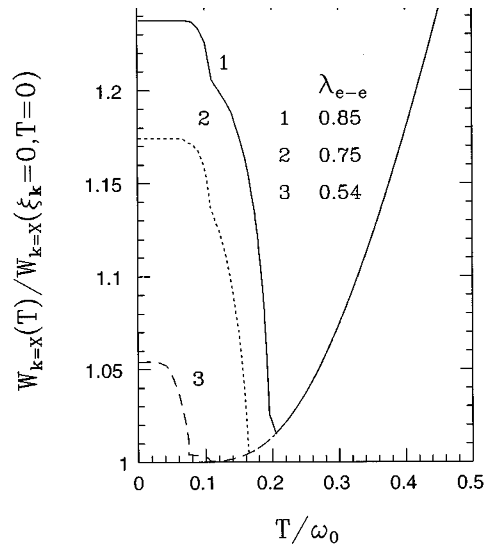

FIG. 6. Enhancement in the zero-point fluctuations [i.e., Eq. (26)] as a function of temperature for the same coupling constant values as in Fig. 2; (the solid line, the dashed line, and the dotted line are respectively $\lambda_{e-e}=0.85$; $\lambda_{e-e}=0.75$; $\lambda_{e-e}=0.54$ as above).

A. The Debye-Waller factor

In Eq. (39), the Debye-Waller factor $W_{\mathbf{k}}$ is identified by

$$W_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{k}'}\frac{\hbar}{2M\omega_{\mathbf{k}'}}|\mathbf{k}\cdot\mathbf{e}_{\mathbf{k}'}|^2\exp(4\xi_{\mathbf{k}'})(2N_{\mathbf{k}'}+1). \tag{40}$$

For $\xi_{\mathbf{k}}=0$, Eqs. (39) and (40) reduce to their well-known harmonic limit. In real crystals, the anomalous temperature dependence of the Debye-Waller factor is usually considered as a signature for anharmonic multiphonon interaction.[25,26] However, such anharmonic effects are usually calculated either perturbatively or by using self-consistent harmonic approximation without inquiring in detail the specific properties of the nonperturbative dynamics at low temperatures. The temperature anomalies arise from the temperature dependence of $\xi_{\mathbf{k}}$. Once $\xi_{\mathbf{k}}$ is calculated, the temperature dependence of the Debye-Waller factor can be examined in the vicinity of T_c. Below T_c, two factors contribute to the anomalous temperature dependence of the structure factor. These are the dynamically enhanced electron-phonon interaction due to the induced correlations and the low-temperature anharmonic phonons. Both factors increase the amplitude of the zero-point vibrations which results in an enhancement in the Debye-Waller factor below T_c. In this work we only consider the former and leave the anharmonic phonon scattering to be examined elsewhere. On the other hand, above T_c the phonon modes are not dynamically correlated (i.e., $\xi_{\mathbf{k}}=0$), but the harmonic Debye contribution continues to produce the standard cotangent-hyperbolic increase in Debye-Waller factor with respect to the temperature. The numerical solution of $S(\mathbf{k},\omega_0)$ as a function of temperature is given in Fig. 5. The structure factor data of Arai *et al.*[10] is shown in the inlet. The theory has the qualitative as well as quantitative features of the data within a reasonable range of coupling constants.

The temperature dependence of $W_{\mathbf{k}}$ scaled with respect to its zero-temperature harmonic limit is shown in Fig. 6. In their XAFS measurements, Conradson *et al.*[27] have reported the observation of similar effects on the apical oxygen z-polarized zero point fluctuation. Very recently Booth *et al.*[28] confirmed in their XAFS correlated-Debye-Waller factor measurements a similar behavior for the collective vibrations of the Cu1-O4 and Cu2-O4 ions.

B. The low-temperature ion momentum fluctuations

Another crucial quantity to examine here is the fluctuations in the phonon momentum given by Eq. (27). The thermal behavior above T_c for $\langle(P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2\rangle$ is expected to be the same as that of the Debye-Waller factor in Fig. 6 since the difference arises only below T_c where $\xi_{\mathbf{k}}\neq 0$. We also do not consider high-temperature anharmonic phonon scattering above T_c. At low temperatures when $\xi_{\mathbf{k}}$ is real and positive, the factor $\exp\{-4\xi_{\mathbf{k}}\}$ suppresses the momentum fluctuations below the harmonic limit.

Using resonant neutron absorption spectroscopy Mook *et al.*[9] have measured the average atomic vibrational energy of the planar Cu resonances as a function of temperature for single-crystal $Bi_2Sr_2CaCu_2O_8$ compound. In this compound, Cu atoms are only present in the Cu-O planes indicating that the anomalies should be associated with the electron-phonon interaction in the planes. The average atomic vibrational energy $\langle P_{\mathbf{k}}^2\rangle_T/2M$ is closely linked with the ion momentum fluctuations as defined in Eq. (27) and can be studied within our model. The numerical results for $\langle(P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2\rangle_T$ normalized by itself at $\xi_{\mathbf{k}}=0$ and $T=0$ is presented in Fig. 7 below. The data by Mook *et al.*[9] is shown by triangles in the inlet as well as the harmonic solution (solid line) as a function of temperature. In order to facilitate the comparison with the calculations as well as to minimize the dependence on the particular compound, the data is also normalized similarly. The pair-correlation model examined here quantitatively reproduces the phonon anomaly below T_c whereas it

