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STRONG INTERACTION OF CORRELATED ELECTRONS WITH PHONONS: EXCHANGE OF PHONON CLOUDS BY POLARONS

V. A. Moskalenko *

Joint Institute for Nuclear Research
141980, Dubna, Moscow region, Russia

P. Entel **

Theoretische Physik, Gerhard-Mercator-Universität Duisburg
47048, Duisburg, Germany

M. Marinaro ***

Dipartimento di Scienze Fisiche E. R. Caianiello, Universita degli Studi di Salerno
84081, Baronissi, Italy

D. F. Digor ****

Institute of Applied Physics, Moldova Academy of Sciences
2028, Chisinau, Moldova

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We investigate the interaction of strongly correlated electrons with phonons in the framework of the Hubbard–Holstein model. The electron–phonon interaction is considered to be strong and is an important parameter of the model in addition to the Coulomb repulsion of electrons and the band filling. This interaction with nondispersive optical phonons is transformed to the problem of mobile polarons using the canonical transformation of Lang and Firsov. We discuss the case where the on-site Coulomb repulsion is exactly canceled by the phonon-mediated attractive interaction. We suggest that polarons exchanging phonon clouds can lead to polaron pairing and superconductivity. The fact that the frequency of the collective mode of phonon clouds is larger than the bare frequency then determines the superconducting transition temperature.

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1. INTRODUCTION

Since the discovery of high-temperature superconductivity by Bednorz and Müller [1], the Hubbard model and related models such as RVB and t-J have widely been used to discuss the physical properties of the normal and superconducting states [2–6]. However, a unanimous explanation of the origin of the condensate in high-temperature superconductors has not emerged so far. One of the unsolved questions is how far phonons can be involved in the formation of the superconducting state. In experimental and theoretical works, the change of phonon frequencies and phonon lifetimes associated with the superconducting transition were mostly discussed. For example, the decrease of frequencies of Raman-active phonons at the transition [7], observation of the isotope effect for not optimally doped superconductors [8], and the observation of a phonon-induced structure in the tunnel characteristics [9] evidence in favor of strong electron–phonon coupling in the cuprates.

The aim of the present paper is to gain further insight into the mutual influence of strong on-site Coulomb repulsion and strong electron–phonon interaction using the single-band Hubbard–Holstein model and a recently developed diagram approach [10–14].

*E-mail: moskalen@thsun1.jinr.ru
**E-mail: entel@thp.uni-duisburg.de
***E-mail: marinaro@sa.infn.it
****E-mail: statphys@asm.md

For simplicity, we consider coupling to dispersionless phonons only, although this might not be the most interesting case as regards superconductivity. However, previous investigations [15–17] have shown that the Hubbard–Holstein model [18, 19] constitutes a formidable problem of its own. Other authors have also intensively studied this model Hamiltonian [20–23].

Because the interactions between electrons and electrons and phonons are strong, we include the Coulomb repulsion in the zero-order Hamiltonian and apply the canonical transformation of Lang and Firsov [24] to eliminate the linear electron–phonon interaction. In the strong electron–phonon coupling limit, the resulting Hamiltonian of hopping polarons (i.e., hopping electrons surrounded by clouds of phonons) can lead to an attractive interaction among electrons mediated by the phonons. In this limit, the chemical potential, the on-site Coulomb energy, and the frequency of the collective mode of phonon clouds (which is much larger than the bare frequency of the Einstein oscillators) are strongly renormalized [17, 25, 26], which affects the dynamical properties of the polarons and the character of the superconducting transition. In discussing this, we assume that the renormalized on-site Coulomb repulsion and attractive electron–electron interaction completely cancel each other. We suggest that the resulting superconducting state with polaronic Cooper pairs is mediated by the exchange of phonon clouds during the hopping processes of the electrons.

2. THEORETIC APPROACH

2.1. The Lang–Firsov transformation of the Hubbard–Holstein model

The initial Hamiltonian of correlated electrons coupled to optical phonons with bare frequency ω_0 is given by

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}^0_{ph} + \mathcal{H}_{e-ph}, \tag{1}$$

$$\mathcal{H}_e = \sum_{i,j,\sigma} \{t(j-i) - \epsilon_0 \delta_{ij}\}\, a^\dagger_{j\sigma} a_{i\sigma} + U \sum_i n_{i_\uparrow} n_{i_\downarrow}, \tag{2}$$

$$\begin{gathered} \mathcal{H}^0_{ph} = \sum_i \hbar\omega_0 \left(b^\dagger_i b_i + \frac{1}{2} \right), \\ \mathcal{H}_{e-ph} = g \sum_i n_i q_i, \end{gathered} \tag{3}$$

$$\begin{gathered} n_i = \sum_\sigma n_{i\sigma}, \quad n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}, \\ q_i = \frac{1}{\sqrt{2}} \left(b_i + b^\dagger_i \right), \end{gathered} \tag{4}$$

where $a^\dagger_{i\sigma}$ ($a_{i\sigma}$) and $b^\dagger_i$ (b_i) are creation (annihilation) operators of electrons and phonons, respectively, i refers to the lattice site and σ to the spin, q_i is the phonon coordinate, g is the electron–phonon interaction constant, U is the on-site Coulomb repulsion, $t(j-i)$ is the two-center transfer integral, and $\epsilon_0 = \bar{\epsilon}_0 - \mu$ with the local energy $\bar{\epsilon}_0$ and chemical potential μ. The Fourier representation of $t(j-i)$ is related to the tight-binding dispersion $\varepsilon(\mathbf{k})$ of bare electrons,

$$t(j-i) = \frac{1}{N} \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \exp\{-i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_i)\},$$

with the band width W. The energy scale of this model is fixed by the parameters W, U, g, and $\hbar\omega_0$. An additional parameter is given by the band filling.

After applying the Lang–Firsov transformation [24]

$$\begin{gathered} \mathcal{H}_p = e^S \mathcal{H} e^{-S}, \quad c_{i\sigma} = e^S a_{i\sigma} e^{-S}, \\ c^\dagger_{i\sigma} = e^S a_{i\sigma} e^{-S} \end{gathered} \tag{5}$$

with

$$\begin{gathered} S = -i\bar{g} \sum_i n_i p_i, \quad \bar{g} = \frac{g}{\hbar\omega_0}, \\ p_i = \frac{i}{\sqrt{2}} \left(b^\dagger_i - b_i \right), \end{gathered} \tag{6}$$

where p_i is the phonon momentum and $\bar{g}$ is the dimensionless interaction constant, we obtain the polaron Hamiltonian

$$\mathcal{H}_p = \mathcal{H}^0_p + \mathcal{H}^0_{ph} + \mathcal{H}_{int}, \tag{7}$$

$$\mathcal{H}^0_p = \sum_i \mathcal{H}^0_{ip}, \quad \mathcal{H}^0_{ip} = \epsilon \sum_\sigma n_{i\sigma} + \bar{U} n_{i\uparrow} n_{i\downarrow}, \tag{8}$$

$$\mathcal{H}_{int} = \sum_{i,j,\sigma} t(j-i) c^\dagger_{j\sigma} c_{i\sigma}, \tag{9}$$

where

$$c^\dagger_{i\sigma} = a^\dagger_{i\sigma} \exp(-i\bar{g}p_i), \quad c_{i\sigma} = a_{i\sigma} \exp(i\bar{g}p_i), \tag{10}$$

$$\begin{gathered} \epsilon = \bar{\epsilon}_0 - \bar{\mu}, \quad \bar{\mu} = \mu + \alpha\hbar\omega_0, \\ \bar{U} = U - 2\alpha\hbar\omega_0, \quad \alpha = \frac{1}{2}\bar{g}^2. \end{gathered} \tag{11}$$

To derive the polaron Hamiltonian, it was necessary to include the shift of the phonon coordinate q_i of the form

$$e^S q_i e^{-S} = q_i - \bar{g} n_i,$$

which is responsible for the elimination of the linear electron–phonon interaction. The polaron Hamiltonian is a polaron–phonon operator by its nature, i.e., the creation operator $c^\dagger_{i\sigma}$ and the destruction operator $c_{i\sigma}$ entering $\mathcal{H}_p$ must be interpreted as creation and destruction operators of polarons (electrons dressed with displacements of ions) that couple dynamically to the momentum of the optical phonon. In the zero-order approximation (omitting $\mathcal{H}_{int}$), polarons and phonons are localized with the strongly renormalized chemical potential $\bar{\mu}$ and on-site Coulomb interaction $\bar{U}$. The operator $\mathcal{H}_{int}$ describes tunneling of polarons between lattice sites, i.e., tunneling of electrons surrounded by clouds of phonons.

