Interaction of strongly correlated electrons and acoustical phonons

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We investigate the interaction of correlated electrons with acoustical phonons using the extended Hubbard-Holstein model in which both, the electron-phonon interaction and the on-site Coulomb repulsion are considered to be strong. The Lang-Firsov canonical transformation allows to obtain mobile polarons for which a new diagram technique and generalized Wick's theorem is used. This allows to handle the Coulomb repulsion between the electrons emerged into a sea of phonon fields (phonon clouds). The physics of emission and absorption of the collective phonon-field mode by the polarons is discussed in detail. Moreover, we have investigated the different behavior of optical and acoustical phonon clouds when propagating through the lattice. Initially the optical phonon fields are located at the lattice sites and do not spread out through the crystal and their evolution is limited by a time \( T \), which means that the exchange of polarons by the phonon clouds is localized and occurs at one and the same lattice site. Hence, the renormalization of local polaron propagators due to optical phonons conserves the hopping matrix elements and the electronic band width. In the opposite case, when the phonon fields are of acoustical nature, the propagation of the fields is delocalized from the beginning and correlations lead band narrowing effects. In addition, there is the possibility of electron transfer without being accompanied by phonon fields. In this case only the local electron propagators are changed while the tunneling matrix elements remain unaffected. In the strong-coupling limit of the electron-phonon interaction, and in the normal as well as in the superconducting phase, chronological thermodynamical averages of products of acoustical phonon-cloud operators can be expressed by one-cloud operator averages. While the normal one-cloud propagator has the form of a Lorentzian, the anomalous one is of Gaussian form and considerably smaller. Therefore, the anomalous electron Green’s functions can be considered to be more important than corresponding polarons functions, i.e., pairing of electrons without phonon-clouds is easier to achieve than pairing of polarons with such clouds.

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I. INTRODUCTION

Since the discovery of high-temperature superconductivity by Bednorz and Müller¹ 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 states²–⁶. 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 can phonons be involved in the formation of the superconducting state. The aim of the present paper is to gain further insight into the mutual influence of strong on-site Coulomb repulsion using the single-band Hubbard-Holstein model⁷,⁸ and a recently developed diagram technique⁹–¹³. We consider now the most interesting case, namely superconductivity of correlated electrons coupled to dispersive acoustical phonons. This investigation differs from our previous studies¹⁴–¹⁹ of electrons coupled to dispersionless optical phonons, which was addressed by most other authors²⁰–²⁵.

Because the interaction between electrons and phonons is strong, we include the Coulomb repulsion in the zero-order Hamiltonian and apply the canonical transformation of Lang and Firsov²⁴ 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 phonon clouds) can lead to an attractive interaction among electrons mediated by the phonons. In this limit, the chemical potential, the on-site and inter-site Coulomb energies as well as the frequency of the collective phonon-cloud mode (which is much larger than the bare acoustical phonon frequencies) are strongly renormalized¹⁷–²⁰. This affects the dynamical properties of the polarons and the character of the superconducting transition. We suggest that the resulting superconducting state with polaronic Cooper pairs is mediated by the exchange of phonon clouds and their collective mode during the hopping of the polarons.

II. THEORETICAL APPROACH

A. The Lang-Firsov transformation of the Hubbard-Holstein model

The initial Hamiltonian of correlated electrons coupled to longitudinal acoustical phonons (the polarization index is omitted) has the form

\[
H = H_e + H_{ph} + H_{e-ph},
\]  

(1)
where

\[ H_e = \sum_{ij, \sigma} \{ t(j-i) + \varepsilon_0 \delta_{ij} \} a_{i \sigma}^\dagger a_{j \sigma} + U_0 \sum_i n_i \varepsilon n_i \varepsilon + \frac{1}{2} \sum_{ij} V_{ij} n_i n_j, \]  

(2)

\[ H_p^0 = \sum_k \hbar \omega_k \left( \frac{1}{2} b_k^\dagger b_k + \frac{i}{2} \right), \]  

(3)

\[ H_{\text{c-ph}} = \sum_{ij} \frac{g(i-j)}{\hbar \omega_k} q_i n_j, \]  

(4)

\[ n_i = \sum_{\sigma} n_{i \sigma}, \quad n_{i \sigma} = a_{i \sigma}^\dagger a_{i \sigma}. \]

Here \( a_{i \sigma} (a_{i \sigma}^\dagger) \) are annihilation (creation) operators of electrons at lattice site \( i \) with spin \( \sigma \), \( b_k (b_k^\dagger) \) are phonon operators with wave vector \( k \); \( q_i (p_i) \) is the phonon coordinate (momentum) at site \( i \), which is related to the phonon operators by

\[ q_i = \frac{1}{\sqrt{V}} \left( b_i + b_i^\dagger \right), \quad p_i = \frac{i}{\sqrt{V}} \left( -b_i + b_i^\dagger \right). \]

The Fourier representation of these quantities have the form

\[ b_i = \frac{1}{\sqrt{N}} \sum_k b_k e^{-ikR_i}, \quad b_i^\dagger = \frac{1}{\sqrt{N}} \sum_k b_k^\dagger e^{ikR_i}, \]  

\[ q_i = \frac{1}{\sqrt{N}} \sum_k q_k e^{-ikR_i}, \quad p_i = \frac{1}{\sqrt{N}} \sum_k p_k e^{ikR_i}, \]  

(5)

\[ q_k = \frac{1}{\sqrt{2}} \left( b_k + b_k^\dagger \right), \quad p_k = \frac{i}{\sqrt{2}} \left( b_k^\dagger - b_k \right). \]

In this Hamiltonian \( U_0 \) and \( V_{ij} \) are the on-site and intersite Coulomb interactions, \( t(i-j) \) is the nearest neighbor two-center transfer integral (which may be extended to include also next-nearest neighbor hopping of electrons), \( g(i-j) \) is the matrix element of the electron-phonon interaction, \( \varepsilon_0 = \varepsilon_0 - \mu_0 \), where \( \varepsilon_0 \) is the local electron energy and \( \mu_0 \) is the chemical potential of the system.

The Fourier representation of \( t(i-j) \) is related to the tight-binding dispersion \( \varepsilon(k) \) of the bare electrons with band width \( W \),

\[ t(R) = \frac{1}{N} \sum_k \varepsilon(k) e^{-ikR}, \]

with \( R \) as the nearest neighbor distance. Apparently the energy scale of the model Hamiltonian is fixed by the parameters \( W, U, \varepsilon \) and \( \hbar \omega_k \). The band filling \( n \) is an additional parameter. After applying the displacement transformation of Lang-Firsov,\(^\text{\text{2b}}\), we obtain the polaron Hamiltonian in the form:

\[ H_p = H_p^0 + H_p^0 + H_{\text{int}}, \]  

(8)

\[ H_p^0 = \sum_i \frac{h}{\omega_k} \left( \frac{1}{2} b_k^\dagger b_k + \frac{i}{2} \right), \]

\[ H_{\text{int}} = \sum_{ij} \frac{g(i-j)}{\hbar \omega_k} q_i n_j, \]  

(10)

where

\[ c_{i \sigma}^\dagger = a_{i \sigma} e^{-i\mu_0}, \quad c_{i \sigma} = a_{i \sigma} e^{i\mu_0}, \]

\[ \eta_i = \frac{1}{\sqrt{N}} \sum_k g(k) p_k e^{ikR_i} = \sum_k p_k g(R_i - R_i), \]  

(12)

\[ g = \varepsilon - \mu - \mu_0 + \frac{1}{2} V_p^0, \quad U = U_0 - V_p^0, \]  

and

\[ V_p^0(i-j) = \frac{1}{N} \sum_k \frac{g(k) g(-k)}{\hbar \omega_k} e^{-ik(R_i - R_j)}. \]  

(14)

Hence, the effective intersite interaction is \( V_{ij} = V_{ij}^0 - V_{ij}^p \) with \( V_{ij}^p = 0 \). The frequency \( \omega_k \) of acoustical phonons is linear in \( k \) for sufficiently small wave vectors. In order to have a reasonable expression for the parameter \( S(k) \) of the canonical transformation, it is necessary that the condition \( g(k = 0) = 0 \) is fulfilled. This condition means that the movement of phonons with infinite wave length, which is equivalent to the macroscopic displacement of the system, cannot influence its properties and must be omitted. Therefore, the Fourier representation of the direct attraction mediated by phonons must also vanish in this limit: \( V_p^0(k = 0) = 0 \). It is important to note that the Fourier representation of the Coulomb part of the inter-site interaction must also vanish for vanishing wave vector: \( V^c(k = 0) = 0 \) as a consequence of required charge neutrality of the system. Therefore, the resulting direct interaction between electrons, \( V(R) = V^c(R) - V_p^0(R) \), fulfills \( V(k = 0) = 0 \). This will be used when analyzing the corresponding diagrammatic contribution.

When deriving the polaron Hamiltonian, it was necessary to include the shift of the polaron coordinate \( \eta_k \) by

\[ e^{i\eta_k} e^{-i\eta_k} = q_k - \frac{1}{\sqrt{N}} \sum_k g(k) n_k e^{ikR_k}, \]

which helps to eliminate the linear electron-phonon interaction.

The polaron Hamiltonian is by nature a polaron-phonon operator because the new creation and annihilation operators \( c_{i \sigma}^\dagger \) and \( c_{i \sigma} \) entering \( H_p \) must be interpreted as operators of polarons, i.e., electrons dressed with displacements of ions that couple dynamically to the momentum of acoustical phonons. In the zero-order approximation (omitting \( H_{\text{int}} \)) polarons are localized and
phonons are free with a strongly renormalized chemical potential $\mu$ and on-site interaction $U$. This last quantity can become negative if the phonon mediated attraction $V_{2k}$ is strong enough to overcome the direct Coulomb repulsion. The first term of the perturbation operator $H_{\text{int}}$ describes tunneling of polarons between lattice sites, i.e., tunneling of electrons surrounded by clouds of phonons. The second term of this operator describes the renormalized polaron-polaron inter-site interactions.

B. Averages of electron and phonon operators

One problem is to deal properly with the impact of electronic correlations on the polaron formation involving operators like (11) for the electron and phonon subsystems. This can be done best by using Green’s functions provided one finds a way to deal with the spin and charge degrees of freedom. In order to achieve this in the limit of large $U$, the Hubbard term can be included in the zero-order Hamiltonian. As a consequence, 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 using Wick’s theorem and conventional Feynman diagrams.

In order to have a systematic description of correlated electrons, Hubbard proposed a graphical expansion around the atomic limit in powers of hopping integrals. This diagrammatic approach was reformulated by Slobodyan and Stasyuk\cite{25} for the single-band Hubbard model and independently by Zaitsev\cite{26} and further developed by Izyumov\cite{27}. In these approaches, the complicated algebraic structure of the projection or Hubbard operators was used.

We have found an alternative way in the sense that our diagram technique involves simpler creation and annihilation operators for electrons at all intermediate stages of the theory and Hubbard and related operators only when evaluating final expressions\cite{9-13}. In this approach, averages of chronological products of interactions are reduced to n-particle Matsubara Green’s functions of the atomic system. These functions can be factorized into independent local averages using a generalization of Wick’s theorem (GWT) which takes strong local correlators into account, see Refs. 9, 10 and 17 for details. 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 formulated by Metzner\cite{28}. But in the latter work the Dyson equation for the renormalized one-particle Green’s function was not derived, nor the correlation function which appears as main element of this equation. It is the purpose of this paper to check in how far we can use the GWT for the extended Hubbard-Holstein model given by Eq. (1).

With respect to the transformed Hubbard-Holstein model, phonon operators are averaged using ordinary Wick’s theorem by taking into account the factorization of the phonon partition function in k space of phonon wave vectors. We define the temperature Green’s function for the polarons in the interaction representation by

$$G_p(x, x', \tau | x, x', \tau') = -\langle T c_{x\sigma}(\tau) \bar{c}_{x'\sigma'}(\tau') U(\beta) \rangle_0^c, \quad (15)$$

with

$$c_{x\sigma}(\tau) = e^{iH_0\tau + c_{x\sigma} e^{-iH_0\tau}}, \quad \bar{c}_{x\sigma}(\tau) = e^{iH_0\tau} c_{x\sigma} e^{-iH_0\tau},$$

$$\pi_x(\tau) = e^{iH_0\tau} \pi_x e^{-iH_0\tau},$$

for the polaron and phonon operators, respectively, with $H_\text{ph} = H_\text{p} + H_\text{ph}$. Instead of $i, j$ we now use $x, x'$ as site indices; $\tau, \tau'$ are imaginary time variables with $0 < \tau < \beta$; $\beta$ is the time ordering operator and $\beta$ the inverse temperature. The evolution operator is given by

$$U(\beta) = \text{e}^{-\beta H_\text{p}} = \sum_0^\beta \text{e}^{-\beta H_{\text{int}}(\tau)}. \quad (16)$$

The statistical averages $\langle \cdots \rangle_0$ are evaluated with respect to the zero-order density matrix of the grand canonical ensemble of localized polarons and free acoustical phonons.

$$\langle \cdots \rangle_0 = \frac{\text{e}^{-\beta H_\text{p}}}{\text{Tr} e^{-\beta H_\text{p}}} \prod_i \frac{\text{e}^{-\beta \omega_k \pi_k}}{\text{Tr} e^{-\beta \omega_k \pi_k}} \prod_k \text{e}^{-\beta \omega_k \pi_k}. \quad (17)$$

The subscript $c$ in Eq. (15) indicates that only connected diagrams have to be taken into account. The polaron part of the density matrix (17) is factorized with respect to the lattice sites. The on-site polaron Hamiltonian contains the polaron-polaron interaction which is proportional to the renormalized parameter $U$. Therefore, this Hamiltonian can be diagonalized only by using Hubbard operators\cite{8}. At this stage no special assumption is made about the value of the quantity $U$ and its sign. So we can set up the equations of motion for the dynamical quantities in this general case. Wick’s theorem of weakly coupled quantum field theory can be used to evaluate statistical averages of phonon operators, including the propagator of phonon clouds.

C. Phonon-cloud propagators

The zero-order one-phonon Matsubara Green’s function has the form

$$\sigma(x, x') = \langle \pi_x(\tau) \pi_{x'}(\tau') \rangle_0 = \frac{1}{2N} \sum_k \langle \mathcal{g}(k)^2 \cos k(x - x') \rangle_0 \times \frac{\cosh \hbar \omega_k \beta/2 - |\tau - \tau'|}{\sinh \hbar \omega_k \beta/2}, \quad (18)$$

with

$$\pi_x(\tau) = \sum_j p_j(\tau) \mathcal{g}(R_j - R_x).$$
Here $x$ is again the position and $\tau$ the imaginary time while $x$ in Eq. (18) stands for $(\mathbf{x}, \tau)$.