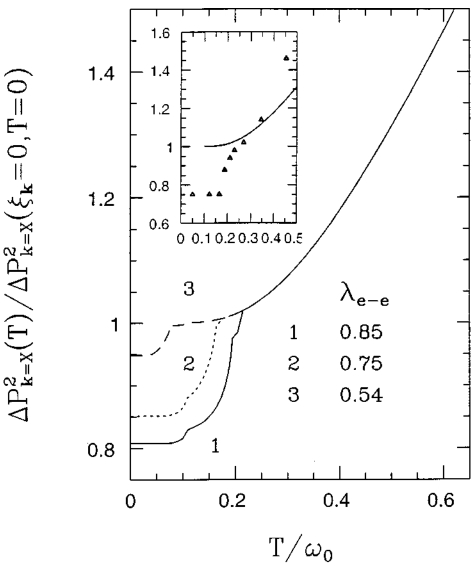

FIG. 7. Temperature dependence of the phonon momentum fluctuations in Eq. (27) normalized by its value at $T=0$ and $\xi_{\mathbf{k}}=0$. The data by Mook *et al.* (Ref. 9) is shown in the inlet. (The solid line, the dashed line, and the dotted line are respectively $\lambda_{e-e}=0.85$; $\lambda_{e-e}=0.75$; $\lambda_{e-e}=0.54$.) Here $\Delta P_{\mathbf{k}}=\langle (P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2\rangle^{1/2}$.

underrates the experiment at $T_c<T$. There are two possible effects which can contribute to the $T_c<T$ behavior in Fig. 7. The first is due to the likely presence of the high-temperature anharmonic phonon scattering. It is known that such high-temperature effects increase the fluctuations[27] which are not embodied in our model. The importance of these high-temperature corrections is obvious and understanding these effects can shed light on the anharmonic lattice properties in these materials. The second effect is the density-density fluctuations created within the normal state. This effect can be formulated in a more refined analysis incorporating the dielectric formulation and linear response theory into the self-consistent picture presented here. These corrections are to be examined in separate reports.

The zero-point fluctuations are pure low-temperature quantum effects. The enhancement observed in $\langle (Q_{\mathbf{k}}-\langle Q_{\mathbf{k}}\rangle)^2\rangle$ and suppression observed in $\langle (P_{\mathbf{k}}-\langle P_{\mathbf{k}}\rangle)^2\rangle$ are manifestations of quantum mechanics at low temperatures.

V. CONCLUSION

To summarize, we examined the effects of low-temperature anomalous phonon correlations on the electron-phonon interaction and on the phonon *wave function* in the presence of superconducting pairs. In particular, we examined our formalism in the context of recently observed anomalous temperature behavior in the Debye-Waller factor, the dynamical structure factor, and the averaged ion vibrational energy measurements in certain HTS.

The charge-density-fluctuation driven phonon anomalies are examined and shown that they result from second-order effects in the polaronic ground state. These effects are only visible if one goes beyond the conventional polaronic models. They do not only induce mere enhancement of superconductivity, but they also consistently amplify the low-temperature quantum fluctuations. A variety of other temperature anomalies (specific heat, penetration depth, thermal conduction, isotope effect, etc.) appear to be relevant for future extension which should be investigated to find whether they are correlated, in part, with anomalies examined here. The current approach suggests that the anomalous rise of the structure factor[10,11] and softening of the momentum fluctuations[9] near T_c are common in origin and connected with the dynamical correlations induced in the polaronic ground state.

The anomalous softening (hardening) of certain phonon modes at the onset of superconductivity as observed by Friedl, Thomsen, and Cardona[29] should also be examined within this scheme, provided that our approach is properly incorporated into the strong-coupling formalism of Zeyher and Zwicknagl.[8] In that respect we believe that, the theory presented here might be of relevance to a wider spectrum of experimental data where anomalous phonons and electron-phonon interactions play important role. Another direction to go is to examine realistic microscopic HTS models which incorporate the chain-plane and planar charge transfer mechanisms with the ideas presented here. The charge transfer is believed to be important in the T_c dependent temperature anomalies,[30,31] in particular, if the coupling of the planar z-polarized B_{1g} and A_{1g} modes to O-O and Cu-O charge fluctuations[32,33] are also incorporated.

Finally, the authors are well aware of the fact that the present state of high-temperature superconductivity does not permit to make definitive statements on the nature of a single active superconducting mechanism. In particular, our basic approach is neither based on, nor favored by a particular mechanism of superconductivity. The authors also believe that the results, although they are based on an oversimplified model, should be extended to more realistic ones conserving the qualitative aspects presented here in search for additional evidence concerning the importance of the electron-phonon interaction. It should be noted that in the central theme of this paper is the presence of charge-density fluctuation induced anomalies driven by the superconducting electron-phonon ground state. On the other hand, in HTS strong antiferromagnetic spin fluctuations are also present in the Cu-O planes in a wide range of dopand concentrations. A more realistic model should consistently embody the spin and charge fluctuations together, which, amounts to extending the presented picture to manifest both spin and charge degrees of freedom.

We came across a recent publication[34] of the generation of time-dependent, pair-correlated phonon ground state in $KTaO_3$ stimulated externally at low temperatures by femtosecond laser pulses. In Ref. 15 we have investigated the influence of the externally driven phonon pair correlations on the phonon mediated superconducting state. The current article is somewhat orthogonal to this picture in the consideration of internally driven dynamical mechanisms generating the pair correlations in the superconducting state. It would be of utmost interest if somewhat similar experiments as in Ref. 34 could be performed on HTS, in particular, for those where the phonon anomalies examined here have been observed.

ACKNOWLEDGMENTS

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