2.2. Expansion around the atomic limit

The problem is now to deal properly with the impact of electronic correlations on the polaron problem. This can be done best using the Green's functions provided one finds a key to deal with the spin and charge degrees of freedom. In the general case where $\bar{U}$ is different from zero, the Coulomb interaction must be included in the zero-order Hamiltonian. As a consequence, the conventional perturbation theory of quantum statistical mechanics is not an adequate tool because it relies on the expansion of the partition function around the noninteracting state (achieved using the traditional Wick theorem and conventional Feynman diagrams). A similar situation occurs for composite particles like polarons,

$$c_{i\sigma} = a_{i\sigma} \exp(i\bar{g}p_i),$$

involving operators for the electron and phonon subsystems.

Hubbard [27] proposed a graphical expansion for correlated electrons about the atomic limit in powers of the hopping integrals. This diagram approach was systematically reformulated for the single-band Hubbard model by Slobodyan and Stasyuk [28] and independently by Zaitsev [29] and further developed by Izyumov [30]. In these approaches, the complicated algebraic structure of the projection or Hubbard operators was used. It therefore appeared to be more appropriate to develop a diagram technique involving simpler creation and annihilation operators for electrons at all intermediate stages of the theory (see Refs. [10, 11] for details). In the latter approach, the averages of chronological products of interactions are reduced to the n-particle Matsubara Green's functions of the atomic system. These functions can be factorized into independent local averages using a generalization of the Wick theorem (GWT), which takes strong local correlations into account (details are given in Refs. [10, 11, 25]). Application of the GWT yields new irreducible on-site many-particle Green's functions, or Kubo cumulants. These new functions contain all local spin and charge fluctuations. A similar linked-cluster expansion for the Hubbard model around the atomic limit was recently reformulated by Metzner [31].

2.3. Averages of phonon operators

We define the temperature Green's function for the polarons in (7) in the interaction representation by

$$\mathcal{G}(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T\, c_{\mathbf{x}\sigma}(\tau) \bar{c}_{\mathbf{x}'\sigma'}(\tau')\, U(\beta) \rangle_0^c \quad (12)$$

with

$$c_{\mathbf{x}\sigma}(\tau) = \exp(\mathcal{H}^0 \tau) c_{\mathbf{x}\sigma} \exp(-\mathcal{H}^0 \tau),$$
$$\bar{c}_{\mathbf{x}\sigma}(\tau) = \exp(\mathcal{H}^0 \tau) c^\dagger_{\mathbf{x}\sigma} \exp(-\mathcal{H}^0 \tau),$$

where $\mathcal{H}^0 = \mathcal{H}^0_p + \mathcal{H}^0_{ph}$ and the evolution operator is given by

$$U(\beta) = T \exp\left(- \int_0^\beta d\tau\, H_{int}(\tau) \right), \quad (13)$$

$\mathbf{x}$, $\mathbf{x}'$ are site indices, and τ, τ' stand for the imaginary time with $0 < \tau < \beta$; T is the time ordering operator and β is the inverse temperature. The statistical average $\langle \ldots \rangle_0^c$ is evaluated with respect to the zero-order density matrix of the grand canonical ensemble of the localized polarons and phonons,

$$\frac{\exp(-\beta \mathcal{H}^0)}{\mathrm{Tr} \exp(-\beta \mathcal{H}^0)} = \prod_i \frac{\exp(-\beta \mathcal{H}^0_{ip})}{\mathrm{Tr} \exp(-\beta \mathcal{H}^0_{ip})} \frac{\exp(-\beta \mathcal{H}^0_{i\,ph})}{\mathrm{Tr} \exp(-\beta \mathcal{H}^0_{i\,ph})}. \quad (14)$$

The superscript «c» in (12) indicates that only connected diagrams must be taken into account. Density matrix (14) is factorized with respect to the lattice sites. The phonon part is easily diagonalized using the free phonon operators b_i and $b^\dagger_i$, while the on-site polaron Hamiltonian contains the polaron–polaron interaction that is proportional to the renormalized parameter $\bar{U}$, which only can be diagonalized using Hubbard operators [18]. At this stage, no special assumption is made about the quantity $\bar{U}$ and its sign; we set up the equations of motion for the dynamical quantities in this general case, but investigate the equations in detail only in the special case where $\bar{U}=0$.

The Wick theorem of weakly coupled quantum field theory can be used in evaluating statistical averages of phonon operators, e.g., the propagator of the phonon cloud,

$$\Phi(\tau_1|\tau_2)=\Phi(\tau_1-\tau_2)\equiv\langle T\exp\{i\bar{g}\,[p(\tau_1)-p(\tau_2)]\}\rangle_0= \\ =\exp\left(-\frac{1}{2}\bar{g}^2\langle T\,[p(\tau_1)-p(\tau_2)]^2\rangle_0\right)= \\ =\exp\left(-\sigma(\beta)+\sigma(|\tau_1-\tau_2|)\right), \quad (15)$$

$$\Phi(\tau_1,\tau_2|\tau_3,\tau_4)\equiv \\ \equiv\langle T\exp\{i\bar{g}[p(\tau_1)+p(\tau_2)-p(\tau_3)-p(\tau_4)]\}\rangle_0= \\ =\exp\left(-\frac{1}{2}\bar{g}^2\langle T\,[p(\tau_1)+p(\tau_2)-p(\tau_3)-p(\tau_4)]^2\rangle_0\right)= \\ =\exp\{\sigma(|\tau_1-\tau_3|)+\sigma(|\tau_1-\tau_4|)+\sigma(|\tau_2-\tau_3|)+ \\ +\sigma(|\tau_2-\tau_4|)-\sigma(|\tau_1-\tau_2|)-\sigma(|\tau_3-\tau_4|)-2\sigma(\beta)\}, \quad (16)$$

where

$$\sigma\left(|\tau_1-\tau_2|\right)=\bar{g}^2\langle T\,p(\tau_1)p(\tau_2)\rangle_0= \\ =\alpha\,\frac{\operatorname{ch}\left(\hbar\omega_0\left\{\dfrac{\beta}{2}-|\tau_1-\tau_2|\right\}\right)}{\operatorname{sh}\left(\dfrac{\beta\hbar\omega_0}{2}\right)}. \quad (17)$$

We now discuss the problem of calculating chronological averages of combinations of polaron operators. We here use the above-mentioned new diagram technique and the GWT [10, 11]. The many-particle on-site irreducible Green's functions are the main element of diagrams in this approach.

3. POLARON AND PHONON GREEN'S FUNCTIONS

In the zero-order approximation, the one-polaron Green's function is given by

$$\mathcal{G}_p^0(x|x')=-\langle T\,c_{\mathbf{x}\sigma}(\tau)\bar{c}_{\mathbf{x}'\sigma'}(\tau')\rangle_0= \\ =-\langle T\,a_{\mathbf{x}\sigma}(\tau)\bar{a}_{\mathbf{x}'\sigma'}(\tau')\rangle_0\Phi(\tau|\tau')= \\ =\mathcal{G}^{(0)}(x|x')\,\Phi(\tau|\tau'), \quad (18)$$

where $x=(\mathbf{x},\sigma,\tau)$. The simplest new element of the diagram technique is the two-particle irreducible Green's function, or Kubo cumulant, which is equal to

$$\mathcal{G}_2^{(0)\,ir}(x_1,x_2|x_3,x_4)=\delta_{\mathbf{x}_1,\mathbf{x}_2}\delta_{\mathbf{x}_1,\mathbf{x}_3}\delta_{\mathbf{x}_1,\mathbf{x}_4}\times \\ \times\,\mathcal{G}_2^{(0)\,ir}(\sigma_1,\tau_1;\sigma_2,\tau_2|\sigma_3,\tau_3;\sigma_4,\tau_4), \quad (19)$$

where

$$\mathcal{G}_2^{(0)\,ir}(\sigma_1,\tau_1;\sigma_2,\tau_2|\sigma_3,\tau_3;\sigma_4,\tau_4)= \\ =\langle T\,c_{\sigma_1}(\tau_1)\,c_{\sigma_2}(\tau_2)\bar{c}_{\sigma_3}(\tau_3)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0- \\ -\langle T\,c_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0\langle T\,c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\rangle_0+ \\ +\langle T\,c_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_3}(\tau_3)\rangle_0\langle T\,c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0. \quad (20)$$