This function makes an essential contribution for small values of distances $|x - x'|$ and $|\tau - \tau'|$ close to zero or $\beta$. For $x = x'$ the minimum value of this function is obtained for $|\tau - \tau'| = \beta/2$. Since all approximations in this paper concern the strong-coupling limit of the electron-phonon interaction, we will use the series expansion of $\sigma(x, x')$ near $\tau = 0$ and $\tau = \beta$:

$$
\sigma(0|\tau) = \begin{cases} 
\sigma(0)|0\rangle - h\omega_c\tau, & \tau \geq 0 \\
\sigma(0)|0\rangle + h\omega_c(\tau - \beta), & \tau \leq \beta
\end{cases}
$$

with

$$
\omega_c = \frac{1}{2N} \sum_k |\mathbf{g}(k)|^2 \omega_k
$$

as collective phonon cloud frequency\(^{17,18}\). Besides the one-phonon propagator we have also many-phonon cloud propagators. There are two kind of one-cloud propagators, of which $\phi(x|x')$ is the normal-state one and $\varphi(x|x')$ the anomalous one of the superconducting state, given by

$$
\begin{align*}
\phi(x|x') &= \phi(x - x'|\tau - \tau') = \langle T e^{i\pi x(r-r')/\beta} \rangle_0 \\
&= \exp(-\frac{1}{\beta}(T [\pi_x(\tau) - \pi_x'(\tau')]^2)_0) \\
&= \exp[\sigma(0|0) + \sigma(x - x'|\tau - \tau')],
\end{align*}
$$

$$
\begin{align*}
\varphi(x|x') &= \varphi(x - x'|\tau - \tau') = \langle T e^{i\pi x(r)^2 + \pi_x'(r')} \rangle_0 \\
&= \exp(-\frac{1}{\beta}(T [\pi_x(\tau) + \pi_x'(\tau')]^2)_0) \\
&= \exp[\sigma(0|0) - \sigma(x - x'|\tau - \tau')].
\end{align*}
$$

For the first function the maximum value of the one-phonon propagator $\sigma(x|x')$ is favored while for the second one the corresponding minimum value is preferred. The Fourier representations in $\tau$-space have the form

$$
\begin{align*}
\phi(0|\tau) &= \frac{1}{\beta} \sum_{\Omega} e^{-i\Omega \tau} \tilde{\phi}(i\Omega_n), \\
\varphi(0|\tau) &= \frac{1}{\beta} \sum_{\Omega} e^{-i\Omega \tau} \tilde{\varphi}(i\Omega_n),
\end{align*}
$$

where

$$
\begin{align*}
\tilde{\phi}(i\Omega_n) &= \int_0^\beta dr e^{i\Omega r} e^{-\sigma(0|0) + \sigma(0|r)}, \\
\tilde{\varphi}(i\Omega_n) &= \int_0^\beta dr e^{i\Omega r} e^{-\sigma(0|0) - \sigma(0|r)}.
\end{align*}
$$

Here is $\Omega_n$ the even Matsubara frequency $\Omega_n = 2\pi n/\beta$. In order to find the Fourier representations of these functions we have used the peculiarities of the $\sigma$-propagator in the strong-coupling limit of the electron-phonon interaction. As proven in Appendix A, the first propagator can be written as

$$
\phi(x|x') \simeq \phi(x)\phi(0) - \delta(x,0)
$$

with

$$
\tilde{\phi}(i\Omega_n) \approx \frac{2\omega_c}{(\Omega_n)^2 - (h\omega_c)^2}, \quad \tilde{\varphi}(i\Omega_n) \approx 1.
$$

A more realistic value for $\tilde{\varphi}(i\Omega_n)$ is obtained by using the dependence of $\sigma(x|x')$ on small values of $x$. In this more precise approximation we find

$$
\tilde{\varphi}(i\Omega_n) = \left(\frac{2\pi}{\sigma_1}\right)^{3/2} e^{-\sigma_1 x^2/2\sigma_2}, \quad \phi(x) \simeq e^{-\sigma_1 x^2/2},
$$

where

$$
\sigma_1 = \frac{1}{6N} \sum_k |g(k)|^2 k^2 \coth \frac{1}{2} h\omega_c \beta.
$$

This result has been obtained by an expansion of $\cos kx$ in terms of $x$. We also assume that $g(k)$ depends on $k$ only through its module $|k|$. Then, the Fourier representation of the normal phonon cloud propagator is a Lorentzian and therefore the time dependence of this phonon cloud corresponds to that of an oscillator with the large collective frequency $\omega_c$. For the anomalous one-cloud propagator $\varphi(x|x')$ we obtain in this approximation a Gaussian representation, see Appendix A:

$$
\tilde{\varphi}(i\Omega_n) = \sqrt{2\pi/\sigma_2} \exp \left[ \frac{1}{2} \beta \Omega_n - \sigma(0|0) - \sigma(0|\beta/2) - (\Omega_n)^2/(2\sigma_2) \right],
$$

where

$$
\sigma_2 = \sigma''(0|\beta/2).
$$

The space dependence of $\varphi(x|i\Omega_n)$ is more complicated compared to the space dependence of $\phi(x|i\Omega_n)$ because we cannot restrict the discussion to small values of $|x|$. In the following, we will discuss many-cloud propagators, both in the normal and superconducting states. We start with the two-cloud propagators [as before, $x = (x, \tau)$]:

$$
\begin{align*}
\phi_2(x_1, x_2, x_3, x_4) &= \langle T \exp \left[ \pi_{x_1}(\tau_1) + \pi_{x_2}(\tau_2) - \pi_{x_3}(\tau_3) - \pi_{x_4}(\tau_4) \right] \rangle_0 \\
&= \exp \left( -\frac{1}{\beta} \langle T \left[ \pi_{x_1}(\tau_1) + \pi_{x_2}(\tau_2) - \pi_{x_3}(\tau_3) - \pi_{x_4}(\tau_4) \right]^2 \rangle_0 \right) \\
&= \exp \left( \sum_{x} \langle x, \tau_1; x_2, \tau_2| x_3, \tau_3; x_4, \tau_4 \rangle \right).
\end{align*}
$$
\[ \varphi_2(x_1, x_2, x_3 | z_4) = \langle T \exp \left[ i \left( \pi_{x_1}(r_1) + \pi_{x_2}(r_2) + \pi_{x_3}(r_3) - \pi_{x_4}(r_4) \right) \right] \rangle 
= \exp \left( -\frac{1}{2} \langle T \left( \pi_{x_1}(r_1) + \pi_{x_2}(r_2) + \pi_{x_3}(r_3) - \pi_{x_4}(r_4) \right)^2 \rangle \right) 
= \exp \left( \Sigma(x_1, r_1; x_2, r_2; x_3, r_3 | x_4, r_4) \right), \]  

(31)

where

\[ \Sigma(x_1, r_1; x_2, r_2 ; x_3, r_3; x_4, r_4) = \sigma(x_1 - x_3 | r_1 - r_3) + \sigma(x_1 - x_4 | r_1 - r_4) + \sigma(x_2 - x_4 | r_2 - r_4) \]

(32)

\[ \Sigma(x_1, r_1; x_2, r_2 ; x_3, r_3; x_4, r_4) = \sigma(x_1 - x_4 | r_1 - r_4) + \sigma(x_2 - x_4 | r_2 - r_4) \]

(33)

The following relations exist between two- and one-cloud Green’s functions:

\[ \phi_2(x_1, x_2 | x_3, x_4) = \phi(x_1 | x_3) \phi(x_2 | x_4) \exp \left[ \sigma(x_1 | x_3) + \sigma(x_2 | x_4) - \sigma(x_1 | x_2) - \sigma(x_3 | x_4) \right] \]

(34a)

\[ \phi_2(x_1, x_2 | x_3, x_4) = \phi(x_1 | x_3) \phi(x_2 | x_4) \exp \left[ \sigma(x_1 | x_3) + \sigma(x_2 | x_4) - \sigma(x_1 | x_2) - \sigma(x_3 | x_4) \right] \]

(34b)

\[ \varphi_2(x_1, x_2, x_3 | x_4) = \varphi(x_1 | x_2) \varphi(x_3 | x_4) \exp \left[ \sigma(x_1 | x_2) + \sigma(x_3 | x_4) - \sigma(x_1 | x_3) - \sigma(x_2 | x_4) \right] \]

(35a)

\[ \varphi_2(x_1, x_2, x_3 | x_4) = \varphi(x_1 | x_2) \varphi(x_3 | x_4) \exp \left[ \sigma(x_1 | x_2) + \sigma(x_3 | x_4) - \sigma(x_1 | x_3) - \sigma(x_2 | x_4) \right] \]

(35b)

\[ \varphi_2(x_1, x_2, x_3 | x_4) = \varphi(x_1 | x_2) \varphi(x_3 | x_4) \exp \left[ \sigma(x_1 | x_2) + \sigma(x_3 | x_4) - \sigma(x_1 | x_3) - \sigma(x_2 | x_4) \right] \]

(35c)

Many-cloud phonon propagators will be present in all diagrams of the thermodynamical perturbation theory to be formulated here. As above equations show, all sites of the diagrams are joint and appear to be connected in the presence of acoustical phonons. In order to classify the diagrams as connected and disconnected ones, it is necessary to have the analogy of Wick’s theorem for many-cloud propagators similar to the theorem we had formulated for correlated electrons. In the absence of such a theorem we cannot prove the existence of a linked-cluster theorem for the thermodynamical potential and for other extensive quantities.

This problem has been discussed in detail in Ref. 30, however, only now we are able to present a solution. In order to obtain this solution, we observe that the two-cloud functions determined by Eqs. (34) and (35) have their maximum values when the arguments of the normal one-cloud functions \( \varphi(x | x’) \) coincide (\( x = x’ \)) and the corresponding exponential factors close to these arguments approach one. There are several possibilities to achieve this and all of them have to be taken into account. We assume that as main approximation the following expressions for the two-cloud propagators will result,

\[ \phi_2(x_1, x_2 | x_3, x_4) = \phi(x_1 | x_3) \phi(x_2 | x_4) + \phi(x_1 | x_4) \phi(x_2 | x_3) + \phi_2^{(2)}(x_1, x_2 | x_3, x_4), \]  

(36)

\[ \varphi_2(x_1, x_2, x_3 | x_4) = \varphi(x_1 | x_2) \varphi(x_3 | x_4) + \varphi(x_1 | x_3) \varphi(x_2 | x_4) + \varphi(x_2 | x_3) \varphi(x_1 | x_4) \]

(36)

These last equations also define the irreducible parts of the two-cloud propagators or phonon-cloud cumulants. In the strong-coupling limit the irreducible functions are small and can be omitted as shown below. The validity of this statement is discussed in Appendix A, in which the Fourier representation of the normal two-cloud propagator,

\[ \phi_2(x_1, i \Omega_1; x_2, i \Omega_2 | x_3, i \Omega_3; x_4, i \Omega_4) = \int_0^\beta \ldots \int_0^\beta d\tau_1 \ldots d\tau_4 \]

\[ \times \exp (i \Omega_1 \tau_1 + i \Omega_2 \tau_2 - i \Omega_3 \tau_3 - i \Omega_4 \tau_4) \]

\[ \times \phi_2(x_1, \tau_1; x_2, \tau_2; x_3, \tau_3; x_4, \tau_4), \]

(38)

has been calculated in the strong-coupling limit leading to

\[ \phi_2(x_1, i \Omega_1; x_2, i \Omega_2 | x_3, i \Omega_3; x_4, i \Omega_4) \]

\[ \simeq \phi(x_1 - x_2 | i \Omega_1) \delta_{\Omega_1 \Omega_2} \phi(x_2 - x_4 | i \Omega_2) \delta_{\Omega_2 \Omega_3} \]

\[ + \phi(x_1 - x_4 | i \Omega_1) \delta_{\Omega_1 \Omega_3} \phi(x_2 - x_3 | i \Omega_2) \delta_{\Omega_2 \Omega_3}. \]

(39)

The last equation shows that in this limit the irreducible function is not relevant and Wick’s theorem has a simple form, which does not contain significant irreducible contributions. Similarly we obtain for \( \varphi_2 \) a form without irreducible contributions,

\[ \varphi_2(x_1, i \Omega_1; x_2, i \Omega_2; x_3, i \Omega_3 | x_4, i \Omega_4) \]
\begin{align}
\int_0^\beta \ldots \int_0^\beta dt_1 \ldots dt_4 \ e^{-i(\Omega t_1 + \delta t_2 t_2 + \delta t_3 t_3 - \Omega t_4 t_4)} \\
\times \varphi_2 (x_1, \tau_1; x_2, \tau_2; x_3, \tau_3 | x_4, \tau_4)
\end{align}

\begin{align}
\approx \varphi (x_1 - x_2 | \Omega_1) \delta_{\Omega_1, -\Omega}, \varphi (x_1 - x_4 | \Omega_4) \delta_{\Omega_4, -\Omega} \\
+ \varphi (x_1 - x_2 | \Omega_1) \delta_{\Omega_1, -\Omega}, \varphi (x_2 - x_4 | \Omega_2) \delta_{\Omega_2, -\Omega} \\
+ \varphi (x_2 - x_3 | \Omega_2) \delta_{\Omega_2, -\Omega}, \varphi (x_1 - x_3 | \Omega_3) \delta_{\Omega_3, -\Omega} 
\end{align}

These results correspond to our preliminary estimates that the irreducible parts in Eqs. (36) and (37) can be omitted because they are not important in the strong-coupling limit, see Appendix A. Hence, without the irreducible parts the equations assume a form corresponding to Wick’s theorem applied to two-cloud propagators. This can easily be generalized to the case of a larger number of clouds. Thus, there is an analogy of having a generalized Wick’s theorem for the case of correlated electrons \(^9\) and a corresponding theorem for correlated phonon clouds. This allows us now to develop a thermodynamical perturbation theory for correlated electrons interacting strongly with phonons.

As is shown below the tunneling of polars between lattice sites can be accompanied by either preserving or by exchanging phonon clouds. In the strong-coupling limit these clouds are heavy, therefore, in case of preserving the cloud, the effective matrix transfer matrix element is considerably diminished leading to band narrowing effects. In the other case, when clouds are exchanged, the transfer matrix element and the electronic band width remain unchanged.

### III. POLARON GREEN’S FUNCTIONS

#### A. Local approximation

The zero-order one-polaron Green’s function is given by

\[
G_0(x, x') = -\langle T c_{\sigma} (\tau) \bar{c}_{\sigma} (\tau') \rangle_0 \\
= -\langle T c_{\sigma} (\tau) \bar{c}_{\sigma} (\tau') \rangle_0 \phi (x, \tau | x', \tau') \\
= \delta_{x, x'} \delta_{\sigma, \sigma'} G_0^{\sigma} (\tau - \tau') \phi (\tau - \tau'),
\]

where \( x \) stands now for \( x = (x, \sigma, \tau) \). In order to discuss the influence of the collective mode on \( G_0^{\sigma} (x, x') \), we write down its Fourier transformation by making use of Eqs. (25) (see Ref. 19):

\[
\mathcal{G}_0^{\sigma} (i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G_0^{\sigma} (\tau),
\]

\[
\mathcal{G}_0^{\sigma} (i\omega_n) = \frac{1}{Z_0} \left[ e^{-\beta E_0 + \overline{\omega}_c} \epsilon (e^{-\beta E_0} + e^{-\beta E_2}) \right] \\
\times \frac{1}{i\omega_n + E_0 - E_2 - \omega_c} \\
+ \frac{e^{-\beta E_2} + \overline{\omega}_c} {i\omega_n + E_0 - E_2 + \omega_c}
\]

where \( \omega_n \) is the odd Matsubara frequency and

\[
Z_0 = 1 + e^{-\beta E_2} + e^{-\beta E_1} + e^{-\beta E_1},
\]

\[
E_0 = 0, \quad E_{\pm \sigma} = \epsilon, \quad E_2 = U + 2\epsilon,
\]

\[
\overline{\omega}_c = (e^{\beta \epsilon} - 1)^{-1}, \quad \overline{\omega}_c = (e^{\beta \omega_c} - 1)^{-1}.
\]

Equation (44) shows that the on-site transition energies of polars are changed by the energy \( \omega_c \) of the collective mode. The delocalization of polars due to hopping and intersite Coulomb interaction leads to broadening of the polaronic energy levels. The polaron propagator has the following antisymmetry property:

\[
\mathcal{G}_0^{\sigma} (i\omega_n; \epsilon; \omega_c) = -\mathcal{G}_0^{\sigma} (-i\omega_n; -\epsilon - U; \omega_c)
\]

#### B. Expansion around the atomic limit

We will now investigate polaron delocalization under the influence of \( H_{\text{pot}} \) in Eq. (10) by making use of thermodynamical perturbation theory in the interaction representation. The averages of chronological products of interactions are reduced to n-particle Green’s functions of the atomic system, which can be factorized into independent local averages of electron operators and chronological products of phonon operators. The procedure relies on a generalized Wick’s theorem for electron operators, which takes into account the strong local electronic correlations, and Wick’s theorem for phonon cloud operators. In addition to the normal one-polaron propagator in Eq. (15), we will also investigate the anomalous propagators defined by

\[
F_{\sigma} (x | x') = -\langle T c_{\sigma} (x) c_{\sigma} (x') \rangle_0^0,
\]

\[
\mathcal{F}_x (x | x') = -\langle T x_{\sigma} (x) x_{\sigma} (x') \rangle_0^0
\]

As before, \( x \) stands for \( (x, \sigma, \tau) \). The easiest way to establish (47) is to make use of a local source term of Cooper pairs,

\[
H_\Delta = \Delta \sum_i \left( a_i^\dagger a_i^\dagger + a_i a_i^\dagger \right),
\]

which is added to the local Hamiltonian (2) and switched off at the end of the calculation.