The first term in the right-hand side of Eq. (20) is

$$\langle T\,c_{\sigma_1}(\tau_1)\,c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0= \\ =\langle T a_{\sigma_1}(\tau_1)a_{\sigma_2}(\tau_2)\bar{a}_{\sigma_3}(\tau_3)\bar{a}_{\sigma_4}(\tau_4)\rangle_0\times \\ \times\,\Phi(\tau_1,\tau_2|\tau_3,\tau_4). \quad (21)$$

As the number of polaron operators increases, more complicated irreducible Green's functions like $\mathcal{G}_n^{(0)ir}(x_1\ldots x_n|x_1'\ldots x_n')$ with $n\geq 3$ and all possible terms of their products appear. The sum of all strongly connected diagrams (i.e., those that cannot be divided into two parts by cutting a single hopping line) containing all kinds of irreducible Green's functions in the perturbation expansion of the evolution operator defines the special function $Z(x|x')$ (see Refs. [10, 11] for details). This function contains all contributions from charge and spin fluctuations. Together with the mass operator (which is the hopping matrix element in our case), it allows us to formulate a Dyson-type equation for the one-polaron Green's function [10–14],

$$\mathcal{G}(x|x')=\Lambda(x|x')+\sum_{1,2}\Lambda(x|1)t(1-2)\mathcal{G}(2|x'), \quad (22)$$

where

$$\Lambda(x|x')=\mathcal{G}_p^{(0)}(x|x')+Z(x|x'), \quad (23)$$

$$t(x-x')=\delta_{\sigma,\sigma'}\delta(\tau-\tau')\,t(\mathbf{x}-\mathbf{x}'). \quad (24)$$

Here, x again denotes $\mathbf{x},\sigma,\tau$ and the sum is over the discrete indices and includes integration over τ. Using the Fourier representation for these quantities,

$$\mathcal{G}_\sigma(\mathbf{x}|\tau) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\beta}\sum_{\omega_n} \exp(-i\mathbf{k}\cdot\mathbf{x} - i\omega_n\tau)\mathcal{G}_\sigma(\mathbf{k}|i\omega_n),$$

$$\Lambda_\sigma(\mathbf{x}|\tau) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\beta}\sum_{\omega_n} \exp(-i\mathbf{k}\cdot\mathbf{x} - i\omega_n\tau)\Lambda_\sigma(\mathbf{k}|i\omega_n), \quad (25)$$

$$\mathcal{G}_\sigma(\mathbf{x}|i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau \exp(i\omega_n\tau)\mathcal{G}_\sigma(\mathbf{x}|\tau),$$

$$\Lambda_\sigma(\mathbf{x}|i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau \exp(i\omega_n\tau)\Lambda_\sigma(\mathbf{x}|\tau),$$

we obtain the Dyson equation for the renormalized one-polaron Green's function,

$$\mathcal{G}_\sigma(\mathbf{k}|i\omega_n) = \frac{\Lambda_\sigma(\mathbf{k}|i\omega_n)}{1 - \varepsilon(\mathbf{k})\,\Lambda(\mathbf{k}|i\omega_n)}, \quad (26)$$

where

$$\omega_n = \frac{(2n+1)\pi}{\beta}$$

is the odd Matsubara frequency.

To discuss $\mathcal{G}_\sigma(k|i\omega)$ further, we need the Fourier representation of the zero-order one-polaron Green's function $\mathcal{G}_p^{(0)}$ defined in (18). In order to facilitate the investigation, we have evaluated the propagator of the phonon cloud (16) in the strong-coupling limit $\alpha \gg 1$ [15, 16, 26],

$$\Phi(\tau) = \frac{1}{\beta}\sum_{\Omega_n} \exp(-i\Omega_n(\tau))\bar{\Phi}(i\Omega_n), \quad (27)$$

$$\bar{\Phi}(i\Omega_n) = \frac{\exp(-\sigma(\beta))}{2}\int_{-\beta}^{\beta} d\tau \exp(i\Omega_n\tau + \sigma(|\tau|)), \quad (28)$$

where $\Omega_n = 2n\pi/\beta$. To find $\bar{\Phi}(i\Omega_n)$, we use the Laplace approximation [32] for integral (28), which contains an exponential function with the parameter α. In the strong-coupling limit $\alpha \gg 1$, we obtain

$$\bar{\Phi}(i\Omega_n) \approx \frac{2\omega_c}{\Omega_n^2 + \omega_c^2}, \quad \omega_c = \hbar\alpha\omega_0 = \frac{g^2}{2\hbar\omega_0}. \quad (29)$$

This term is the harmonic propagator of the collective mode of phonons belonging to the polaron clouds. There are further terms describing anharmonic deviations. For $\alpha \gg 1$, these terms can be omitted because they are small compared with the harmonic contribution. Using the Laplace approximation [32] and

$$\Phi(\tau_1, \tau_2|\tau_3, \tau_4) = \frac{1}{\beta^4}\sum_{\Omega_1 \ldots \Omega_4} \bar{\Phi}(i\Omega_1, i\Omega_2|i\Omega_3, i\Omega_4) \times \exp(-i\Omega_1\tau_1 - i\Omega_2\tau_2 + i\Omega_3\tau_3 + i\Omega_4\tau_4), \quad (30)$$

$$\bar{\Phi}(i\Omega_1, i\Omega_2|i\Omega_3, i\Omega_4) = \int_0^\beta \ldots \int_0^\beta d\tau_1 \ldots d\tau_4 \times \exp(i\Omega_1\tau_1 + i\Omega_2\tau_2 - i\Omega_3\tau_3 - i\Omega_4\tau_4) \times \Phi(\tau_1, \tau_2|\tau_3, \tau_4), \quad (31)$$

we then obtain the Fourier representation of the phonon correlation function

$$\bar{\Phi}(i\Omega_1, i\Omega_2|i\Omega_3, i\Omega_4) \approx [\delta_{\Omega_1,\Omega_3}\delta_{\Omega_2,\Omega_4} + \delta_{\Omega_1,\Omega_4}\delta_{\Omega_2,\Omega_3}]\,\bar{\Phi}(i\Omega_1)\,\bar{\Phi}(i\Omega_2), \quad (32)$$

which corresponds to

$$\Phi(\tau_1, \tau_2|\tau_3, \tau_4) \approx \Phi(\tau_1|\tau_3)\,\Phi(\tau_2|\tau_4) + \Phi(\tau_1|\tau_4)\,\Phi(\tau_2|\tau_3). \quad (33)$$

This implies that in what follows, we can keep only the free collective oscillations of phonon clouds (29) surrounding the polarons and use the Hartree–Fock approximation (32) and (33) for their two-particle correlation functions. In particular, we investigate the influence of the absorption and emission of this collective mode by polarons on the superconducting phase transition.

With the harmonic mode given by (29), the Fourier representation of the local polaron Green's function

$$\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\ \exp(i\omega_n\tau)\bar{\mathcal{G}}_{p\sigma}^{(0)}(\tau) \quad (34)$$

becomes

$$\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n) \approx \frac{1}{Z_0} \times \left(\frac{\exp(-\beta E_0) + \bar{N}(\omega_c)(\exp(-\beta E_0) + \exp(-\beta E_\sigma))}{i\omega_n + E_0 - E_\sigma - \omega_c} + \frac{\exp(-\beta E_\sigma) + \bar{N}(\omega_c)(\exp(-\beta E_0) + \exp(-\beta E_\sigma))}{i\omega_n + E_0 - E_\sigma + \omega_c} + \frac{\exp(-\beta E_{-\sigma}) + \bar{N}(\omega_c)(\exp(-\beta E_\sigma) + \exp(-\beta E_2))}{i\omega_n + E_{-\sigma} - E_2 - \omega_c} + \frac{\exp(-\beta E_2) + \bar{N}(\omega_c)(\exp(-\beta E_\sigma) + \exp(-\beta E_2))}{i\omega_n + E_{-\sigma} - E_2 + \omega_c}\right), \quad (35)$$

where

$$Z_0 = 1 + \exp(-\beta E_\sigma) + \\ + \exp(-\beta E_{-\sigma}) + \exp(-\beta E_2), \quad (36a)$$

$$E_0 = 0, \quad E_{\pm\sigma} = \epsilon, \quad E_2 = \bar{U} + 2\epsilon, \quad (36b)$$

$$\bar{n}(\epsilon) = (\exp(\beta\epsilon) + 1)^{-1}, \\ \bar{N}(\omega_c) = (\exp(\beta\omega_c) - 1)^{-1}. \quad (37)$$

Equation (35) shows that the on-site transition energies of polarons are changed by the collective-mode energy $\pm\omega_c$ of the phonon clouds. The delocalization of polarons due to their hopping between lattice sites causes the broadening of the polaron energy levels. Equation (35) can be further simplified for a small on-site interaction energy $\bar{U}$ of polarons. For $\bar{U} = 0$, we obtain

$$\bar{\mathcal{G}}^{(0)}_{p\sigma}(i\omega_n|\epsilon) = \frac{\bar{N}(\omega_c) + 1 - \bar{n}(\epsilon)}{i\omega_n - \epsilon - \omega_c} + \frac{\bar{N}(\omega_c) + \bar{n}(\epsilon)}{i\omega_n - \epsilon + \omega_c} = \\ = \frac{(i\omega_n - \epsilon)\,\mathrm{cth}(\beta\omega_c/2) + \omega_c\,\mathrm{th}(\beta\epsilon/2)}{(i\omega_n - \epsilon)^2 - \omega_c^2}. \quad (38)$$

This function has the antisymmetry property

$$\bar{\mathcal{G}}^{(0)}_{p\sigma}(-i\omega_n| - \epsilon) = -\bar{\mathcal{G}}^{(0)}_{p\sigma}(i\omega_n|\epsilon) \quad (39)$$

which also holds for the renormalized polaron quantities,

$$\Lambda_\sigma(-\mathbf{k}, -i\omega_n| - \epsilon) = -\Lambda_\sigma(\mathbf{k}, i\omega_n|\epsilon), \\ \mathcal{G}_\sigma(-\mathbf{k}, -i\omega_n| - \epsilon) = -\mathcal{G}_\sigma(\mathbf{k}, i\omega_n|\epsilon). \quad (40)$$

Setting $\bar{U} \approx 0$, we assume that the strong on-site Coulomb repulsion of polarons can be canceled by the attraction induced by the strong electron–phonon interaction. We consider this as a model case that allows a transparent discussion of the polarons exchanging phonon clouds during hopping between lattice sites.

4. TWO-PARTICLE IRREDUCIBLE CORRELATION FUNCTIONS

In what follows, we discuss the influence of a strong electron–phonon interaction on the two-particle irreducible Green's function. For $\bar{U} = 0$, the electronic correlation function in (22) is given by

$$\langle T a_{\sigma_1}(\tau_1)\, a_{\sigma_2}(\tau_2)\, \bar{a}_{\sigma_3}(\tau_3)\, \bar{a}_{\sigma_4}(\tau_4)\rangle_0 = \\ = \langle T\, a_{\sigma_1}(\tau_1)\bar{a}_{\sigma_4}(\tau_4)\rangle_0 \langle T\, a_{\sigma_2}(\tau_2)\bar{a}_{\sigma_3}(\tau_3)\rangle_0 - \\ - \langle T\, a_{\sigma_1}(\tau_1)\bar{a}_{\sigma_3}(\tau_3)\rangle_0 \langle T\, a_{\sigma_2}(\tau_2)\bar{a}_{\sigma_4}(\tau_4)\rangle_0 \quad (41)$$

because the standard Wick theorem is now applicable. Using (33), we obtain the relation

$$\mathcal{G}^{(0)\,ir}_2(\sigma_1, \tau_1; \sigma_2, \tau_2|\sigma_3, \tau_3; \sigma_4, \tau_4) = \\ = \delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}\mathcal{G}^{(0)}_{\sigma_1}(\tau_1 - \tau_4)\mathcal{G}^{(0)}_{\sigma_2}(\tau_2 - \tau_3) \times \\ \times \Phi(\tau_1 - \tau_3)\,\Phi(\tau_2 - \tau_4) - \\ - \delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\, \mathcal{G}^{(0)}_{\sigma_1}(\tau_1 - \tau_3)\, \mathcal{G}^{(0)}_{\sigma_2}(\tau_2 - \tau_4) \times \\ \times \Phi(\tau_1 - \tau_4)\,\Phi(\tau_2 - \tau_3) \quad (42)$$

for the two-particle irreducible Green's function (21). In the absence of the exchange of phonon clouds by polarons, this quantity must vanish. Indeed, if the electrons keep their initial phonon clouds during the time of propagation of two polarons, then the irreducible two-polaron Green's function (21) vanishes for $\bar{U} = 0$. But because two electrons can be exchanged (independently of the exchange of phonon clouds), we obtain new contributions corresponding to two polarons with the exchanged phonon clouds. Alternatively, we can say that for $\bar{U} = 0$, the Wick theorem applies separately to free electrons and free phonons; however, it does not apply to polarons as composite particles, and their cumulants do not therefore vanish.

The Fourier representation of (42),

$$\mathcal{G}^{(0)\,ir}_2(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_3, i\omega_3; \sigma_4, i\omega_4) = \\ = \int_0^\beta \ldots \int_0^\beta d\tau_1 \ldots d\tau_4 \times \\ \times \mathcal{G}^{(0)\,ir}_2(\sigma_1, \tau_1; \sigma_2, \tau_2|\sigma_3, \tau_3; \sigma_4, \tau_4) \times \\ \times \exp(i\omega_1\tau_1 + i\omega_2\tau_2 - i\omega_3\tau_3 - i\omega_4\tau_4), \quad (43)$$

is given by

$$\mathcal{G}^{(0)\,ir}_2(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_3, i\omega_3; \sigma_4, i\omega_4) = \\ = \beta\,\delta_{\omega_1+\omega_2,\omega_3+\omega_4} \times \\ \times \bar{\mathcal{G}}^{(0)\,ir}_2(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_3, i\omega_3; \sigma_4, i\omega_4) = \\ = \beta\,\delta_{\omega_1+\omega_2,\omega_3+\omega_4}\,\{\delta_{\sigma_1,\sigma_4}\,\delta_{\sigma_2,\sigma_3} \times \\ \times A_{\sigma_1,\sigma_2}(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_2, i\omega_3; \sigma_1, i\omega_4) - \\ - \delta_{\sigma_1,\sigma_3}\,\delta_{\sigma_2,\sigma_4} \times \\ \times A_{\sigma_1,\sigma_2}\,(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_1, i\omega_4; \sigma_2, i\omega_3)\}, \quad (44)$$

where

$$A_{\sigma_1,\sigma_2}(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_2, i\omega_3; \sigma_1, i\omega_4) = \frac{1}{\beta}\sum_\Omega \frac{(2\omega_c)^2}{[i\omega_1 - i\Omega - \epsilon][i\omega_3 - i\Omega - \epsilon][\Omega^2 + \omega_c^2][(\Omega + \Omega_1)^2 + \omega_c^2]} \quad (45)$$

with $\Omega_1 = \omega_2 - \omega_3$. The summation leads to

$$A_{\sigma_1,\sigma_2}(\sigma_1, i\omega_1; \sigma_2, i\omega_2|\sigma_2, i\omega_3; \sigma_1, i\omega_4) = \\ = 2(\omega_c)^2 \left\{ \frac{\operatorname{th}(\beta\epsilon/2)\,[i\omega_1 + i\omega_2 - 2\epsilon][2\omega_c^2 - (i\omega_1 - \epsilon)(i\omega_4 - \epsilon) - (i\omega_2 - \epsilon)(i\omega_3 - \epsilon)]}{[(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]} - \right. \\ - \frac{2\omega_c[i\omega_1 + i\omega_2 - 2\epsilon]^2 \operatorname{cth}(\beta\omega_c/2)\,[2\omega_c^2 - (i\omega_1 - \epsilon)(i\omega_3 - \epsilon) - (i\omega_2 - \epsilon)(i\omega_4 - \epsilon)]}{[(i\Omega_1)^2 - (2\omega_c)^2][(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]} - \\ \left. - \frac{\operatorname{cth}(\beta\omega_c/2)}{\omega_c[(i\Omega_1)^2 - (2\omega_c)^2]} \left[\frac{(i\omega_1 - \epsilon)(i\omega_3 - \epsilon) + 3\omega_c^2}{[(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2]} + \frac{(i\omega_2 - \epsilon)(i\omega_4 - \epsilon) + 3\omega_c^2}{[(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]} \right] \right\}. \quad (46)$$

The function A_{σ_1,σ_2} contains contributions of the different spin channels to the two-particle on-site Green's function. The spin structure in Eq. (44) is due to the conservation law for the spins of the polarons.