In first order perturbation theory the contributions to the normal polaron Green’s function (15) and anomalous Green’s function (47a) are shown in Fig. 1(a) and Fig. 1(b), respectively.

The diagrammatic elements are self-explanatory (see caption of Fig. 1). Since the correlation functions \( \Gamma^\sigma_0 (x, x' | i) \) and \( \mathcal{G}_0^{\sigma} (x, x' | i) \) and the two-particle irreducible
FIG. 1: The simplest diagrams contributing to the normal (a) and anomalous (b) one-polaron Green's functions. Solid lines with arrows in same direction represent normal ($G^0$) and lines with arrows in opposite directions anomalous ($\tilde{G}^0$) propagators, respectively. Short-dashed lines are for the hopping matrix elements $t(i-j)$, long-dashed lines represent the direct polaron-polaron interactions $V(i-j)$, the wiggly lines stand for the normal phonon (cloud) propagators $\phi(x|x')$, and the zigzag lines are the anomalous phonon (cloud) propagators $\varphi(x|x')$. Rectangles depict the correlation functions $\Gamma^0$ and $\tilde{\Gamma}^0$.

function $G^0_2|_{x_1,x_2|x_3,x_4}$ are local quantities, all site indices are equal:

$$
\Gamma^0_2(x,x'|i) = \delta_{x,x'} \delta_{i,i} \Gamma^0_2(\sigma,\tau;\sigma',\tau'|n),
$$

$$
\tilde{\Gamma}^0_2(x,x'|i) = \delta_{x,x'} \delta_{i,i} \tilde{\Gamma}^0_2(\sigma,\tau;\sigma',\tau'|n),
$$

(48a)

(48b)

where

$$
\Gamma^0_2(\sigma,\tau;\sigma',\tau'|\eta) = \langle \Gamma a_\sigma(\tau) a_{\sigma'}(\tau') | n(\eta) \rangle_0
$$

$$
\tilde{\Gamma}^0_2(\sigma,\tau;\sigma',\tau'|\eta) = \langle \Gamma a_\sigma(\tau) a_{\sigma'}(\tau') | n(\eta) \rangle_0
$$

$$
\langle \Gamma a_\sigma(\tau) a_{\sigma'}(\tau') | n(\eta) \rangle_0 - \langle \Gamma a_\sigma(\tau) | n(\eta) \rangle_0 \langle a_{\sigma'}(\tau') | n(\eta) \rangle_0,
$$

$$
\tilde{\Gamma}^0_2(\sigma,\tau;\sigma',\tau'|\eta) = \langle \Gamma a_\sigma(\tau) a_{\sigma'}(\tau') | n(\eta) \rangle_0
$$

$$
-\langle \Gamma a_\sigma(\tau) | n(\eta) \rangle_0 \langle a_{\sigma'}(\tau') | n(\eta) \rangle_0.
$$

(49a)

(49b)

These functions can be compared with the two-particle irreducible quantities of Ref. 9,10 defined by

$$
G^0_2|_{x_1,x_2|x_3,x_4} = \delta_{x_1,x_3} \delta_{x_2,x_4}
$$

$$
G^0_2|_{x_1,x_2|x_3,x_4} = \delta_{x_1,x_3} \delta_{x_2,x_4}
$$

(49c)

(49d)
\[ G_{2}^{0,x}[\sigma_{1} \mid \sigma_{2}] = \sum_{\sigma_{1}, \sigma_{2}} G_{2}^{0,x}[\sigma_{1} \mid \sigma_{2}] = \sum_{\sigma_{1}, \sigma_{2}} G_{2}^{0,x}[\sigma_{1} \mid \sigma_{2}], \quad (50a) \]

\[ G_{2}^{0,x}[x_{1}, x_{2}, x_{3} | x_{4}] = \delta_{x_{1}, x_{2}} \delta_{x_{1}, x_{3}} \delta_{x_{1}, x_{4}}, \quad (50b) \]

where

\[ G_{2}^{0,x}[\sigma_{1} \mid \sigma_{2}] = \langle (\sigma_{1} \sigma_{2} \sigma_{3})^{0} | (\sigma_{1} \sigma_{2} \sigma_{3})^{0} \rangle \]

The second function, \( G_{2}^{0,x}[x_{1}, x_{2}, x_{3} | x_{4}] \), can be obtained from Eq. (51) by replacing the operator \( \sigma_{x} \) by \( \sigma_{y} \) and corresponds to an anomalous superconducting contribution. Between the non-full cumulant \( \Gamma_{3}^{0}(\sigma \mid \sigma' \mid \sigma') \) and the full one \( G_{2}^{0,x} \) exists the following relation

\[ \Gamma_{3}^{0}(\sigma \mid \sigma' \mid \sigma') = - \sum_{\sigma} G_{2}^{0,x}[\sigma \mid \sigma_{1} \mid \sigma_{1} \mid \sigma' \mid \sigma'] \]

In second order perturbation theory we have to deal with more complicated functions like

\[ \Gamma_{3}(x_{1}, x_{2} \mid i_{1}, i_{2}) = \delta_{x_{1}, x_{2}} \delta_{x_{1}, x_{2}} \Gamma_{3}(\sigma \mid \sigma' \mid \sigma' \mid \sigma_{1}, \sigma_{2}), \quad (53a) \]

\[ \Gamma_{3}(\sigma \mid \sigma' \mid \sigma' \mid \sigma_{1}, \sigma_{2}) = \langle (\sigma_{1} \sigma_{2} \sigma_{3})^{0} | (\sigma_{1} \sigma_{2} \sigma_{3})^{0} \rangle \]

with the following relation between the non-full and full three-particle cumulants,

\[ \Gamma_{3}(\sigma \mid \sigma' \mid \sigma_{1}, \sigma_{2}) = - \sum_{\sigma_{1}, \sigma_{2}} G_{3}^{0,x}[\sigma \sigma_{1} \sigma_{2}] \sum_{\sigma_{1}, \sigma_{2}} G_{3}^{0,x}[\sigma_{1} \sigma_{2} \sigma_{3}] \]

\[ - \sum_{\sigma_{1}, \sigma_{2}} G_{3}^{0,x}[\sigma \sigma_{1} \sigma_{2}] G_{3}^{0,x}[\sigma_{1} \sigma_{2} \sigma_{3}] G_{3}^{0,x}[\sigma_{3} \sigma_{4} \sigma_{5}] \]

\[ - \sum_{\sigma_{1}, \sigma_{2}} G_{3}^{0,x}[\sigma \sigma_{1} \sigma_{2}] G_{3}^{0,x}[\sigma_{1} \sigma_{2} \sigma_{3}] G_{3}^{0,x}[\sigma_{3} \sigma_{4} \sigma_{5}] \]

where

\[ n^{2c} = \langle (\hat{n} - \langle \hat{n} \rangle)^{2} \rangle, \quad n^{3c} = \langle (\hat{n} - \langle \hat{n} \rangle)^{3} \rangle, \quad n^{4c} = \langle (\hat{n} - \langle \hat{n} \rangle)^{4} \rangle - 3 \langle (\hat{n} - \langle \hat{n} \rangle)^{2} \rangle^{2}. \]

The first diagram of the right-hand part of Fig. 1(a) is a local normal electron propagator \( G_{2}^{0}(x \mid x') \) represented by a solid line, which is renormalized by the phonon-cloud propagator \( \phi(x \mid x') \). The corresponding first diagram in Fig. 1(b) is the anomalous electron Green's function renormalized by the phonon-cloud. In this case the renormalization is determined by the anomalous function \( \phi(x \mid x') \), which is smaller than the corresponding contribution from the propagator \( \phi(x \mid x') \). The diagrams (b)-(e) of Fig. 1(a) and (b)-(g) of Fig. 1(b) take into account intersite tunneling, of which the corresponding last diagrams describe direct polaron-polaron intersite interaction.

Among these diagrams we have also weakly connected ones, e.g., diagram (b) in Fig. 1(a) and diagrams (b) and (e) in Fig. 1(b), which can be divided into two parts by cutting one tunneling line. All other diagrams are strongly connected. All contributions of Fig. 1(b) for the anomalous Green's functions contain the phonon-cloud propagator \( \phi(x \mid x') \) and are therefore less important than the corresponding diagrams of Fig. 1(a).

In second order perturbation theory there are both groups of weakly and strongly-connected diagrams. The weakly connected ones are the simple repetition of the first-order diagrams. Therefore, in Figs. 2-4 only the strongly-connected diagrams for the normal and anomalous polaron Green's functions are shown.

The diagrams (a)-(i) in Figs. 2 and 3 originate from polaron tunneling processes. In the group of more complex diagrams the contributions from (f) appear only because of the electron-phonon interaction. Diagrams (g)-(k), each with a rectangle, are special contributions characteristic of strongly correlated electron systems. The diagrams (h) and (i) contain the phonon (cloud) correlation function \( \phi_{2}(x_{1} x_{2} | x'_{1} x'_{2}) \), each consisting of six terms with different order of phonon propagation. To illustrate this, the corresponding diagrammatical representation for one of the anomalous Green's functions is shown in Fig. 4 (without resolving the structure of the less important phonon-cloud propagator \( \phi_{n} \)).

With respect to the full normal Green's function \( G \) we now introduce the correlation function \( Z(x \mid x') \) in analogy with previous works. In diagrammatical form typical contributions to this function are given by (c)-(f) in Fig. 1(a) and by all contributions from Figs. 2 and 3 and by corresponding strongly-connected contributions from higher order perturbation theory. If we then connect the strongly-connected diagrams in all possible ways by the weakly connected diagrams with non-renormalized tunneling matrix elements, we are able to formulate a
Dyson-like equation,
\[ G_{\sigma\sigma'}(x, \tau | x', \tau') = \Lambda_{\sigma\sigma'}(x, \tau | x', \tau') \]
\[ + \int d\tau_1 \sum_{x_1, x_2} \sum_{\sigma_1} \Lambda_{\sigma\sigma_1}(x, \tau | x_1, \tau_1) \times t(x_1 - x_2) G_{\sigma_1\sigma'}(x_2, \tau_1 | x', \tau'), \]
where
\[ \Lambda_{\sigma}(x | x') = G^0_p(x | x') + Z_p(x | x'), \]
which in Fourier representation,
\[ G_{\sigma\sigma'}(x | x') = \frac{1}{\beta N} \sum_{\omega_n} \sum_{k} G_{\sigma\sigma'}(k | \omega_n) e^{-ik(x-x')} e^{-\omega_n(\tau-\tau')}, \]
has a simple algebraical form:
\[ G_{\sigma\sigma}(k | \omega_n) = \frac{\Lambda_{\sigma\sigma}(k | \omega_n)}{1 - \varepsilon(k) \Lambda_{\sigma\sigma}(k | \omega_n)}, \]
with the tight-binding dispersion \( \varepsilon(k) \) of the bare electrons defined before.

Here we have assumed a paramagnetic ground state and spin conservation \( \sigma' = \sigma \). It is important to note that the form of the Dyson equation is the same for both the superconducting and normal states of the system. The states differ with respect to the correlation function \( Z \). This situation is somewhat different from the Hubbard-Holstein model for optical phonons, where in the superconducting state normal and anomalous Green's functions are interrelated. However, here two anomalous polaron Green's functions are proportional to the anomalous one-phonon-cloud propagator \( \varphi(x | x') \). Nevertheless, Dyson's equation for the anomalous polaron Green's functions requires the knowledge of the normal polaron Green's function. Then, by summing of corresponding diagrams we obtain:
\[ F_{\sigma\sigma}(x, \tau | x', \tau') = \Omega_{\sigma\sigma}(x, \tau | x', \tau') \]
\[ + \sum_{x_1, x_2} \int d\tau_1 \Lambda_{\sigma\sigma}(x, \tau | x_1, \tau_1) \times t(x_1 - x_2) F_{\sigma\sigma}(x_2, \tau_1 | x', \tau') \]
\[ \times G_{\sigma\sigma}(x', \tau | x_2, \tau_1) \]
with
\[ \Omega_{\sigma}(x | x') = F^0_p(x | x') + Y_p(x | x'), \]
where $\Psi_p(x|x')$ is the sum of all strongly-connected diagrams for the anomalous Green’s functions. This quantity is analogous to the function $Z(x|x')$ but differs from it by the direction of external electron lines. The Fourier representation of Eq. (60) has the form:

$$
F_{\rho\sigma}(k|\omega_n) = \Omega_{\rho\sigma}(k|\omega_n) \left[ 1 - \varepsilon(k) \Lambda_{\rho\sigma}(k|\omega_n) \right] \\
\times \left[ 1 + \varepsilon(-k) G_{\rho\sigma}(k|\omega_n) \right].
$$

We obtain by making use of Eq. (59):

$$
F_{\rho\sigma}(k|\omega_n) = \frac{\Omega_{\rho\sigma}(k|\omega_n)}{1 - \varepsilon(k) \Lambda_{\rho\sigma}(k|\omega_n)} \\
\times \frac{1}{1 - \varepsilon(-k) G_{\rho\sigma}(k|\omega_n)}
$$

The anomalous quantities $\Omega_{\rho\sigma}$, $\Lambda_{\rho\sigma}$, $F_p$ and $\Phi_p$ are proportional to the anomalous one-phonon-cloud propagator $\varphi$, which in the strong-coupling limit is an exponentially small quantity. Therefore, it is more important to consider the propagators $F_e(x|x')$ and $\Phi_e(x|x')$ defined in terms of the electron operators $a_e(\tau)$ and $\bar{a}_e(\tau)$ and not in terms of the polaron operators $c(\tau)$ and $\bar{c}(\tau)$. In addition we have to discuss the normal electron propagator $G_e(x|x')$. These functions are defined by

$$
G_e(x|x') = -\langle T a_{\rho\sigma}(\tau) a_{\rho\sigma}^{\dagger}(\tau') U(\beta) \rangle_0, \\
F_e(x|x') = -\langle T \bar{a}_{\rho\sigma}(\tau) \bar{a}_{\rho\sigma}^{\dagger}(\tau') U(\beta) \rangle_0, \\
\Phi_e(x|x') = -\langle T \bar{a}_{\rho\sigma}(\tau) \bar{a}_{\rho\sigma}^{\dagger}(\tau') U(\beta) \rangle_0.
$$

Diagrammatical contributions to the first two functions are shown in Fig. 5 and 6, respectively.