5. SUPERCONDUCTING PHASE TRANSITION

In what follows, we check whether the polaronic system can have a superconducting instability in the absence of a direct attractive interaction for the polarons, i.e., for $\bar{U} = 0$. In this case, the attraction is only induced dynamically by polarons exchanging the phonon clouds. To describe superconductivity, we need the anomalous propagators [33] in addition to the normal state Green's function (13). For simplicity, we limit the discussion to the s-wave superconductivity as in previous investigations of superconducting instabilities in the Hubbard model [13, 14] and in the Hubbard–Holstein model in the strong-coupling limit $\alpha \gg 1$ [26].

To describe the superconducting state, we need three irreducible functions Λ_σ, $Y_{\sigma,-\sigma}$, and $\bar{Y}_{-\sigma,\sigma}$ that represent infinite sums of diagrams containing irreducible many-particle Green's functions. In order to obtain a close set of equations, we restrict ourselves to a class of rather simple contributions, which nevertheless contain the most important charge, spin, and pairing correlations; see Ref. [26] for details. This class of diagrams is obtained by neglecting contributions for which the Fourier representation of the superconducting order parameters $Y_{\sigma,-\sigma}$ and $\bar{Y}_{-\sigma,\sigma}$ depend on the polaron momentum $\mathbf{k}$. In this approximation, $Y_{\sigma,-\sigma}$ is to be obtained from

$$Y_{\sigma,-\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l} \frac{\varepsilon(\mathbf{k})\,\varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega_l)}{D_\sigma(\mathbf{k}, i\omega_l)} \times \\ \times \bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, -i\omega|\sigma, i\omega_l; -\sigma, -i\omega_l). \quad (47)$$

In the same approximation, Λ_σ is to be computed from

$$\Lambda_\sigma(i\omega) = \mathcal{G}_{p\sigma}^{(0)}(i\omega) - \frac{1}{\beta N} \times \\ \times \sum_{\mathbf{k},\omega_l} \frac{\varepsilon^2(\mathbf{k})}{D_\sigma(\mathbf{k}, i\omega_l)} \{\Lambda_\sigma(i\omega_l)[1 - \varepsilon(-\mathbf{k})\,\Lambda_{-\sigma}(-i\omega_l)] - \\ - \varepsilon(\mathbf{k})\,Y_{\sigma,-\sigma}(i\omega_l)\,\bar{Y}_{-\sigma,\sigma}(i\omega_l)\} \times \\ \times \bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; \sigma, i\omega_l|\sigma, i\omega_l; \sigma, i\omega) - \\ - \frac{1}{\beta N}\sum_{\mathbf{k},\omega_l} \frac{\varepsilon^2(\mathbf{k})}{D_\sigma(\mathbf{k}, i\omega_l)} \{\Lambda_{-\sigma}(-i\omega_l) \times \\ \times [1 - \varepsilon(\mathbf{k})\Lambda_\sigma(i\omega_l)] - \varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega_l)\bar{Y}_{-\sigma,\sigma}(i\omega_l)\} \times \\ \times \bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, -i\omega_l| - \sigma, -i\omega_l; \sigma, i\omega) \quad (48)$$

with

$$D_\sigma(\mathbf{k}, i\omega) = [1 - \varepsilon(\mathbf{k})\Lambda_\sigma(i\omega)][1 - \varepsilon(-\mathbf{k})\Lambda_{-\sigma}(-i\omega)] + \\ + \varepsilon(\mathbf{k})\varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega)\bar{Y}_{-\sigma,\sigma}(i\omega). \quad (49)$$

The corresponding equation for $\bar{Y}_{-\sigma,\sigma}(i\omega)$ can be obtained from the expression for $Y_{\sigma,-\sigma}(i\omega)$.

Together with the equations for the one- and two-particle Green's functions, the above equations completely determine the properties of the superconducting phase, provided it exists. In order to gain a further insight into the physics contained in (47) and (48), we linearize the equations in terms of the order parameter $Y_{\sigma,-\sigma}(i\omega)$ that determines the critical temperature T_c. The resulting equation for the order parameter is

$$Y_{\sigma,-\sigma}(i\omega) = \\ = -\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l} \frac{\varepsilon(\mathbf{k})\varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega_l)}{[1 - \varepsilon(\mathbf{k})\Lambda_\sigma(i\omega_l)][1 - \varepsilon(-\mathbf{k})\Lambda_{-\sigma}(-i\omega_l)]} \times \\ \times \bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, -i\omega|\sigma, i\omega_l; -\sigma, -i\omega_l). \quad (50)$$

This equation must be solved together with the equation for $\Lambda_\sigma(i\omega)$ that can be approximated by setting the order parameters to zero, with the result

$$\Lambda_\sigma(i\omega) = \mathcal{G}^{(0)}_{p\sigma}(i\omega) - \frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon^2(\mathbf{k})\Lambda_\sigma(i\omega_l)}{1-\varepsilon(\mathbf{k})\Lambda_\sigma(i\omega_l)}\times$$
$$\times\bar{\mathcal{G}}^{(0)\,ir}_2(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega) - \frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon^2(\mathbf{k})\Lambda_{-\sigma}(i\omega_l)}{1-\varepsilon(-\mathbf{k})\Lambda_{-\sigma}(i\omega_l)}\bar{\mathcal{G}}^{(0)\,ir}_2(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega). \quad (51)$$

To determine T_c, we must solve (51) for Λ_σ and insert the result in (50). The irreducible functions in (50) and (51) can be written as

$$\bar{\mathcal{G}}^{(0)\,ir}_2(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega) = \frac{(\omega-\omega_l)^2}{\Delta^2\Delta_l^2}\Big\{2\omega_c^2(x+x_l)\,\mathrm{th}(\beta\epsilon/2) -$$
$$-\frac{\mathrm{cth}(\beta\omega_c/2)}{\omega_c[(i\omega-i\omega_l)^2-4\omega_c^2]}\left[(xx_l+\omega_c^2)(\Delta\Delta_l+8\omega_c^4)-2\omega_c^2(\Delta+\Delta_l)(xx_l-\omega_c^2)\right]\Big\}, \quad (52)$$

$$\bar{\mathcal{G}}^{(0)\,ir}_2(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega) = -\frac{2\omega_c}{\Delta^2\Delta_l^2}\Big\{\omega_c(x+x_l)(\Delta+\Delta_l)\,\mathrm{th}(\beta\epsilon/2) +$$
$$+\mathrm{cth}(\beta\omega_c/2)(x+x_l)^2(xx_l-\omega_c^2)\Big\} + \frac{\mathrm{cth}(\beta\omega_c/2)(xx_l+3\omega_c^2)}{\omega_c\Delta\Delta_l}, \quad (53)$$

$$\bar{\mathcal{G}}^{(0)\,ir}_2(\sigma,i\omega;-\sigma,-i\omega|\sigma,i\omega_l;-\sigma,-i\omega_l) =$$
$$= -\frac{2\epsilon(2\omega_c)^2\,\mathrm{th}(\beta\epsilon/2)[i\omega\, i\omega_l+\epsilon^2-\omega_c^2]}{[\omega^2+(\epsilon+\omega_c)^2][\omega^2+(\epsilon-\omega_c)^2][\omega_l^2+(\epsilon+\omega_c)^2][\omega_l^2+(\epsilon-\omega_c)^2]} +$$
$$+\frac{2\omega_c\,\mathrm{cth}(\beta\omega_c/2)[i\omega\, i\omega_l+2\omega_c(\epsilon-\omega_c)-(\epsilon-\omega_c)^2]}{[\omega^2+(\epsilon-\omega_c)^2][\omega_l^2+(\epsilon-\omega_c)^2][(\omega-\omega_l)^2+(2\omega_c)^2]} +$$
$$+\frac{2\omega_c\,\mathrm{cth}(\beta\omega_c/2)[i\omega\, i\omega_l-2\omega_c(\epsilon+\omega_c)-(\epsilon+\omega_c)^2]}{[\omega^2+(\epsilon+\omega_c)^2][\omega_l^2+(\epsilon+\omega_c)^2][(\omega-\omega_l)^2+(2\omega_c)^2]}, \quad (54)$$

where

$$x = i\omega-\epsilon,\quad \Delta = (i\omega-\epsilon)^2-\omega_c^2, \quad (55a)$$
$$x_l = i\omega_l-\epsilon,\quad \Delta_l = (i\omega_l-\epsilon)^2-\omega_c^2. \quad (55b)$$