Figure 5 shows the diagrams contributing to the normal one-electron propagator in the presence of acoustical phonons (clouds). For simplicity we have used similar drawing elements as before although now we discuss electron propagators. We again find weakly connected diagrams which can be divided into two parts by cutting one electron line like $c_1-c_7$. Furthermore, we introduce normal, $\Sigma(x|x')$, and anomalous, $\Xi(x|x')$ and $\Xi(x|x')$, mass operators, of which the simplest contributions are shown in Fig. 7. For example, diagram $a_1$ is the renormalized tunneling matrix element, whereas (b) and (c) are the simplest contributions to the anomalous mass operators. In analogy to the rectangles representing irreducible
Green’s functions, $G_n^0$, or non-full cumulants, $\Gamma_n^0$, $\Xi_n^0$, and $\overline{\Xi}_n^0$ in Figs. 5 and 6, we introduce here the correlation functions $Z_e(x|x’)$ for the normal state and $Y_e(x|x’)$ and $\overline{Y}_e(x|x’)$ for the superconducting state. For example, to (d) and (e) in Fig 5 corresponding diagrams contribute here to $Z_e(x|x’)$, while to (d) and (e) in Fig. 6 corresponding diagrams contribute to the correlation function $Y_e(x|x’)$, which leads to

$$\Lambda_e(x|x’) = G^0(x|x’) + Z_e(x|x’),$$

(65a)

$$\Omega_e(x|x’) = \Gamma^0(x|x’) + Y_e(x|x’),$$

(65b)

$$\overline{\Omega}_e(x|x’) = \overline{\Gamma}^0(x|x’) + \overline{Y}_e(x|x’).$$

(65c)

Thus we have introduced the main dynamical quantities which determine the to Fig. 5 and 6 corresponding diagrammatical structure. This allows us to derive Dyson equations for the electron Green’s function system. The full electron Green’s functions can be expressed as

$$G_e(x|x’) = \Lambda_e(x|x’) + \Lambda_e(x|x_1) \Sigma_e(x_1|x_2) G_e(x_2|x’),$$

$$- \Lambda_e(x|x_1) \Xi_e(x_1|x_2) \overline{F}_e(x_2|x’),$$

$$- \Omega_e(x|x_1) \Sigma_e(x_2|x_1) F_e(x_2|x’),$$

$$- \Omega_e(x|x_1) \Xi_e(x_1|x_2) \overline{G}_e(x_2|x’),$$

(66a)

$$F_e(x|x’) = \Omega_e(x|x’) + \Omega_e(x|x_1) \Sigma_e(x_2|x_1) G_e(x_2|x’),$$

$$- \Omega_e(x|x_1) \Xi_e(x_1|x_2) F_e(x_2|x’),$$

$$- \Lambda_e(x|x_1) \Sigma_e(x_1|x_2) \overline{G}_e(x_2|x’),$$

$$+ \Lambda_e(x|x_1) \Xi_e(x_1|x_2) \overline{F}_e(x_2|x’),$$

(66b)

$$\overline{F}_e(x|x’) = \overline{\Omega}_e(x|x’) + \overline{\Omega}_e(x|x_1) \Sigma_e(x_2|x_1) G_e(x_2|x’),$$

$$- \overline{\Omega}_e(x|x_1) \Xi_e(x_1|x_2) \overline{F}_e(x_2|x’),$$

$$- \Lambda_e(x|x_1) \Sigma_e(x_1|x_2) \overline{G}_e(x_2|x’),$$

$$+ \Lambda_e(x|x_1) \Xi_e(x_1|x_2) \overline{G}_e(x_2|x’),$$

(66c)

Here $x$ stands for $(\mathbf{x}, \sigma, \tau)$. Double repeated indices im-
ply summation over \( x \) and \( \sigma \) and integration over \( \tau \). All quantities in these equations are renormalized functions containing all diagrammatic contributions to the normal and anomalous one-electron Green's functions. The Fourier representation of the first two equations can be written as \( [k = \mathbf{k}, i\omega_n] \):

\[
\begin{align*}
\Lambda^\sigma_{\sigma'}(-k) &= G^\sigma_{\sigma'}(-k) \left[ 1 - \Lambda_{\sigma'}(k) \Sigma^\sigma_{\sigma'}(-k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right] \\
&+ F^\sigma_{\sigma'}(k) \left[ \Lambda^\sigma_{\sigma'}(-k) \Xi^\sigma_{\sigma'}(k) + \Omega^\sigma_{\sigma'}(k) \Sigma^\sigma_{\sigma'}(k) \right], \quad (67a) \\
\Omega^\sigma_{\sigma'}(k) &= F^\sigma_{\sigma'}(k) \left[ 1 - \Lambda^\sigma_{\sigma'}(k) \Sigma^\sigma_{\sigma'}(k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right] \\
&- G^\sigma_{\sigma'}(-k) \left[ \Omega^\sigma_{\sigma'}(k) \Sigma^\sigma_{\sigma'}(-k) + \Lambda^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right]. \quad (67b)
\end{align*}
\]

The solutions of these equations are

\[
G^\sigma_{\sigma'}(-k) = \frac{1}{d^\sigma(k)} \left[ \Lambda^\sigma_{\sigma'}(-k) - \Sigma^\sigma_{\sigma'}(k) \Lambda^\sigma_{\sigma'}(-k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right], \quad (68a)
\]

\[
F^\sigma_{\sigma'}(k) = \frac{1}{d^\sigma(k)} \left[ \Omega^\sigma_{\sigma'}(k) \right] \\
+ \Xi^\sigma_{\sigma'}(k) \left[ \Lambda^\sigma_{\sigma'}(k) \Lambda^\sigma_{\sigma'}(-k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right], \quad (68b)
\]

\[
\Xi^\sigma_{\sigma'}(k) = \frac{1}{d^\sigma(k)} \left[ \Omega^\sigma_{\sigma'}(k) \right] \\
+ \Xi^\sigma_{\sigma'}(k) \left[ \Lambda^\sigma_{\sigma'}(k) \Lambda^\sigma_{\sigma'}(-k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right], \quad (68c)
\]

where

\[
d^\sigma(k) = 1 - \Lambda^\sigma_{\sigma'}(k) \Sigma^\sigma_{\sigma'}(k) + \Lambda^\sigma_{\sigma'}(-k) \Sigma^\sigma_{\sigma'}(-k) \\
+ \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \\
+ \left[ \Lambda^\sigma_{\sigma'}(k) \Lambda^\sigma_{\sigma'}(-k) + \Omega^\sigma_{\sigma'}(k) \Xi^\sigma_{\sigma'}(k) \right]
\]
\[
\times \left[ \Sigma^\varphi_\sigma(k) \Sigma^\varphi(-k) + \Xi^\varphi_\sigma(k) \Xi^\varphi(-k) \right].
\] (69)

The functions \( F, \Omega \) and \( \Xi \) obey the following symmetry relations:

\[
F^\varphi_\sigma(k) = -F^\varphi_\sigma(-k), \quad \Omega^\varphi_\sigma(k) = -\Omega^\varphi_\sigma(-k),
\]

\[
\Xi^\varphi_\sigma(k) = -\Xi^\varphi_\sigma(-k),
\]

and hence,

\[
d^\varphi_\sigma(k) = d^\varphi(-k). \tag{71}
\]

These equations for the renormalized electron Green’s functions are exact. Since they do not contain the exponentially small anomalous phonon-cloud propagator \( \varphi(x|x') \), superconducting pairing is easier to achieve by electrons without phonon clouds but moving in the environment of the clouds belonging to other polarons, than by polarons moving in the same environment. We can now switch off the superconducting source term, which means that \( F^0 \) and \( F^f \) are identically zero. However, the functions \( \Omega_{\varphi,\sigma} \) and \( \Omega_{\varphi,\sigma}^f \) survive in this limit and are equal to the order parameters of the superconducting state, \( Y_{\varphi,\sigma} \) and \( Y_{\varphi,\sigma}^f \), respectively.
IV. SOLVABLE LIMITS

The three correlation functions \( Z_{ee}, Y_{e\sigma\sigma} \) and \( Y_{e\sigma\sigma} \) are the infinite sums of diagrams which contain both partially and completely irreducible many-particle Green's functions. In order to obtain a closed set of equations which can be solved (at least numerically), we restrict ourselves to a class of rather simple diagrams which, however, contain the most important spin, charge and pairing correlations.

One way to do this, is to check how the individual diagrams are influenced by the phonon fields, for example by distinguishing the case of moderate coupling, when Eq. (26) can be used, from the strong-coupling case where Eq. (25) holds. This helps to eliminate from the diagrams the less important ones. For example, in the strong-coupling limit \( \phi(x|x') \propto \delta_{x,x'} \) holds, which allows to discard all renormalized tunneling matrix elements of the form \( t(x'-x) \phi(x-x'|0) \). In this limiting case the narrowing of the electronic energy band is maximum, i.e., its width is equal to zero. Since this extreme case is a bit unrealistic, we will in the following consider the case of moderate electron-phonon coupling when also the band narrowing is moderate and Eq. (26) must be used. After summing the infinite series of the most important contributions we obtain the result which is shown graphically in Fig. 8.

It is evident that in this approximation for the correlation functions no closed set of equations is obtained because of the complicated nature of mass operators. So we have to simplify the latter quantities of which the simplest diagrams are depicted in Fig. 7. For the normal mass operator we will use the contribution (a) in Fig. 7 which is given by

\[
\Sigma_e(x|x') = \sum_{i} (x| x') \phi(x - x'|0)
\]

\[\approx t(x - x') \exp(-\sigma_1 (x - x')^2/2)\]

For simplicity we replace in the exponential function the distance \( |x - x'| \) by the lattice constant \( a \) being a characteristic length over which the electrons tunnel:

\[
\Sigma_e(x|x') = t(x - x') \delta(\tau - \tau')
\]

\[= t(x - x') \exp(-W_p) \delta(\tau - \tau'), \quad \text{(72a)}\]

\[W_p = \frac{1}{2} \sigma_1 (a^2). \quad \text{(72b)}\]

This result means that tunneling of phonon-fields leads to electronic band-narrowing effects by which the bare energy \( \varepsilon(k) \) is replaced by \( \tilde{\varepsilon}(k) = \varepsilon(k) e^{-W_p} \). For moderate electron-phonon interaction the quantity \( W_p \) is about unity. With respect to the anomalous mass operators, \( \Xi_e \) and \( \Xi_{e,s} \), we observe that they are smaller than the normal one and can therefore safely be neglected. This will be used when expanding the equations close to the superconducting transition temperature.

Another approximation is related to a simplification of the exact Dyson Eqs. (68) by omitting all anomalous mass operators, which yields \( [k = (k, i\omega)] \)

\[G_{e\sigma}(k) = \frac{i}{D^c_{\sigma}(k)} \left\{ A_{e\sigma}^c(k) \left[ 1 - \tilde{\varepsilon}(-k) A_{e\sigma}^c(-k) \right] \right\}
\]

\[-\tilde{\varepsilon}(-k) Y_{e\sigma\sigma}^c(k) \overline{Y}_{\sigma\sigma}^c(-k) \right\}, \quad \text{(73a)}\]

\[F_{\sigma\sigma}^c(k) = \frac{Y_{\sigma\sigma}^c(k)\overline{Y}_{\sigma\sigma}^c(-k)}{D^c_{\sigma}(k)}, \quad \text{(73b)}\]

\[D_{\sigma}^c(k) = \left[ 1 - \tilde{\varepsilon}(k) A_{e\sigma}^c(k) \right] \left[ 1 - \tilde{\varepsilon}(-k) A_{e\sigma}^c(-k) \right]
\]

\[+ \tilde{\varepsilon}(k) \tilde{\varepsilon}(-k) Y_{e\sigma\sigma}^c(k) \overline{Y}_{\sigma\sigma}^c(-k), \quad \text{(73c)}\]

\[A_{e\sigma}^c(k) = G_{e\sigma}^0(k) + Z_{e\sigma}(k). \quad \text{(73d)}\]

These equations are identical in form with the Dyson equations for polaron superconductivity mediated by optical phonons\(^7\). The difference to the previous work is
related to the appearance of the renormalized energy $\tilde{\varepsilon}(k)$ and new correlation functions shown in Fig. 8. These irreducible functions depicted by rectangles are on-site quantities with equal site indices. Hence, all right-hand parts in Eq. 8 are proportional to $\delta_{x,x'}$ meaning that $Z_{e,\sigma}$ and $Y_{e,\sigma}$ are also local functions and corresponding Fourier representations to be independent of the polaron momentum $k$. In the diagrams $x$ and $i_{1}$ stand for $(x,\sigma,\tau, x') (i_{1},\sigma,\tau_{1})$, respectively, whereby summation over $i_{1}, i_{2}, j_{1}, j_{2}$ and $\sigma_{1}, \sigma_{2}$ and integration over $\tau_{1}$ and $\tau_{2}$ is assumed. These quantities have the following analytical structure:

\[
Z_{e}(x,\sigma,\tau|x',\sigma',\tau') = -\frac{1}{2}\delta_{x,x'} \sum_{j} V^{2}(x-j) \times \int_{0}^{\beta} d\tau_{1} d\tau_{2} \Gamma_{3}(\sigma,\tau;\sigma',\tau'|\tau_{1},\tau_{2}) n_{x,\tau} - \delta_{x,x'} \\
\times \sum_{\sigma_{1},\sigma_{2}} \sum_{ij} \int_{0}^{\beta} d\tau_{1} d\tau_{2} G_{2}^{0\varphi}[\sigma,\sigma;\tau_{1},\tau_{2}] F_{\sigma}'(i,\tau_{1},\tau_{2}) G_{e}(i,\sigma,\tau_{1} j, \sigma, \tau_{2}) - \delta_{x,x'} \\
\times \int_{0}^{\beta} d\tau_{1} d\tau_{2} G_{2}^{0\varphi}[\sigma,\tau;\sigma_{1},\tau_{2}] \phi(0|\tau_{1} - \tau_{2}) G_{p}(i,\sigma,\tau_{2} j, \sigma_{1}, \tau_{1}),
\]

(74)

\[
Y^{e}(x,\sigma,\tau|x',\sigma',\tau') = -\frac{1}{2}\delta_{x,x'} \sum_{\sigma_{1},\sigma_{2}} \sum_{i, j} \int_{0}^{\beta} d\tau_{1} d\tau_{2} G_{2}^{0\varphi}[\sigma,\tau;\sigma_{1},\tau_{2}] \tilde{f}(x-i_{1}) \tilde{f}(x-i_{2}) \\
\times F^{e}(i_{1},\sigma_{1},\tau_{1} | i_{2},\sigma_{2},\tau_{2}) - \frac{1}{2}\delta_{x,x'} \\
\times \sum_{\sigma_{1},\sigma_{2}} \sum_{i, j} G_{2}^{0\varphi}[\sigma,\tau;\sigma_{1},\tau_{2}] \tilde{f}(x-i_{1}) \\
\times \tilde{f}(x-i_{2}) F^{e}(i,\sigma_{1},\tau_{1} | i_{2},\sigma_{2},\tau_{2}) \phi(0|\tau_{1} - \tau_{2}) \\
\times \phi(0|\tau_{2} - \gamma),
\]