To analyze (50) and (51) further, we introduce the notation

$$\phi_\sigma(i\omega) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\varepsilon^2(\mathbf{k})\Lambda_\sigma(i\omega)}{1-\varepsilon(\mathbf{k})\Lambda_\sigma(i\omega)} = \frac{1}{N}\sum_{\mathbf{k}}\frac{\varepsilon(\mathbf{k})}{1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega)}, \quad (56)$$

$$g_\sigma(i\omega) = \mathcal{G}_\sigma(\mathbf{x}=\mathbf{x}'|i\omega) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\Lambda_\sigma(i\omega)}{1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega)}, \quad (57)$$

$$\phi^{sc}_\sigma(i\omega) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\varepsilon(\mathbf{k})\varepsilon(-\mathbf{k})}{[1-\varepsilon(\mathbf{k})\Lambda_\sigma(i\omega)][1-\varepsilon(-\mathbf{k})\Lambda_{-\sigma}(-i\omega)]} = \frac{\phi_\sigma(i\omega)-\phi_{-\sigma}(-i\omega)}{\Lambda_\sigma(i\omega)-\Lambda_{-\sigma}(-i\omega)}. \quad (58)$$

We also assume that $\varepsilon(\mathbf{k})=\varepsilon(-\mathbf{k})$ holds with

$$\sum_{\mathbf{k}}\varepsilon(\mathbf{k}) = \sum_{\mathbf{k}}\varepsilon^3(\mathbf{k}) = 0.$$

We replace sums with integrals,

$$\frac{1}{N}\sum_{\mathbf{k}} = \int d\varepsilon\,\rho_0(\varepsilon), \quad (59)$$

$$\rho_0(\varepsilon) = \frac{4}{\pi W}\sqrt{1-\left(\frac{2\varepsilon}{W}\right)^2} \times \begin{cases} 1, & |\varepsilon| < \dfrac{W}{2}, \\ 0, & |\varepsilon| > \dfrac{W}{2}, \end{cases} \qquad (60)$$

where W is the band width and ρ_0 is the model density of states of a semielliptic form. Because we do not consider magnetic states here, the spin subscript can be omitted in the paramagnetic phase,

$$\Lambda_\sigma(i\omega) = \Lambda_{-\sigma}(i\omega) = \Lambda(i\omega), \qquad (61a)$$

$$\phi_\sigma(i\omega) = \phi_{-\sigma}(i\omega) = \phi(i\omega), \qquad (61b)$$

$$\phi^{sc}_\sigma(i\omega) = \phi^{sc}_{-\sigma}(i\omega) = \phi^{sc}(i\omega). \qquad (61c)$$

However, the spin subscript is essential for the superconducting order parameter $Y_{\sigma,-\sigma}(i\omega)$,

$$Y_{\sigma,-\sigma}(i\omega) = g_{\sigma,-\sigma} Y(i\omega), \qquad (62a)$$

$$g_{\sigma,-\sigma} = \delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}, \qquad (62b)$$

where $Y(i\omega)$ is an even function of the frequency,

$$Y(i\omega) = Y(-i\omega). \qquad (63)$$

We finally add the equation that determines the chemical potential,

$$\frac{1}{\beta}\sum_{\omega_n}\sum_{\sigma} \mathcal{G}_\sigma(\mathbf{x}=\mathbf{x}'|i\omega)\exp(i\omega_n 0^+) = \frac{2}{\beta}\sum_{\omega_n} g_\sigma(i\omega)\exp(i\omega_n 0^+) = \frac{N_p}{N}, \qquad (64)$$

where N_p is the number of polarons and N is the number of lattice sites. With (59) and (60), functions (56) and (57) can be written as

$$\phi(i\omega) = \frac{W}{2}\,\frac{\left(1-\sqrt{1-\lambda^2(i\omega)}\right)^2}{\lambda^3(i\omega)} = \frac{W}{2}\,\frac{\lambda(i\omega)}{\left(1+\sqrt{1-\lambda^2(i\omega)}\right)^2}, \qquad (65)$$

$$g(i\omega) = \frac{4}{W}\,\frac{\left(1-\sqrt{1-\lambda^2(i\omega)}\right)^2}{\lambda(i\omega)} = \frac{4}{W}\,\frac{\lambda(i\omega)}{\left(1+\sqrt{1-\lambda^2(i\omega)}\right)^2}, \qquad (66)$$

where

$$\lambda(i\omega) = (W/2)\Lambda(i\omega).$$

In order to check whether the state determined from Eq. (51) is metallic or dielectric, we must analyze the renormalized density of states given by

$$\rho(E) = -\frac{1}{\pi}\,\mathrm{Im}\, g(E+i0^+) = -\frac{1}{\pi}\,\mathrm{Im}\left(\frac{1-\sqrt{1-\lambda^2(E+i0^+)}}{\lambda(E+i0^+)}\right), \qquad (67)$$

where $\lambda(E+i0^+)$ is the analytic continuation of $\lambda(i\omega)$.

6. ANALYTIC SOLUTIONS

The expressions for $\Lambda(i\omega)$ and $Y(i\omega)$ can be simplified using notation (56) and (57) and symmetry property (62),

$$Y(i\omega) = \frac{1}{\beta}\sum_{\omega_l}\phi^{sc}(i\omega_l) \times \bar{\mathcal{G}}^{(0)\,ir}(\sigma,i\omega;-\sigma,-i\omega|\sigma,i\omega_l;-\sigma,-i\omega_l)Y(i\omega_l), \qquad (68)$$

$$\Lambda(i\omega) = \mathcal{G}^{(0)}_p(i\omega) - \frac{1}{\beta}\sum_{\omega_l}\phi(i\omega_l)\left[\bar{\mathcal{G}}^{(0)\,ir}(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega) + \bar{\mathcal{G}}^{(0)\,ir}(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega)\right]. \qquad (69)$$

To find a solution of Eq. (68), we insert (54), replace $Y(i\omega_n)$ with

$$Y(i\omega_n) = \phi^{sc}(z_0)\,\chi(i\omega_n)\,Y(z_0), \quad z_0 \approx 0, \qquad (70)$$

$$\chi(i\omega_n) = \frac{1}{\beta}\sum_{\omega_l}\bar{\mathcal{G}}^{(0)\,ir}(\sigma,i\omega_n;-\sigma,-i\omega_n|\sigma,i\omega_l;-\sigma,-i\omega_l) = \frac{2\omega_c[\omega_c-\epsilon\,\mathrm{th}(\beta\epsilon/2)\,\mathrm{ch}(\beta\omega_c/2)] + \mathrm{ch}(\beta\omega_c)(-\omega_c^2+\epsilon^2+\omega_n^2)(\mathrm{ch}(\beta\omega_c)-1)^{-1}}{[\omega_n^2+(\omega_c+\epsilon)^2][\omega_n^2+(\omega_c-\epsilon)^2]}, \qquad (71)$$

and use the Poisson summation formula

$$\frac{1}{\beta}\sum_{\omega_n} f(i\omega_n) = -\frac{1}{2\pi i}\int\limits_C dz\,\frac{f(z)}{e^{\beta z}+1}, \quad (72)$$

where C denotes the usual counterclockwise contour of the imaginary axis. With the help of the analytically continued function $\chi(z)$ for $Z = Z_0 = 0$, we then obtain an equation for the critical temperature T_c from Eq. (68),

$$\chi(0|\epsilon)\,\phi^{sc}(0|\epsilon) = 1, \quad (73)$$

$$\chi(0|\epsilon) = \Bigl(2\omega_c[\omega_c - \epsilon\,\mathrm{th}(\beta_c\epsilon/2)\,\mathrm{cth}(\beta_c\omega_c/2)] + \\ + \frac{(\epsilon^2-\omega_c^2)\,\mathrm{ch}(\beta_c\omega_c)}{\mathrm{ch}(\beta_c\omega_c)-1}\Bigr)\left(\omega_c^2-\epsilon^2\right)^{-2}. \quad (74)$$

This quantity is even in ϵ, and therefore only the absolute value of $\epsilon = \bar\epsilon_0 - \bar\mu$ determines $k_BT_c = \beta_c^{-1}$. From (58) and (65), we can make a rough guess for the quantity $\phi^{sc}(0)$,

$$\phi^{sc}(0) \approx \left(\frac{W}{4}\right)^2\frac{1}{\gamma^2}, \\ \gamma = \frac{1}{2}\left(1+\sqrt{1-\lambda^2(0+i\delta)}\right), \quad (75)$$

where γ must satisfy the equation $\gamma(-\epsilon) = \gamma(\epsilon)$. This quantity can be obtained self-consistently from Eq. (64) for the chemical potential. For simplicity, we here replace $[1+\sqrt{1-\lambda^2(0+i\delta)}]$ with 2γ. Then (64) can be written as

$$\frac{2}{\gamma}\frac{1}{\beta}\sum_{\omega_n}\Lambda(i\omega_n)\exp(i\omega_n 0^+) = \frac{N_p}{N}. \quad (76)$$

Using (69) together with (52) and (53), we can express $\Lambda(i\omega_n)$ as

$$\Lambda(i\omega_n) = \frac{(i\omega_n-\epsilon)A_1(\epsilon)+\omega_cB_1(\epsilon)}{(i\omega_n-\epsilon)^2-\omega_c^2} + \\ + \frac{\omega_c^2[(i\omega_n-\epsilon)A_2(\epsilon)+\omega_cB_2(\epsilon)]}{[(i\omega_n-\epsilon)^2-\omega_c^2]^2} \quad (77)$$

with unknown coefficients A_i and B_i. They can be found from Eq. (69) or more easily from the asymptotic behavior of (77) as $|\omega_n|\to\infty$,

$$\Lambda(i\omega_n)\underset{|\omega_n|\to\infty}{=} \frac{A_1}{i\omega_n} + \frac{A_1\epsilon+\omega_cB_1}{(i\omega_n)^2} + \\ + \frac{A_1(\omega_c^2+\epsilon^2)+2\epsilon\omega_cB_1+\omega_c^2A_2}{(i\omega_n)^3} + \\ + \frac{A_1(\epsilon^3+3\epsilon\omega_c^2)+B_1(\omega_c^3+3\epsilon^2\omega_c)+\omega_c^2(3\epsilon A_2+\omega_cB_2)}{(i\omega_n)^4}+\ldots \quad (78)$$

If we compare this with the asymptotic behavior of the full one-polaron Green's function (see the Appendix) by invoking the methods of moments together with the asymptotic behavior of $g(i\omega_n)$ in (66), we obtain

$$A_1(\epsilon) = 1, \quad (79a)$$

$$B_1(\epsilon) = -\frac{1}{\omega_c}[M_1+\epsilon], \quad (79b)$$

$$A_2(\epsilon) = \frac{1}{\omega_c^2}\left[M_2+2\epsilon M_1+\epsilon^2-\omega_c^2-\left(\frac{W}{4}\right)^2\right], \quad (79c)$$

$$B_2(\epsilon) = \\ = \frac{1}{\omega_c^3}\left[-M_3-3\epsilon M_2+M_1\left(\omega_c^2-3\epsilon^2+3\left(\frac{W}{4}\right)^2\right)+\right. \\ \left. +\epsilon\omega_c^2-\epsilon^3+3\epsilon\left(\frac{W}{4}\right)^2\right], \quad (79d)$$

where M_i is the ith moment of the one-polaron Green's function. The results in (A.5) for the moments in the lowest order allow us to evaluate A_i and B_i, see (A.7). $A_1 = 1$ describes the asymptotic freedom of the polarons. $B_1 = \mathrm{th}(\beta\epsilon/2)$ is identical with its value in the zero-order polaron Green's function (38). The two new quantities A_2 and B_2 are small, being proportional to $\omega_0/\omega_c = 1/\alpha$.

Inserting (77) in the left-hand side of Eq. (76) and performing the summation, we obtain

$$\frac{1}{\beta}\sum_{\omega_n}\Lambda(i\omega_n)\exp(i\omega_n0^+) = \bar n(\epsilon) + \\ + \frac{\mathrm{th}(\beta\epsilon/2)[\mathrm{th}(\beta\omega_c/2)-1][1-\mathrm{th}^2(\beta\epsilon/2)]}{2[1-\mathrm{th}^2(\beta\omega_c/2)\,\mathrm{th}^2(\beta\epsilon/2)]} + \\ + \frac{B_2(\epsilon)}{4}\,\mathrm{th}(\beta\omega_c/2)\frac{1-\mathrm{th}^2(\beta\epsilon/2)}{1-\mathrm{th}^2(\beta\epsilon/2)\,\mathrm{th}^2(\beta\omega_c/2)} - \\ - \frac{\beta\omega_c}{16}\left[\frac{A_2(\epsilon)+B_2(\epsilon)}{\mathrm{ch}^2[\beta(\omega_c+\epsilon)/2]} - \frac{A_2(\epsilon)-B_2(\epsilon)}{\mathrm{ch}^2[\beta(\omega_c-\epsilon)/2]}\right], \quad (80)$$

which is equal to $(\gamma/2)(N_p/N)$ in accordance with Eq. (76). Because the collective frequency is large, $\beta\omega_c \gg 1$, we can omit exponentially small quantities like $\exp(-\beta\omega_c)$. Since we are interested in results for electron numbers that are close to half filling ($\epsilon = 0$), also $|\epsilon| \ll \omega_c$ holds. We also neglect contributions of the order $1/\alpha$. Then the equation for chemical potential (74) is simply

$$\bar n(\epsilon) = \gamma n_p/2, \quad n_p = N_p/N. \quad (81)$$

If we set $\gamma = 1$ (free polarons), we obtain from (75) that

$$\phi^{sc}(0) = (W/4)^2, \quad (82)$$

which allows us to write the equation for the critical temperature T_c as

$$\epsilon^2 + \omega_c^2 - 2\epsilon\omega_c \operatorname{th}(\beta\epsilon/2) = (\omega_c^2 - \epsilon^2)^2 (4/W)^2. \quad (83)$$

In this approximation, T_c depends only on the local parameters, but we expect that close to half filling, this should give an indication which of the local quantities is most important for superconductivity in the strong-coupling limit of the Hubbard–Holstein model. Precisely at half filling, Eq. (83) can only be satisfied if $\omega_c = W/4$. This may perhaps be an unphysically large value for a renormalized quantity. It also shows that the specific limit $\bar{U} = 0$ is probably the critical value for the occurence of superconductivity in the framework of the Hubbard–Holstein model. It is clear that superconductivity is possible for $\bar{U} < 0$, but in this case, it would have to compete in energy with the energies of charge-ordered states.

For the special case where $\omega_c = W/4$, we obtain

$$\left(\frac{\epsilon}{\omega_c}\right)^2 \left[3 - \left(\frac{\epsilon}{\omega_c}\right)^2\right] = \frac{2|\epsilon|}{\omega_c} \operatorname{th}\left(\frac{\beta_c|\epsilon|}{2}\right). \quad (84)$$

Because $\epsilon/\omega_c < 3$ holds (which we do not discuss in detail), we can seek solutions in the case where $|\epsilon| \ll \omega_c$, leading to

$$k_B T_c = \frac{\omega_c}{3}\left[1 - \frac{5}{12}\left(\frac{\epsilon}{\omega_c}\right)^2 + \ldots\right] = \frac{W}{12}\left[1 - \frac{20}{3}\left(\frac{\epsilon}{W}\right)^2 + \ldots\right]. \quad (85)$$

In spite of the many approximations used (all of which are reasonable, however) the result for T_c is remarkable because it shows that the critical temperature depends on the band width (corresponding to the largest cut-off energy of the model) and not on the effective mass of the ions. For small deviations from half filling, T_c decreases and is independent of the sign of ϵ.

For different values of ω_c,

$$\omega_c = W/4 - y, \quad (86)$$

with $y \neq 0$, there are only solutions not at half filling. In this case, Eq. (84) can be written as

$$\beta_c|\epsilon| = \ln\frac{1+\kappa}{1-\kappa}, \quad (87)$$

$$\kappa = \frac{\epsilon^2 + \omega_c^2 - (4/W)^2(\omega_c^2 - \epsilon^2)^2}{2|\epsilon|\omega_c}, \quad 0 < \kappa < 1. \quad (88)$$

The condition $\kappa < 1$ is equivalent to

$$|\epsilon| + \omega_c < W/4. \quad (89)$$

On the other hand, the condition $\kappa > 0$ reformulates differently depending on the parameter y,

$$\omega_c < W/4, \quad y > 0: \quad (W/4 - \omega_c)^2 < \epsilon^2 < \epsilon_{max}^2, \quad (90)$$

$$\omega_c > W/4, \quad y < 0: \quad \epsilon_{min}^2 < \epsilon^2 < \epsilon_{max}^2, \quad (91)$$

$$\epsilon_{max,min}^2 = \omega_c^2 + \frac{1}{2}\left(\frac{W}{4}\right)^2 \pm \pm \left(\frac{W}{8}\right)\sqrt{\left(\frac{W}{4}\right)^2 + 8\omega_c^2}. \quad (92)$$

For small y, we can simplify (87) and (88) as

$$\kappa \approx \frac{2}{W|\epsilon|}\left\{\epsilon^2\left[3 - \epsilon^2\left(\frac{4}{W}\right)^2\right] + y\left[\frac{W}{2} - \frac{4\epsilon^2}{W} - \epsilon^4\left(\frac{4}{W}\right)^3\right]\right\}, \quad (93)$$

with the following restrictions for ϵ:

$$y > 0: \quad y^2 < \epsilon^2 < 3\left(\frac{W}{4}\right)^2 - \frac{5}{6}Wy + \frac{29}{27}y^2, \quad (94)$$

$$y < 0: \quad \frac{W}{6}|y| + \frac{25}{27}y^2 < \epsilon^2 < 3\left(\frac{W}{4}\right)^2 + \frac{5}{6}W|y| + \frac{29}{27}y^2. \quad (95)$$

Large values of T_c can be achieved for $\kappa \lessapprox 1$ and in the vicinity of half filling ($\epsilon \neq 0$),

$$k_B T_c \approx \frac{W\delta}{12(\delta - 1)}, \quad \delta = \frac{6\epsilon^2}{W|y|} > 1, \quad y = \frac{W}{4} - \omega_c, \quad (96)$$

but only for $y < 0$, and hence $\omega_c > W/4$.