(75)

and corresponding Eq. for $Y_{e,\sigma}$. Since Eqs. (74) and (75) are the result of summing an infinite series of diagrams, the thin lined representing one-particle propagators are replaced by full normal electron ($G_{e}$) and polaron ($G_{p}$) and anomalous ($F_{\sigma}$) functions. Fourier transformation of these quantities leads in case of spin-singlet channel of superconductivity to

\[
Z_{e,\sigma}(i\omega) = -\frac{1}{2}\sum_{\omega_{1},K,\sigma_{1}} \tilde{\tilde{\varepsilon}}(k) \tilde{\tilde{\varepsilon}}(k) \\
\times G_{e,\sigma_{1},\sigma_{1}}(i\omega_{1}) G_{2}^{0\varphi}[\sigma,\omega_{1};\sigma_{1},i\omega_{1} | \sigma_{1},i\omega_{1}] - \frac{1}{\beta N} \sum_{k,\omega_{1},\Omega} \varepsilon^{2}(k) G_{e,\sigma_{1},\sigma_{1}}(k|i\omega_{1} + \Omega) \phi(i\Omega) \\
\times G_{2}^{0\varphi}[\sigma,\omega_{1};\sigma_{1},i\omega_{1} | \sigma_{1},i\omega_{1};\sigma_{1},i\omega_{1}],
\]

(76)

\[
Y_{e,\sigma}(i\omega) = -\frac{1}{2\beta N} \sum_{k,\omega_{1},\sigma_{1}} \tilde{\tilde{\varepsilon}}(k) \tilde{\tilde{\varepsilon}}(k) F_{e,\sigma_{1},-\sigma_{1}}(k|i\omega_{1}) \\
\times G_{2}^{0\varphi}[\sigma,\omega_{1};-\sigma,-i\omega_{1} | \sigma_{1},i\omega_{1};-\sigma_{1},-i\omega_{1}] \\
- \frac{1}{2N} \sum_{\sigma_{1},K} \sum_{\omega_{1},\Omega_{1},\Omega_{2}} \tilde{\tilde{\varepsilon}}(k) \tilde{\tilde{\varepsilon}}(k) \\
\times F_{e,\sigma_{1},-\sigma_{1}}(k|i\omega_{1},\Omega_{1} + \Omega_{2}) \phi(i\Omega_{1}) \phi(i\Omega_{2}).
\]
× \tilde{G}_{2}^{\sigma}[\sigma, \omega; \omega_{1}, \omega_{2}] = \frac{\beta U^{2}[1 - \delta_{\omega, \omega_{1}}(1 + e^{\beta \mu})(e^{\beta \mu} + e^{\beta(2\mu - U)})]}{Z_{0}^{2} \lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{2})}, \quad (80a)

\tilde{G}_{2}^{\sigma}[\sigma, \omega; \sigma, \omega_{1}, \omega_{2}] = \frac{U}{Z_{0}} \left\{ \frac{\beta U e^{2\beta \mu}(e^{\beta U} - 1)}{Z_{0} \lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{1})} - \frac{\beta U e^{2\beta \mu} \delta_{\omega, \omega_{1}}}{\lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{1})} \right\} - \frac{(e^{\beta(2\mu - U)} - 1)[\lambda(\omega) + \lambda(\omega_{1})]}{[\lambda(\omega) + \lambda(\omega_{1})]^{2} \lambda(\omega) \lambda(\omega_{1})} \left[ \frac{1}{\lambda(\omega) \lambda(\omega_{1})} \times \left( \frac{1}{\lambda(\omega)} + \frac{1}{\lambda(\omega_{1})} \right) \right] - \frac{2}{\lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{1})} \right\}, \quad (80b)

\tilde{G}_{2}^{\sigma}[\sigma, \omega; -\sigma, -\omega_{1}, -\sigma, -\omega_{1}] = \frac{U}{Z_{0}} \left\{ \frac{\beta U}{\lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{1})} \right\} - \frac{(e^{\beta(2\mu - U)} - 1)[\lambda(\omega) - \lambda(\omega_{1})]}{[\lambda(\omega) - \lambda(\omega_{1})]^{2} \lambda(\omega) \lambda(\omega_{1})} \left[ \frac{1}{\lambda(\omega) \lambda(\omega_{1})} \times \left( \frac{1}{\lambda(\omega)} - \frac{1}{\lambda(\omega_{1})} \right) \right] - \frac{2}{\lambda(\omega) \lambda(\omega_{1}) \lambda(\omega_{2}) \lambda(\omega_{1})} \right\}, \quad (80c)

where \delta_{\omega, \omega_{1}} is the Kronecker symbol for Matsubara frequencies and

\[ Z_{0} = 1 + 2 e^{\beta \mu} + e^{\beta(2\mu - U)} \]
\[ \lambda(\omega) = i \omega + \mu, \quad \lambda(\omega_{1}) = i \omega + \mu - U, \quad \sigma = -\sigma. \quad (81) \]

For the present study \mu and U in Eqs. (80a-c) and (81) have to be replaced by the renormalized quantities of Eq. (13). The foregoing equations are generalized Eliashberg equations of strong-coupling superconductivity for the case that strong electron correlations have been taken into account in a self-consistent way. In spite of the approximations involved the equations are rather complicated. In order to gain further insight into the physics behind Eqs. (77) and (79), we will linearize the equations in terms of the order parameter \textbf{Y}_{\sigma,\sigma'}, but not in terms of \Lambda_{\sigma}. Then the critical temperature \textbf{T}_{c} of the superconducting transition can be obtained from
\[
Y_{\sigma_1,\sigma_2}(i\omega) = -\frac{1}{\beta N} \sum_{k} \left[ \frac{\tilde{\varepsilon}(k) \tilde{\varepsilon}(-k) G^0_{\sigma_1}(i\omega) \tilde{G}^0_{\sigma_2}[\sigma, i\omega; \sigma, -i\omega]}{[1 - \tilde{\varepsilon}(k) \Lambda_{\sigma_1}(i\omega)][1 - \tilde{\varepsilon}(-k) \Lambda_{\sigma_2}(-i\omega)]} \right]
\]
\[
- \frac{1}{\beta N} \sum_{k} \frac{1}{2} \sum_{\Omega_1, \Omega_2} \left[ \frac{\tilde{\varepsilon}(k) \tilde{\varepsilon}(-k) Y_{\sigma_1,\sigma_2}(i(\omega_1 - \Omega_1 + \Omega_2)) \phi(i\Omega_1) \phi(i\Omega_2) \tilde{G}^0_{\sigma_1}[\sigma, i\omega; \sigma, -i\omega]}{[1 - \tilde{\varepsilon}(k) \Lambda_{\sigma_1}(i\omega - i\Omega_1 + i\Omega_2)][1 - \tilde{\varepsilon}(-k) \Lambda_{\sigma_2}(-i\omega + i\Omega_1 - i\Omega_2)]} \right].
\]

(82)

\[
\Lambda_{\sigma}(i\omega) = G^0_{\sigma}(i\omega) - \frac{1}{2} V_{\text{nn}} 2 e^2 \Gamma_{\sigma,\sigma}(i\omega) - \frac{1}{\beta N} \sum_{k,\omega_1,\sigma_1} \frac{\tilde{\varepsilon}^2(k) \Lambda_{\sigma\sigma}(i\omega_1) \tilde{G}^0_{\sigma_1}[\sigma, i\omega; \sigma, i\omega_1; \sigma, i\omega]}{1 - \tilde{\varepsilon}(k) \Lambda_{\sigma\sigma}(i\omega)} \tilde{G}^0_{\sigma_2}[\sigma, i\omega; \sigma, i\omega_1; \sigma, i\omega].
\]

(83)

In order to determine \( T_c \) it is necessary to solve Eq. (83) for \( \Lambda_{\sigma}(i\omega) \) and to insert it into Eq. (82). Because electron pairing is more important than polaron pairing, we will not discuss here corresponding results for the polaronic function \( \Lambda_{\sigma}(i\omega) \).

A further reasonable approximation is to replace in Eq (83) the propagator of the phonon field, \( \phi(i\Omega_1) \), by its average value leading to a shift of the energy denominator by \( \pm \hbar \omega_c \). Since \( \hbar \omega_c \) is larger than other typical energies involved, the average value of the energy denominator is moderate coupling strength smaller than all other terms in Eq. (83) and can therefore be omitted, which leaves

\[
\Lambda_{\sigma}(i\omega) = G^0_{\sigma}(i\omega)
\]
\[
- \frac{1}{\beta N} \sum_{k,\omega_1} \frac{\tilde{\varepsilon}^2(k) \Lambda_{\sigma\sigma}(i\omega_1) \tilde{G}^0_{\sigma_1}[\sigma, i\omega; \sigma, i\omega_1; \sigma, i\omega]}{1 - \tilde{\varepsilon}(k) \Lambda_{\sigma\sigma}(i\omega)} \tilde{G}^0_{\sigma_2}[\sigma, i\omega; \sigma, i\omega_1; \sigma, i\omega].
\]

(84)

where

\[
G^0_{\sigma}(i\omega) = G^0_{\sigma}(i\omega) - \frac{1}{2} V_{\text{nn}} 2 e^2 \Gamma_{\sigma,\sigma}(i\omega).
\]

(85)

Equation (84) is identical with the corresponding equation for the single band Hubbard model without phonons if we replace in Eq. (84) the renormalized quantities \( \mu, U, \tilde{\varepsilon}(k) \) and \( G^0_{\sigma}(i\omega) \) by the initial quantities \( \mu_0, U_0 \) and \( \varepsilon(k) \). This means that we have reduced the influence of superconductivity in frame of the Hubbard-Holstein model to the analogous problem with respect to the single band Hubbard model.

It is instructive to analyze the contributions from the two spin channels by considering the quantities

\[
\chi_\uparrow(i\omega) = \frac{1}{\beta N} \sum_{\omega_1} \sum_\mathbf{k} \frac{[\tilde{\varepsilon}(k) \Lambda_{\sigma}(i\omega_1)]}{1 - \tilde{\varepsilon}(k) \Lambda_{\sigma}(i\omega)}
\]

(80a-b)

and using the notation

\[
\phi_\sigma^0(i\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{[\tilde{\varepsilon}(k) \Lambda_{\sigma}(i\omega)]}{1 - \tilde{\varepsilon}(k) \Lambda_{\sigma}(i\omega)} \phi(k).
\]

(87)

Here it is assumed that \( \varepsilon(k) = -\tilde{\varepsilon}(-k) \) holds with \( \sum_k \varepsilon(k) = 0 \). We replace sums by integrals,

\[
\rho_0(\tilde{\varepsilon}) = \frac{4}{\pi W} \sqrt{1 - (2\tilde{\varepsilon}/W)^2} \times \left\{ \begin{array}{ll}
1, & |\tilde{\varepsilon}| \leq \tilde{W}/2 \\
0, & |\tilde{\varepsilon}| > \tilde{W}/2
\end{array} \right.
\]

(89)

\( \tilde{W} \) is the renormalized band width \( \tilde{W} = W e^{-W} \) and \( \rho_0 \) the semieliptic model density of states. Since we do not consider magnetic solutions, the spin index can be omitted.

Making use of (80a-b) for the irreducible functions we obtain

\[
\chi_\uparrow(i\omega) = \frac{\beta U^2 (1 + e^{\beta \mu}) (e^{\beta \mu} + e^{\beta(2\mu - U)})}{Z_\uparrow^0 \chi(i\omega) \chi(i\omega)} \times \left\{ \begin{array}{ll}
\phi^\uparrow(i\omega) - \phi^\downarrow(i\omega) \\
\beta \lambda(i\omega) \chi(i\omega)
\end{array} \right.,
\]

(90a)

\[
\chi_\downarrow(i\omega) = \frac{U}{Z_0} \left\{ \begin{array}{ll}
- 2(\mu - U)(e^{\beta(2\mu - U)} - 1) \phi_\uparrow^0(i\omega) \\
\beta(2\mu - U)[\lambda^2(i\omega) \chi(i\omega)]^2
\end{array} \right.
\]

- \frac{U e^{\beta \mu} \phi_\uparrow^0(i\omega) + (1 + e^{\beta \mu}) U \phi_\downarrow^0(i\omega)}{[\lambda(i\omega) \chi(i\omega)]^2}

(90b)
\[
\begin{align*}
+ \left[ \beta U e^{2\beta \mu (e^{-\beta U} - 1)} \right] \\
\times \left\{ \frac{1}{\lambda(i\omega)} \right. \\
&\left. \left[ \frac{\phi^\epsilon(i\omega)}{\lambda(i\omega)} \right] - \frac{1 + e^{\beta \mu}}{\lambda^2(i\omega)} \right\},
\end{align*}
\]

where

\[
\phi = \frac{1}{\beta} \sum_{w_1} \frac{\phi^\epsilon(i\omega)}{\lambda(i\omega)},
\]

\[
\bar{\phi}_1 = \frac{1}{\beta} \sum_{w_1} \phi^\epsilon(i\omega) \left( \frac{1}{\lambda(i\omega)} - \frac{1}{\lambda^2(i\omega)} \right)^2,
\]

\[
\gamma_0(i\omega) = \frac{1}{\beta} \sum_{w_1} \frac{\lambda(i\omega) + \lambda(i\omega) \psi_{w+w_1} 0 \phi^\epsilon(i\omega)}{\lambda(i\omega)},
\]

and \( \psi_{w+w_1,0} = 1 - \delta_{w+w_1,0} \). In case of half filling when \( \mu = U/2, \lambda(i\omega) = i\omega + \mu, \lambda(i\omega) = i\omega - \mu \), we have the antisymmetry property, \( \phi^\epsilon(-i\omega) = -\phi^\epsilon(i\omega) \), and therefore \( \phi = \phi_1 = 0 \). Furthermore, we find at half filling,

\[
\chi_+(i\omega) = - \frac{\mu^2 \phi^\epsilon(i\omega)}{[i\omega]^2 - \mu^2},
\]

\[
\chi_-(i\omega) = - \frac{2\mu \phi^\epsilon(i\omega)}{[i\omega]^2 - \mu^2} = 2\chi_+(i\omega),
\]

and therefore Eq. (84) is equal to

\[
\chi_+(i\omega) + \chi_-(i\omega) = 3\chi_+(i\omega).
\]

Away from half filling we will for simplicity omit the contribution of the anti-parallel spin channel in Eq. (84) and introduce instead a correction factor \( f_\sigma \), which is three at half filling and different from three at general filling. The final equation to be investigated is then

\[
\Lambda_{\sigma\sigma}(i\omega) = G_V(i\omega)
\]

\[
- \frac{f_\sigma}{\beta N} \sum_{k,\omega} \frac{[\varepsilon(k)]^2 \Lambda_\sigma(i\omega)}{1 - \varepsilon(k) \Lambda_\sigma(i\omega)} \times G_2^{0,1r}[\sigma, i\omega; \sigma, i\omega][\sigma, i\omega; \sigma, i\omega].
\]

Further simplifications can be made regarding Eq. (82) for the critical temperature. We note that the main contribution to the last term results from the minimum values of frequency difference \( \Omega_1 - \Omega_2 \). When \( \Omega_1 = \Omega_2 \) we get after summing over \( \Omega_1 \):

\[
\frac{1}{\beta \hbar \omega_c} \sum_{\Omega_1} [\phi(\Omega_1)]^2 = \frac{1}{\beta \hbar \omega_c} \coth \frac{1}{2} \beta \hbar \omega_c + \frac{1}{2 \sinh^2 \frac{1}{2} \beta \hbar \omega_c},
\]

so that

\[
f_c = 1 + \frac{1}{\beta \hbar \omega_c} \coth \frac{1}{2} \beta \hbar \omega_c + \frac{1}{2 \sinh^2 \frac{1}{2} \beta \hbar \omega_c}
\]

can be used as a common factor in the remaining function for the superconducting order parameter, which is

\[
Y_{\sigma,\sigma}(i\omega) = - \frac{f_c}{\beta N} \sum_{k,\omega} \frac{\varepsilon(k) \varepsilon(-k) Y_{\sigma,\sigma}(i\omega)}{[1 - \varepsilon(k) \Lambda_\sigma(i\omega)][1 - \varepsilon(-k) \Lambda_\sigma(-i\omega)]}.
\]

In order to solve Eq. (97) for \( T_c \), we introduce a new function,

\[
\phi^{\infty}(i\omega) = \frac{1}{N} \sum_k \frac{\varepsilon(k) \varepsilon(-k)}{[1 - \varepsilon(k) \Lambda_\sigma(i\omega)][1 - \varepsilon(-k) \Lambda_\sigma(-i\omega)]} = \frac{\phi^\epsilon(i\omega) - \phi^\epsilon(-i\omega)}{\Lambda_\sigma(i\omega) - \Lambda_\sigma(-i\omega)},
\]

which allows to rewrite Eq. (97) in the form

\[
Y_{\sigma,\sigma}(i\omega) = - \frac{f_c}{\beta N} \sum_{w_1} \phi^{\infty}(i\omega_1) Y_{\sigma,\sigma}(i\omega_1) \times \tilde{G}_2^{0,1r}[\sigma, i\omega; \sigma, -i\omega][\sigma, i\omega_1; \sigma, -i\omega_1].
\]

Using furthermore

\[
\psi_1 = \frac{1}{\beta} \sum_{\omega} \frac{\phi^\epsilon(i\omega) Y_{\sigma,\sigma}(i\omega)}{[\mu^2 - (i\omega)^2]},
\]

\[
\psi_2 = \frac{1}{\beta} \sum_{\omega} \frac{\phi^\epsilon(i\omega) Y_{\sigma,\sigma}(i\omega)}{[\mu - U]^2 - (i\omega)^2},
\]

\[
\zeta = \frac{U^2 f_c}{Z_0} \left\{ e^{\beta \mu} \frac{\phi^{\infty}(i\omega)}{Z_0} \right\},
\]

\[
Q(i\omega) = 1 + \frac{[\mu^2 - (i\omega)^2][\mu - U]^2}{[\mu^2 - (i\omega)^2][\mu - U]^2 - i\omega^2}],
\]

allows to obtain the solution:

\[
Y_{\sigma,\sigma}(i\omega) = - \frac{U f_c [1 + U/(2\mu - U)][1 + e^{\beta \mu}] \psi_1}{Q(i\omega)[\mu^2 - (i\omega)^2]}.
\]
\[ \rho(E) = -\frac{1}{\pi} \text{Im} g(E + i0^+), \]
\[ g(i\omega_n) = \frac{1}{N} \sum_k \frac{\Lambda(i\omega_n)}{1 - \varepsilon(k) \Lambda(i\omega_n)}. \]

where \( \Lambda(i\omega_n) \) has to be calculated from Eq. (94). The integration over \( k \) is again done by using the semieliptical form of model density of states in Eq. (89). This gives for the quantities (87) and (107b) the following result:\n
\[ \phi^*(i\omega) = \frac{1}{2} \tilde{W} \phi^*(i\omega), \]
\[ \phi^*(i\omega) = (1 - [1 - \tilde{\Lambda}^2(i\omega)]^{1/2})/\tilde{\Lambda}(i\omega), \]
\[ \tilde{\Lambda}(i\omega) = \frac{1}{2} \tilde{W} \Lambda(i\omega), \]

yielding for the renormalized density of states (DOS) in Eq. (107a)

\[ \rho(E) \equiv \frac{4 \pi r(E)}{\pi \tilde{W}} = -\frac{4}{\pi \tilde{W}} \text{Im} \left[ 1 - \sqrt{1 - \tilde{\Lambda}^2(E)} \right] / \Lambda(E), \]

where \( \tilde{\Lambda}(E) \) is the analytical continuation of \( \tilde{\Lambda}(i\omega_n) \).

We now address Eq. (94) which determines the normal state of the system. By Using (90a) and (108) we rewrite it in the form:

\[ \tilde{\Lambda}(i\omega) = \frac{1}{2} \tilde{W} G^v(i\omega) - \frac{1}{2} f_s \tilde{W} \chi_+ (i\omega), \]

with \( \chi_+ (i\omega) \) given by Eq. (90a). In the limit \( E \to 0 \) Eq. (111) becomes

\[ \tilde{\Lambda} \left[ 1 - \frac{\tilde{\Lambda}^2}{\Lambda^2} \left( 1 - \sqrt{1 - \tilde{\Lambda}^2} \right)^2 \right] = b, \]

where \( \tilde{\Lambda} = \Lambda(E + i\delta) \) for \( E = 0 \). The two parameters \( a \) and \( b \) and the function \( G^v(0) \) are given by

\[ a^2 = \frac{4 f_s \tilde{W}^2 T^2 (1 + e^{\beta \mu})(e^{\beta \mu} + e^{\beta(2\mu-U)})}{2 \pi Z_0^2 \mu^2 (\mu-U)^2}, \]
\[ b = \frac{1}{2} \tilde{W} G^v(0) - \frac{1}{2} f_s \]
\[ \times \frac{\beta \tilde{W} U^2 (1 + e^{\beta \mu})(e^{\beta \mu} + e^{\beta(2\mu-U)})}{\mu (\mu-U) Z_0^2} \phi, \]

\[ G^v(0) = \frac{1 - \tilde{\pi}_T}{\mu} + \tilde{\pi}_T \]
\[ - \frac{\tilde{\pi}^2 V_0 \beta}{\mu^2} \left[ 1 + \frac{\beta \mu}{1 + e^{\beta \mu}} \right] (1 - \tilde{\pi}), \]
\[ \tilde{\pi} = 2 \tilde{\pi}_T, \]
with \( \bar{\phi} \) given by Eq. (91). The first term in Eq. (113c) is the value of the local one-particle Green's function of the Hubbard model for \( E = 0 \) while the second term is the corresponding contribution from the inter-site Coulomb interaction discussed in Appendix B, see (B16).

Equation (112) has been discussed for the simpler case of half filling when \( b = 0 \) in Refs. 17 and 27. Away from half filling we have \( \bar{\mu} \neq 1, \mu \neq U/2 \) and \( b \neq 0 \). As Eq. (113a-b) show, the parameters \( a \) and \( b \) depend on chemical potential \( \mu \), strong-coupling parameter \( U \) and mean electron number per lattice site \( \bar{\mu} \). Moreover, \( b \) depends on the inter-site Coulomb repulsion. Although parameters \( a \) and \( b \) are not independent of each other, we first try to get information in case that \( b = 0 \), i.e., for \( \bar{\phi} = G^R(\nu) = 0 \), which holds for \( \Lambda(-i\omega) = -\Lambda(i\omega) \). In the half-filled band case when \( \mu = U/2 \) and \( \bar{\mu} = 1 \), the quantity \( a \) is equal to

\[
a = \sqrt{f_s W/U}, \quad f_s = 3, \tag{114}
\]

which allows to determine \( \Lambda \) in Eq. (112) from a simpler relation,

\[
1 - a \left(1 - \frac{1}{\bar{\Lambda}^2} \right) \left[ 1 + a \left(1 - \frac{1}{\bar{\Lambda}^2} \right) \right] = 0.
\tag{115}
\]

For \( a > 1 \) the first factor gives \( \bar{\Lambda}^2 = a(2 - a) \) and hence,

\[
\bar{\Lambda} = \pm \sqrt{a(2 - a)}, \quad a < 2, \tag{116a}
\]

\[
\bar{\Lambda} = \pm i \sqrt{a(2 - a)}, \quad a > 2. \tag{116b}
\]

By inserting these solutions in Eq. (109) for the renormalized DOS we obtain results different from zero only for the expression with lower sign in Eq. (116b), i.e., for \( a > 2 \). Hence we obtain a metallic state at half filling only if the Coulomb interaction is less than a critical value \( \bar{W} \)

\[
U < U_c, \quad U_c = \frac{1}{3} \sqrt{3} \bar{W}. \tag{117}
\]

In this case there is no gap at the Fermi level and the renormalized DOS becomes \( a > 2 \)

\[
\rho(0) = \frac{4}{\pi \bar{W}} r(0), \quad r(0) = \sqrt{a(a - 2)/a} \tag{118}
\]

The insulating (dielectric) phase exists if the inverse condition holds, \( a < 2 \), \( U > U_c \), leading to the opening of an energy gap at the Fermi level.

Away from half-filling, for \( a > 2 \) and \( b \) sufficiently small, the solution of Eq. (112) can be obtained from a series expansion in powers of \( b \)

\[
\bar{\Lambda}_b = \bar{\Lambda} + \frac{(1 - b)(a - 2)}{2(a - 2)} + \frac{(a^2 - 5a + 3)b^2}{8\Lambda(a - 1)(a - 2)^2} + \ldots \tag{119}
\]

where \( \bar{\Lambda} \) is given by Eq. (116) in zero-order approximation. This leads to

\[
r(0) = \sqrt{a(a - 2) + \frac{(2a^3 - 8a^2 + 12a - 5)b^2}{8a^{3/2}(a - 1)^2(a - 2)^{3/2}} + \ldots} \tag{120}
\]

This result shows that not \( b \) but \( b/(a - 2) \) should be taken as expansion parameter. Therefore the expansion is not correct very close to \( a = 2 \). Another peculiarity of Eq. (120) is its even character in \( b \), which follows from the fact that in the solution of Eq. (112), \( \tilde{\Lambda} \), changes sign when the sign of \( b \) is changed. Therefore, if we have the solutions \( \Lambda_1 \pm i\Lambda_2 \) of Eq. (112), then correspondingly \( -\Lambda_1 \mp i\Lambda_2 \) are solutions for \( b < 0 \). The different signs of the real parts do not matter since Eq. (110) depends only on the absolute value of \( \Lambda_1 \). The numerical investigation shows that for \( a > 2 \) the role of \( b \) is not decisive, i.e., the system remains metallic. However, in the range \( 0 < a < 2 \), for which the system is insulating when \( b = 0 \), the influence of \( b \) is decisive because there exists a critical value, \( b_c(a) \approx 1 - a/2 \), such that the system is metallic for \( |b| > b_c \) and insulating for \( |b| < b_c \). Note that there is no critical value \( b_c \) if we take \( a \) and \( b \) to be independent of each other.

The metallic state exists for low and high band filling (small and large values of \( \mu \)) and near half filling, \( \mu \approx U/2 \), provided that \( U < U_c \). The physical role of \( b \) is to enhance in each case the tendency towards metallicity. There is also the case of reappearance of the metallic phase for \( a < 2 \) and \( |b| > b_c(a) \). The variation of \( b_c(a) \) is shown in Fig. 9.

![FIG. 9: Variation of the critical parameter \( b_c(a) \) in the range \( 0 < a < 2 \). For \( |b| > b_c \), the system is metallic while it is insulating for \( |b| < b_c \). For \( a > 2 \) the system is metallic regardless of the value of \( b \).](image-url)
The two limits coincide for \( a = 2 \). But this does not correspond to the low-energy limit. Because of the fast convergence of the sums in Eq. (104) which contain \( \phi^\infty(i\omega) \) and which determine the parameters \( \eta_{ij} \) of Eq. (105), we can rewrite \( \eta_{ij} \) as

\[
\eta_{11} = \frac{U\phi^\infty}{\beta} \sum_{\omega} \frac{(d^2 - z^2)}{Q_1(z)(c^2 - z^2)} \\
= \frac{U\phi^\infty}{\beta} [I_1 + I_2(c^2 - d^2)], \tag{123a}
\]

\[
\eta_{22} = \frac{U\phi^\infty}{\beta} \sum_{\omega} \frac{(c^2 - z^2)}{Q_1(z)(d^2 - z^2)} \\
= \frac{U\phi^\infty}{\beta} [I_1 - I_3(c^2 - d^2)], \tag{123b}
\]

\[
\eta_{12} = \frac{U\phi^\infty}{\beta} \sum_{\omega} \frac{1}{Q_1(z)} = \frac{U\phi^\infty}{\beta} I_1, \tag{123c}
\]

where

\[
I_1 = \frac{1}{\beta} \sum_{\omega} \frac{1}{Q_1(z)}, \tag{124a}
\]

\[
I_2 = \frac{1}{\beta} \sum_{\omega} \frac{1}{Q_1(z),(z^2 - c^2)}. \tag{124b}
\]

\[
I_3 = \frac{1}{\beta} \sum_{\omega} \frac{1}{Q_1(z),(z^2 - d^2)}, \tag{124c}
\]

\[
Q_1(z) = (z^2 - c^2)(z^2 - d^2) + \zeta \phi^\infty, \tag{124d}
\]

and

\[
\zeta \phi^\infty = \frac{\mu}{2} (\mu - U)^2 \left[ \frac{Z_0 e^{\beta \mu} + e^{2\beta \mu}(1 - e^{-\beta U})}{f_0(e^{\beta \mu} + 1)(e^{\beta \mu} + e^{\beta(2\mu - U)})} \right],
\]

\[
c^2 = \mu^2, \quad d^2 = (\mu - U)^2, \quad z = i\omega_n. \tag{125}
\]

In case that \( U > 0 \) the quantity \( \zeta \phi^\infty \equiv \gamma^4 \) is positive. In the other case of very strong electron-phonon interaction we have \( U < 0 \). In this case we will use the notation \( \zeta \phi^\infty = -\theta^4 \) (with negative \( \zeta \)). Although \( U < 0 \) seems not to be the generic case, we believe that in the metallic phase in case of strong electron-phonon interaction an effective attractive interaction is possible, because the local and intersite Coulomb interaction can be largely screened by the electron-ion interaction. However, calculation of self-consistent screening in not the aim of this paper. We just require charge neutrality and take \( U \) as a parameter which allows to discuss the case of effective repulsive as well as attractive interactions. We first discuss the case \( U > 0 \) and then \( U < 0 \).