7. SUMMARY

We have discussed the occurence of superconductivity in the strong-coupling limit ($\bar{g} \gg 1$) of the Hubbard–Holstein model. Strong coupling leads to a renormalization of the one-polaron Green's function already in the local approximation. For $\bar{g} \gg 1$, we found a collective mode for the phonon clouds estimated by evaluating integrals in the Laplace approximation. Because of absorption and emission of this mode by polarons, the on-site energies of polarons are renormalized. Similarly, the irreducible two-particle Green's functions are renormalized. Allowing the exchange of polarons including their phonon clouds leads to a new irreducible Green's function that has been used to study spin–singlet pairing of polarons. Analytic results for the superconducting phase have been obtained in the limiting case where the local repulsion of polarons is exactly canceled by their attractive interaction. The resulting equation for the critical temperature has been obtained by assuming a large collective-mode frequency and a nearly half-filled band case. The parameters that determine T_c are ω_c ($\omega_c \geq W/4$), ϵ (with $\epsilon = 0$ corresponding to half filling), and the band width W. In the strong-coupling limit, we obtain the critical temperature of the order of $\omega_c/3$.

It is interesting to note that a similar result for the value of T_c has been established in [34, 35] for such anomalous low-temperature superconductors as Pb, Hg, and Nb realized within the framework of Eliashberg's theory [36].

In Eliashberg's theory, the retarded nature of the photon-induced interaction and the pseudopotential treatment of the screened Coulomb interaction are taken into account. For example, in [35], the maximum value of the critical temperature T_c^{max} is equal to $\langle\omega\rangle/\exp(3/2)$, where $\langle\omega\rangle$ is the average phonon frequency taken over the phonon density of states, $\langle\omega\rangle \approx 0.5\omega_0$. Our equations involve only the collective frequency $\omega_c = \alpha\omega_0$, $\alpha > 1$.

It is possible to estimate the values of T_c not only analytically but also via calculations using Eq. (83), or more precisely, Eq. (73). Indeed, such numerical results have been obtained by assuming some values of the theory parameters and of the interval of interesting values of T_c. From the three parameteres in our theory (ω_c, W, and e), we first choose the value of the collective frequency ω_c. Assuming that ω_0 is equal to 0.07 eV for cuprates and that the dimensionless interaction constant $\overline{q}$ is equal to 3, we obtain $\alpha = 4.5$ and $\omega_c = 0.315$ eV. We next fix the value of T_c, e.g., to be equal to 100 K. With these values of ω_c and T_c, the following pairs of the other two parameters are compatible:

$$e = 0.10515 \text{ eV} \quad \text{and} \quad W = 1.68057 \text{ eV},$$

$$e = 0.20348 \text{ eV} \quad \text{and} \quad W = 2.07383 \text{ eV},$$

$$e = 0.30149 \text{ eV} \quad \text{and} \quad W = 2.46594 \text{ eV}.$$

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APPENDIX

The method of moments

Using the Heisenberg representation of the one-polaron Green's function

$$\mathcal{G}_\sigma(\mathbf{x}-\mathbf{x}'|\tau-\tau') = \langle T\,\hat{c}_{\mathbf{x}\sigma}(\tau)\,\hat{\bar{c}}_{\mathbf{x}'\sigma'}(\tau')\rangle_H, \qquad (A.1)$$

where

$$\hat{c}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau} c_{\mathbf{x}\sigma} e^{-\mathcal{H}\tau}, \qquad (A.2a)$$

$$\hat{\bar{c}}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau} c^\dagger_{\mathbf{x}\sigma} e^{-\mathcal{H}\tau}, \qquad (A.2b)$$

we can write the asimptotic expansion of the Fourier representation in (25) for $|\omega_n| \to \infty$ as

$$\mathcal{G}_\sigma(\mathbf{x}=0|i\omega_n) = g_\sigma(i\omega_n) = = \frac{1}{i\omega_n} - \frac{M_1}{(i\omega_n)^2} + \frac{M_2}{(i\omega_n)^3} - \frac{M_3}{(i\omega_n)^4} + \ldots, \qquad (A.3)$$

$$M_n = \langle\{c^\dagger_{\mathbf{x}\sigma}, \underbrace{[\mathcal{H}[\mathcal{H}\ldots[\mathcal{H}, c_{\mathbf{x}\sigma}]}_{n}\ldots]\}\rangle_H, \qquad (A.4)$$

where the statistical average $\langle\ldots\rangle_H$ is defined with respect to the full density matrix of the grand canonical ensemble. In the simplest approximation, we obtain the first three moments of the Green's functions as

$$M_1 = -(\epsilon + \omega_c \operatorname{th}(\beta\epsilon/2)), \qquad (A.5a)$$

$$M_2 = \epsilon^2 + \omega_c^2 + (W/4)^2 + 2\epsilon\omega_c \operatorname{th}(\beta\epsilon/2) + + \omega_0\omega_c \operatorname{cth}(\beta\omega_c/2), \qquad (A.5b)$$

$$M_3 = -\{\epsilon^3 + 3\epsilon[\omega_c^2 + \omega_c\omega_0 \operatorname{ch}(\beta\omega_c/2) + (W/4)^2] + + \omega_c \operatorname{th}(\beta\epsilon/2)[3\epsilon^2 + 3(W/4)^2 + \omega_c^2 + \omega_0^2 + + 3\omega_0\omega_c \operatorname{cth}(\beta\omega_0/2)]\}. \qquad (A.5c)$$

The expressions for the moments can be used to determine the unknown coefficients $A_n(\epsilon)$ and $B_n(\epsilon)$ in the relation for $\Lambda_\sigma(i\omega)$, Eq. (78), by also considering the asymptotic behavior of $g_\sigma(i\omega)$ in (66) for small values of $\lambda_\sigma(i\omega)$,

$$g_\sigma(i\omega) = (2/W)\lambda_\sigma(i\omega) \times \times [1 + (\lambda^2/4) + 2(\lambda^2/4)^2 + \ldots]. \quad (A.6)$$

We then insert the asymptotic form of $\lambda_\sigma(i\omega)$ from (78). Comparing the corresponding equations fixes the coefficients $A_n(\epsilon)$ and $B_n(\epsilon)$ as

$$A_1(\epsilon) = 1, \quad (A.7a)$$

$$B_1(\epsilon) = -\frac{1}{\omega_c}[M_1 + \epsilon] \approx \mathrm{th}(\beta\epsilon/2), \quad (A.7b)$$

$$A_2(\epsilon) = \frac{1}{\omega_c^2}\left[M_2 + 2\epsilon M_1 + \epsilon^2 - \omega_c^2 - (W/4)^2\right] \approx \approx \frac{\omega_0}{\omega_c}\,\mathrm{cth}(\beta\omega_0/2), \quad (A.7c)$$

$$B_2(\epsilon) = \frac{1}{\omega_c^3}\left[-M_3 - 3\epsilon M_2 + M_1\left(\omega_c^2 - 3\epsilon^2 + 3(W/4)^2\right) + \epsilon\omega_c^2 - \epsilon^3 + 3\epsilon(W/4)^2\right] \approx \approx \frac{\omega_0}{\omega_c}\,\mathrm{th}(\beta\epsilon/2)\left[\frac{\omega_0}{\omega_c} + 3\,\mathrm{cth}(\beta\omega_0/2)\right]. \quad (A.7d)$$

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