The sums in \( I_n \) have been evaluated by contour integration with the help of Poisson's formula, see Eq. (C2). For the case \( \gamma^4 > (c^2 - d^2)^2/4 \) we obtain the following equation which determines \( T_c \):

\[
0 = 1 + \frac{f_c U\phi^\infty}{2\gamma^4 \sqrt{\gamma^4 + c^2 d^2}} \left\{ \frac{2\gamma^4 - (c^2 - d^2)^2}{4\gamma^4 - (c^2 - d^2)^2} \left[ 1 + \frac{U(1 - e^{\beta(2\mu - U)})}{Z_0(2\mu - U)} \right] \right\} \frac{\alpha_2 \sinh \beta \alpha_1 - \alpha_1 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \\
+ \left[ \frac{U + (2\mu - U)(1 - e^{\beta(2\mu - U)})}{Z_0} \right] \frac{\alpha_1 \sinh \beta \alpha_1 + \alpha_2 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \\
+ \left[ \frac{\tanh \frac{1}{2} \beta d}{d} \left( \frac{\mu}{Z_0} \right) \left( e^{\beta \mu} + e^{\beta(2\mu - U)} \right) - \frac{\mu \tanh \frac{1}{2} \beta c}{c Z_0} (1 + e^{\beta \mu}) \right] 2U \sqrt{\gamma^4 + c^2 d^2} \\
+ \frac{f_c U^2 \mu(\mu - U)(U\phi^\infty)^2(1 + e^{\beta \mu})(e^{\beta \mu} + e^{\beta(2\mu - U)})}{\gamma^4 Z_0} \sqrt{\gamma^4 + c^2 d^2} \left\{ \frac{2\gamma^4 - (c^2 - d^2)^2}{4\gamma^4 - (c^2 - d^2)^2} \right\} \frac{1}{(c^2 - d^2)} \frac{\alpha_2 \sinh \beta \alpha_1 - \alpha_1 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \\
\times \left\{ \frac{\tanh \frac{1}{2} \beta d}{d} - \frac{\tanh \frac{1}{2} \beta d}{c} \right\} \frac{\alpha_2 \sinh \beta \alpha_1 - \alpha_1 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} - \frac{\sinh^2 \beta \alpha_1 + \sin^2 \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2}^{\gamma^2} \right\} \\
\times \left\{ \frac{\tanh \frac{1}{2} \beta d}{d} + \frac{\tanh \frac{1}{2} \beta d}{c} \right\} \frac{\alpha_1 \sinh \beta \alpha_1 + \alpha_2 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \right\}, \tag{126}
\]

where the parameters \( \alpha_1 \) and \( \alpha_2 \) are given by Eq. (C3).

For the special case of half filling when \( \mu = U/2 > 0 \) and

\[
c^2 = d^2 = \mu^2 = (U/2)^2, \quad \phi^\infty = \frac{1}{3} \mu^2,
\]

\[
\gamma^4 = f_c \left( \frac{\mu^4 (e^{\beta \mu} - \frac{1}{3})}{e^{\beta \mu} + 1} \right) > 0,
\]

Eq. (126) is of simpler form.
\[ 0 = 1 + \frac{f_c \mu^5}{3 \gamma^4 \mu^2 \mu} \left\{ \gamma^2 \left(1 - \frac{\beta \mu}{e^{\beta \mu} + 1} \right) \frac{\alpha_2 \sinh \beta \alpha_1 - \alpha_1 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} + 4 \frac{\alpha_1 \sinh \beta \alpha_1 + \alpha_2 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \right\} - \frac{4 \sqrt{\gamma^4 + \mu^4} \tanh \frac{1}{2} \beta \mu}{\mu} + \frac{4 \beta^2 \mu^{10}}{9 \gamma^4 \mu^4} \left\{ \frac{\sinh^2 \beta \alpha_1 + \sin^2 \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} + \frac{\sqrt{\gamma^4 + \mu^4}}{\mu^2} \tanh^2 \frac{1}{2} \beta \mu \right\} + \frac{\gamma^2}{2 \mu} \frac{d}{d \mu} \frac{\tanh \frac{1}{2} \beta \mu}{\mu} \left( \frac{\alpha_2 \sinh \beta \alpha_1 - \alpha_1 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} - \frac{2}{\mu} \tanh \frac{1}{2} \beta \mu \frac{\alpha_1 \sinh \beta \alpha_1 + \alpha_2 \sin \beta \alpha_2}{\cosh \beta \alpha_1 + \cos \beta \alpha_2} \right), \] (128)

where
\[ \alpha_1 = \frac{1}{\sqrt{2}} \left( \sqrt{\gamma^4 + \mu^4} + \mu^2 \right)^{1/2}, \] (129)

If we consider at half filling in addition $$\beta \mu \gg 1$$ and $$\beta \omega_c \gg 1$$ we get $$\gamma^4 = \mu^4$$ and $$f_c = 1$$ and instead of Eq. (129) we obtain
\[ \alpha_1 = \frac{\mu}{\sqrt{2}} \left( \sqrt{2} \pm 1 \right)^{1/2}, \] (130)

and Eq. (128) for $$T = T_c$$ becomes
\[ \beta \mu e^{-\beta \mu} + 1 + 2 \sqrt{2} + 1 \left( 1 + 2 \sqrt{2} + 2 \sqrt{2} + 1 \right) = 0, \] (131)

In the following we will discuss the opposite case, i.e., $$\zeta \phi^c \leq \left( \epsilon^2 - d^2 \right)^2 / 4$$, which includes the possibility to consider the negative values of $$\zeta$$ and hence $$\zeta \phi^c = -\theta^4 < 0$$. This case corresponds to $$U < 0$$. The corresponding equation for $$T_c$$ is then

\[ 0 = 1 - f_c U \phi^c \left( \frac{(\epsilon^2 - d^2)^2 + 2 \theta^4}{\sqrt{(\epsilon^2 - d^2)^2 + 4 \theta^4}} \right) 1 - \frac{U (e^{(2 \mu - U)} - 1)}{U (2 \mu - U)} \left( \frac{\tanh \beta z_1 \tanh \beta z_2}{z_1} \right) \]
\[ + U \left( \frac{(2 \mu - U)(1 - e^{(2 \mu - U)})}{Z_0 (2 \mu - U)} \right) \left( \frac{\tanh \beta z_1}{z_1} + \frac{\tanh \beta z_2}{z_2} \right) \]
\[ + 4 U \left( \frac{(\mu - U) \tanh \beta d (e^{(\mu - U)} - 1)}{Z_0} \right) \mu e^{(\mu - U)} (1 + e^{(2 \mu - U)}) \left( \frac{\tanh \beta z_1}{z_1} + \frac{\tanh \beta z_2}{z_2} \right) \]
\[ + f_c^2 U^4 \frac{(\mu - U)(d^2)^2 + 2 \theta^4}{2 \theta^4 Z_0^2} \left( \frac{\tanh \beta z_1}{z_1} + \frac{\tanh \beta z_2}{z_2} \right) \]
\[ - 2 \left( \frac{\tanh \beta z_1 \tanh \beta z_2}{z_1} \right) \left( \frac{\tanh \beta d}{d} \right) \frac{1}{(c^2 - d^2)} \]
\[ \times \left( \frac{\tanh \beta d}{d} \right) \left( \frac{\tanh \beta z_1}{z_1} - \frac{\tanh \beta z_2}{z_2} \right) \left( \frac{c^2 - d^2)^2 + 2 \theta^4}{(c^2 - d^2)^2 + 4 \theta^4} \right), \] (132)

where
\[ z_1 = \frac{1}{\sqrt{2}} \left( c^2 + d^2 \pm \sqrt{(c^2 - d^2)^2 + 4 \theta^4} \right)^{1/2}. \] (133)

For half filling, $$U < 0$$ and $$\theta^4 < c^2 d^2$$ we have
\[ \zeta \phi^c = -\theta^4 = -\frac{1}{2} f_c \mu^4 \frac{1 - 3 e^{-\beta U/2}}{1 + e^{-\beta U/2}} \] (134)
for sufficiently large $$|U|$$, i.e., $$\ln |U/\beta| > \ln 9$$. 

\[ \]
In case of very small $\theta$ values corresponding to the condition
\[ \ln \beta |\mu| = \ln (\beta \frac{1}{2} |U|) \geq \ln 3 \]  
(135)

Eq. (132) simplifies to ($\theta \to 0$),
\[ 1 - f_c \theta \mathcal{G} \left\{ A_1 \left( 1 - \frac{\beta \mu}{1 + e^{\beta \mu}} \right) + 4 \mu^2 A_2 \right\} - 4 f_c^2 \mu \theta (\phi^2)^2 (A_1 A_3 - A_2^2) = 0, \]  
(136)

where
\[ A_n = \frac{1}{n!} \left( \frac{\tanh \frac{1}{2} \beta \mu}{\mu} \right)^n. \]  
(137)

Because $\beta |\mu|$ is assumed to be larger than 3, the coefficients in Eq. (137) can be approximated by
\[ A_1 \approx \frac{1}{2 |\mu|^3}, \quad A_2 \approx \frac{3}{8 |\mu|^2}, \quad A_3 \approx \frac{5}{16 |\mu|^2}, \]  
(138)

allowing to replace Eq. (136) by
\[ 1 + f_c \frac{1}{3} - \frac{f_c^2}{144} - f_c \beta |\mu| = 0. \]  
(139)

For negative chemical potential, $\mu < 0$, and $f_c = 1 + 1/(\beta \omega_c)$ the equation for the critical temperature has the simple form:
\[ \beta^3 - 46 \beta^2 + (24 y - 191) \beta + 24 y = 0, \]  
(140)

with
\[ t = \frac{k_B T_c}{\hbar \omega_c} \text{, } y = \frac{|\mu|}{\hbar \omega_c}. \]  
(141)

yielding for small $t$ the solution,
\[ t \approx \frac{y}{1 - y} - \frac{46}{191} \frac{y^2}{(1 - y)^3}, \]  
(142)

where
\[ y = \frac{24}{191}, \]  
(143)

with the requirement that $\gamma \ll 1$ is fulfilled. In the simplest approximation $T_c$ is of the order,
\[ k_B T_c \approx \frac{24}{191} |\mu|, \]  

showing that $T_c$ is proportional to the renormalized chemical potential in Eq. (14) and increases linearly with increasing strength of the electron-phonon coupling parameter.

VI. CONCLUSIONS

The interaction of correlated electrons and acoustical phonons has been discussed by using the canonical transformation of Lang-Firsov which results in mobile polarons consisting of electrons surrounded by the acoustical phonon fields (clouds). A kind of generalized Wick’s theorem is used to handle the strong Coulomb repulsion between the electrons emerged into the see of phonon fields.

In the strong-coupling limit of the electron-phonon interaction chronologial thermodynamic averages of products of acoustical phonon-field operators are expressed by averages of one-cloud operators. For the normal one-cloud propagator the Lorentzian form in Eq. (25) while for anomalous one the Gaussian form in Eq. (28) has been found. Because the latter propagator is considerably smaller than the first one, we find that the anomalous electronic Green’s functions are more important than the corresponding polaronic functions. So the superconducting phase transition is determined as usual by the appearance of electronic Cooper pairs, i.e., the pairing of electrons without phonons-clouds is easier to achieve than the pairing of polarons with such clouds.

For the system of renormalized electronic Green’s functions in Eq. (64) the diagrammatical structure is analyzed and the Dyson equations have been derived, see Eqs. (66-69). Besides the self Green’s functions the equations contain also three correlation functions and three mass operators. These quantities have been calculated by summing infinite series of diagrams after performing appropriate approximations of Eq. (68). Resulting Eqs. (77) and (79) for the superconducting state are then linearized in terms of the order parameter $Y_{\alpha,\pi}$ leading to the final Eq. (105) which determines the superconducting transition temperature $T_c$, which is invariant with respect to particle-hole transformation. Further analysis shows that the problem of superconductivity in the frame of the Hubbard-Holstein model is analogous to the discussion of superconductivity in the frame of the single band Hubbard model with appropriately renormalized parameters.

For further discussion the normal state properties given by Eq. (94) are investigated with respect to the metal-insulator transition. For half filling, i.e., one electron per lattice site and $\mu = U/2$, the model yields a metallic state provided the renormalized value of $U$ is smaller than $\sqrt{3}/2\bar{W}$, where $\bar{W}$ is the electron energy band width, which is narrowed by the effect of the phonon fields, see Eqs. (112) and (115). The second parameter $b$ in Eq. (112) determines the deviation from half-filling. It has been shown that away from half filling a metallic state is favored for $U > \sqrt{3}/2\bar{W}$ and $b$ larger than a critical value $b_c$.

The search for superconductivity has then been performed on the basis of Eq. (105) for $s$-wave superconductivity for two cases. In the first case, at half filling, ($\mu = U/2$) with positive $U$, Eq. (105) has been reduced to Eq. (131), which has no solution. In the second case of
negative $U$ the non-trivial solution in Eq. (144) has been found. As mentioned before, in a real solid with correlated electrons the quantity $U$ should be replaced by an effective screened parameter. For an overall attractive interaction mediated by the phonons the Hubbard-Holstein model can have a superconducting solution although the bare value $U_0$ can still be substantially large.

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APPENDIX A: LAPLACE APPROXIMATION

In this section we provide calculational details of the Fourier representations $\tilde{\phi}(\Omega)$ and $\tilde{\sigma}(\Omega)$ defined in Eqs. (24a) and (24b) by making use of the Laplace method of approximation\(^2\). In the strong-coupling limit the integrand is maximal at the end points $\tau = 0$ and $\tau = \beta$ and is considerably smaller at other points of the interval of integration $0, \beta$. Therefore, we can replace the initial integral in Eq. (24a) by one in which the region of integration is limited to the two small intervals $(0, \tau_0)$ and $(\beta - \tau_0, \beta)$. In these intervals insertion of the expansions (19) lead to

$$\tilde{\phi}(\Omega) \approx \int_0^{\tau_0} d\tau \ e^{i\Omega \tau - \hbar \omega_c \tau} + \int_{\beta - \tau_0}^{\beta} d\tau \ e^{i\Omega \tau - \hbar \omega_c (\beta - \tau)}.$$  \hspace{1cm} (A1)

Then, because in the strong-coupling limit the collective frequency $\omega_c$ is large, we can replace $\tau_0$ by infinity, which yields a Lorentzian for (A1),

$$\tilde{\phi}(\Omega) = \frac{2\hbar \omega_c}{(i\Omega)^2 - (\hbar \omega_c)^2}. \hspace{1cm} (A2)$$

If we take into account the space dependence and expand in terms of small distances, $|x|$, we obtain:

$$\sigma(x|\tau) \approx \sigma(0|\tau) - \frac{1}{2} \sigma_1 x^2, \hspace{1cm} (A3)$$

where

$$\sigma_1 = \frac{1}{6N} \sum_k |\mathcal{F}(k)|^2 \frac{\hbar^2 \coth \frac{1}{2\beta} \hbar \omega_c}{\sinh \frac{1}{2\beta} \hbar \omega_c}. \hspace{1cm} (A4)$$

For small values of $|x|$ the function in Eq. (21) can then be written in factorized form,

$$\phi(x|\tau) \approx \phi(x) \phi(0|\tau), \hspace{1cm} (A5)$$

where

$$\phi(0|\tau) = e^{-\sigma(0|\tau + \sigma(0|\tau)} = \frac{1}{\beta} \sum_{\Omega} \tilde{\phi}(\Omega) e^{-i\Omega \tau}, \hspace{1cm} (A6)$$

$$\phi(x) = e^{-\sigma_1 x^2/2} = \frac{1}{\sqrt{2\pi}} \sum_{\Omega} \tilde{\phi}(\Omega) e^{-i\Omega \kappa x}, \hspace{1cm} (A7)$$

$$\tilde{\phi}(\Omega) = (2\pi/\sigma_1)^{3/2} e^{-\beta^2/\sigma_1}. \hspace{1cm} (A8)$$

For the Fourier representation of the anomalous phonon-cloud propagator $\varphi(x|\tau)$ we consider first $|x| = 0$. In this case we need the $\tau$ expansion of $\sigma(0|\tau)$ near the midpoint of the interval $\tau = \beta/2$ where this function is minimal. Near this minimum we use the following expression:

$$\sigma(0|\tau) \approx \sigma(0|\beta) + \frac{1}{2} \sigma''(0|\beta/2) (\tau - \beta/2)^2.$$  

This approximation can be used in the integral (24b), which allows to rewrite it as

$$\tilde{\phi}(i\Omega) \approx \int_{\beta - \tau_0}^{\beta} d\tau \ e^{-\sigma(0|\tau) - \sigma(0|\beta/2)} \times e^{i\Omega \tau - \hbar \omega_c (\beta - \tau)^2} \sigma''(0|\beta/2). \hspace{1cm} (A9)$$

The width of the small interval, $2\tau_0$, is now extended to infinity because the second derivative, $\sigma''(0|\beta/2)$, is large in the strong-coupling limit, which yields a Gaussian distribution,

$$\tilde{\phi}(i\Omega) = \sqrt{\frac{2\pi}{\sigma_2}} e^{-\sigma(0|\tau) - \sigma(0|\beta/2) + i\Omega / 2 \sigma_2 / (2\sigma_2)}, \hspace{1cm} (A10)$$

$$\sigma_2 = \sigma''(0|\beta/2).$$

This allows to get an approximate expression for Eq. (38). With Eqs. (30) and (32) we have, for example, to evaluate

$$\phi_2(x_1, i\Omega_1, x_2, i\Omega_2, x_3, i\Omega_3, x_4, i\Omega_4)$$

$$= \int_{\beta - \tau_0}^{\beta} d\tau \ e^{i\Omega_1 \tau + i\Omega_2 \tau - i\Omega_3 \tau + i\Omega_4 \tau} \times \exp \left\{ \sigma(x_1 - x_2 | \tau - \tau_0) + \sigma(x_1 - x_3 | \tau - \tau_4) + \sigma(x_3 - x_4 | \tau - \tau_4) - \sigma(x_1 - x_3 | \tau - \tau_4) - \sigma(x_1 - x_4 | \tau - \tau_4) - \sigma(x_2 - x_4 | \tau - \tau_4) \right\} - 2\sigma(0|0)). \hspace{1cm} (A11)$$

Equation (A11) leads to a sum of 24 fourfold integrals with different chronological order of $\tau_1, \ldots, 4$ (for example, $\phi_2^{1, 2, 3, 4}$ is defined by from $\beta > \tau_1 > \tau_2 > \tau_3 > \tau_4 > 0$), of which only 16 make an essential contribution in the strong-coupling limit. It is convenient to combine the 16 terms pairwise like

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$

$$[\tau_1 > \tau_2 > \tau_3 > \tau_4]$$
Further pairwise terms are obtained from the chronological orders by changing in the first two groups the order of \( \tau_1 \) and \( \tau_2 \), and in the last two groups the order of \( \tau_1 \) and \( \tau_4 \). All integrals are then calculated by using the maximum possible value of \( \Sigma \) in Eq. (32) in the Laplace approximation, i.e., maximal contributions arise from positive terms in Eq. (32) and coinciding arguments in each \( \sigma \) function. In addition the \( \tau \) space, for which the integrand is maximal, should be large enough. For example, in the integration over the first pairwise terms we take \( |\tau_1 - \tau_3| \) and \( |\tau_2 - \tau_4| \) as well as \(|x_1 - x_3| \) and \(|x_2 - x_4| \) as small quantities. This leads with \( \tau_1 - \tau_3 = t_1 \) and \( \tau_2 - \tau_4 = t_2 \) and, assuming for simplicity, \( x_1 = x_3 \) and \( x_2 = x_4 \), to the following argument of the exponential function in Eq. (A11):

\[
\sigma(0|t_1) + \sigma(0|t_2) + \sigma(x_1 - x_3|\tau_1 - \tau_2) + \sigma(x_2 - x_4|\tau_1 - \tau_2) - \sigma(x_1 - x_3|\tau_2 - \tau_1 + t_2) - 2\sigma(0,0),
\]

(A12)

which simply reduces to \(-\hbar \omega_c(t_1 + t_2)\) when expanding in \( t_1 \) and \( t_2 \). The corresponding integrations over \( t_1 \) and \( t_2 \) in the interval \((0, \tau_0) \rightarrow (0, \infty)\) lead to

\[
\phi_{\tau_1 > \tau_2 > \tau_3 > \tau_4}^{\tau_1 > \tau_2 > \tau_3 > \tau_4} = \int_0^\beta \int_0^\tau_1 dt_2 \int_0^\tau_1 dt_1 e^{i\tau_1(\Omega_1 - \Omega_2) + i\tau_2(\Omega_2 - \Omega_4)} \\
\times \int_0^\tau_2 dt_1 \int_0^\tau_2 dt_2 e^{i\tau_1(\Omega_1 - \Omega_2) + i\tau_2(\Omega_2 - \Omega_4)}
\]

(A13)

\[
\phi_{\tau_1 > \tau_2 > \tau_3 > \tau_4}^{\tau_1 > \tau_2 > \tau_3 > \tau_4} \text{ differs from } \phi_{\tau_1 > \tau_2 > \tau_3 > \tau_4}^{\tau_1 > \tau_2 > \tau_3 > \tau_4} \text{ by the last twofold integrals, which can be written as}
\]

\[
\int_0^\beta \int_0^\tau_2 dt_2 \int_0^\tau_2 dt_1 e^{i\tau_1(\Omega_1 - \Omega_2) + i\tau_2(\Omega_2 - \Omega_4)}
\]

(A14)

By combining the last two integrals, (A13) and (A14), we obtain the law of conservation for the frequencies,

\[
\phi_{\tau_1 > \tau_2 > \tau_3 > \tau_4}^{\tau_1 > \tau_2 > \tau_3 > \tau_4} = \phi_{\tau_1 > \tau_2 > \tau_3 > \tau_4}^{\tau_1 > \tau_2 > \tau_3 > \tau_4}
\]

(A15)

The same procedure can be used for the other 7 groups of integrals, which finally leads to

\[
\phi_2(x_1, i\Omega_1; x_2, i\Omega_2; x_3, i\Omega_3; x_4, i\Omega_4)
\]

\[
= \{\delta_{x_1, x_3} \delta_{x_2, x_4} \beta^2 \delta_{\Omega_1, \Omega_3} \delta_{\Omega_2, \Omega_4} + \delta_{x_1, x_4} \delta_{x_2, x_3} \beta^2 \delta_{\Omega_1, \Omega_2} \delta_{\Omega_3, \Omega_4}
\}

\left[\frac{2\hbar \omega_c}{(i\Omega_1)^2 - (i\Omega_2)^2 - (i\Omega_4)^2}\right].
\]

(A16)

This equation can be rewritten in the form,

\[
\phi_2(x_1, i\Omega_1; x_2, i\Omega_2; x_3, i\Omega_3; x_4, i\Omega_4)
\]

\[
= \phi(x_1, i\Omega_1; x_3, i\Omega_3) \phi(x_2, i\Omega_2; x_4, i\Omega_4) + \phi(x_1, i\Omega_1; x_4, i\Omega_4) \phi(x_2, i\Omega_2; x_3, i\Omega_3),
\]

(A17)

\[
\phi(x_1, i\Omega_1; x_3, i\Omega_3) = \phi_0(i\Omega_1) \beta \delta_{\Omega_1, \Omega_3} \delta_{x_1, x_3}.\]

(A18)

From these equations we finally obtain Eq. (36). In similar manner we calculated the Fourier representation of the two-cloud function \( \varphi_2 \), which leads to Eq. (37).

**APPENDIX B: DETERMINATION OF THE GREEN'S FUNCTION \( \Gamma_{\sigma, \sigma'}(i\omega) \)**

The evaluation of \( \Gamma_{\sigma, \sigma'}(i\omega) \) requires knowledge of the following two- and three-particle Green's functions:

\[
G_0^0[\sigma, \tau; \sigma', \tau'|1] = \langle T a_\sigma(\tau) \bar{\pi}_{\sigma'}(\tau') n(\tau_1) \rangle_{0},
\]

(B1a)

\[
G_0^0[\sigma, \tau; \sigma, \tau'|1, \tau_2] = \langle T a_\sigma(\tau) \bar{\pi}_{\sigma'}(\tau') n(\tau_1) n(\tau_2) \rangle_{0},
\]

(B1b)

where the statistical averaging is determined by the local part of the Hubbard Hamiltonian. In the calculation it is necessary to switch over to Hubbard operators, \( X^{mn} \), where the indices \( m \) and \( n \) denote ionic quantum states, \( m = 0, \pm 1, \pm 2 \).

\[
a_\sigma = X^{0\sigma} + \sigma X^{2\sigma}, \quad a_0^\sigma = X^{0\sigma} + \sigma X^{2\sigma}.
\]

(B2)

We omit calculation details and list only the resulting expressions,
\[
\begin{align*}
&- \theta (\tau' - \tau) \theta (\tau - \tau_1) \left[ e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} + 2e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right] - \theta (\tau' - \tau_1) \theta (\tau - \tau_2) e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \\
&+ \theta (\tau_1 - \tau) \theta (\tau' - \tau) e^{-\beta E_\Gamma + \langle \tau' - \tau \rangle \Xi} - \theta (\tau_1 - \tau_2) \theta (\tau - \tau') \left[ e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} + 2e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right], \tag{B3}
\end{align*}
\]

\[
G_{\sigma, \sigma'}[\tau, \tau'; \tau_1, \tau_2] = \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ \left[ \theta (\tau' - \tau) \theta (\tau' - \tau_1) \theta (\tau_1 - \tau_2) + \theta (\tau' - \tau) \theta (\tau_1 - \tau) \theta (\tau_2 - \tau_1) \right] e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \\
+ \left[ \theta (\tau_1 - \tau) \theta (\tau - \tau') \theta (\tau' - \tau_2) + \theta (\tau_2 - \tau) \theta (\tau_1 - \tau) \theta (\tau' - \tau_1) \right] e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \\
+ \left[ \theta (\tau' - \tau') \theta (\tau - \tau_1) \theta (\tau_1 - \tau_2) + \theta (\tau - \tau_1) \theta (\tau_1 - \tau) \theta (\tau_2 - \tau_1) \right] \left[ e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} + 2e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right] \\
- \left[ \theta (\tau' - \tau) \theta (\tau_1 - \tau_2) \theta (\tau_2 - \tau) + \theta (\tau_2 - \tau) \theta (\tau_1 - \tau) \theta (\tau - \tau') \right] \left[ e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} + 4e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right] \\
- \left[ \theta (\tau' - \tau) \theta (\tau_1 - \tau_2) \theta (\tau_2 - \tau) + \theta (\tau_2 - \tau) \theta (\tau_1 - \tau) \theta (\tau - \tau') \right] e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \\
+ \left[ \theta (\tau_1 - \tau) \theta (\tau - \tau') \theta (\tau' - \tau_2) + \theta (\tau_2 - \tau) \theta (\tau_1 - \tau) \theta (\tau' - \tau_1) \right] e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \\
+ \left[ \theta (\tau_1 - \tau) \theta (\tau - \tau') \theta (\tau_2 - \tau_1) \theta (\tau_1 - \tau) \theta (\tau - \tau') \right] 2e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \\
+ \left[ \theta (\tau_1 - \tau) \theta (\tau - \tau') \theta (\tau_2 - \tau_1) \theta (\tau_1 - \tau) \theta (\tau - \tau') \right] 2e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \\
- \left[ \theta (\tau_1 - \tau) \theta (\tau - \tau') \theta (\tau_2 - \tau_1) \theta (\tau_1 - \tau) \theta (\tau - \tau') \right] 2e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Xi} \right\}, \tag{B4}
\]

where
\[
\Delta = E_0 - E_\sigma = \mu, \quad \Xi = E_\phi - E_2 = \mu - U, \tag{B5}
\]

and \(\theta(x)\) is here the step function. Integration over \(\tau_1\) and \(\tau_2\) yields:

\[
\psi_2(\tau' - \tau') = \int_0^\beta d\tau_1 \left\{ \langle \Gamma \alpha_\sigma(\tau) \pi_{\sigma'}(\tau') n(\tau_1) \rangle \right\}_0 \\
= \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ \theta (\tau' - \tau) (\tau - \tau') e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} \\
+ \theta (\tau' - \tau') (\beta + \tau' - \tau) e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \\
- \theta (\tau' - \tau') \beta + \tau' - \tau) e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Delta} \\
- \theta (\tau' - \tau') (2\beta + \tau' - \tau) e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right\}, \tag{B6}
\]

\[
\psi_3(\tau - \tau') = \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \left\{ \langle \Gamma \alpha_\sigma(\tau) \pi_{\sigma'}(\tau') n(\tau_1) n(\tau_2) \rangle \right\}_0 \\
= \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ \theta (\tau - \tau') (\tau - \tau')^2 e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Delta} \\
+ \theta (\tau - \tau') (\beta + \tau - \tau') e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \\
- \theta (\tau' - \tau) (\beta + \tau' - \tau) e^{-\beta E_\sigma + \langle \tau - \tau' \rangle \Delta} \\
- \theta (\tau' - \tau) (2\beta + \tau' - \tau) e^{-\beta E_\sigma + \langle \tau' - \tau \rangle \Xi} \right\}. \tag{B7}
\]

The Fourier representation of these functions,

\[
\psi_n (\tau - \tau') = \frac{1}{\beta} \sum_{\omega_n} e^{i\omega_n(\tau - \tau')} \psi_n(i\omega_n), \tag{B8}
\]

are given by

\[
\psi_2(i\omega) = \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ \left( e^{-\beta E_\sigma} + e^{-\beta E_\sigma} \right) \left( \frac{1}{\lambda^2(i\omega)} - \frac{1}{\lambda'(i\omega)} \right) \\
+ \left( e^{-\beta E_\sigma} + e^{-\beta E_\sigma} \right) \left( \frac{1}{\lambda(i\omega)} \right) \right\}, \tag{B9}
\]

\[
\psi_3(i\omega) = \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ - \frac{2(e^{-\beta E_\sigma} + e^{-\beta E_\sigma})}{\lambda(i\omega)} \\
+ \frac{2\beta e^{-\beta E_\sigma}}{\lambda'(i\omega)} + \frac{2\beta e^{-\beta E_\sigma}}{\lambda(i\omega)} + \frac{4\beta e^{-\beta E_\sigma}}{\lambda'(i\omega)} \right\}. \tag{B10}
\]

This allows to evaluate the \(\Gamma_{\sigma,\sigma'}(\tau - \tau')\) function,

\[
\Gamma_{\sigma,\sigma'}(\tau - \tau') = \psi_3(\tau - \tau') - 2n_0 \beta \psi_2(\tau - \tau') \\
+ \beta^2 G_{\sigma,\sigma'}^0(\tau - \tau') \left( n^2_0 \right) - 2(n^2_0), \tag{B11}
\]

and to obtain its Fourier representation,

\[
\Gamma_{\sigma,\sigma'}(i\omega) = \frac{\delta_{\sigma, \sigma'} \delta_{\tau, \tau'}}{Z_0} \left\{ - \frac{2(e^{-\beta E_\sigma} + e^{-\beta E_\sigma})}{\lambda^2(i\omega)} \\
+ \frac{2(e^{-\beta E_\sigma} + e^{-\beta E_\sigma})}{\lambda(i\omega)} \right\}. \tag{B10}
\]
\[
\begin{align*}
&+ \frac{2\beta}{\lambda i(\omega)} \left[ e^{-\beta E_x} - \langle n \rangle_0 (e^{-\beta E_0} + e^{-\beta E_x}) \right] \\
&+ \frac{2\beta}{\lambda} \left[ e^{-\beta E_x} + 2e^{-\beta E_z} \right] \\
&- \langle n \rangle_0 (e^{-\beta E_0} + e^{-\beta E_z}) \\
&+ \frac{\beta^2}{\lambda(i\omega)} \left[ - (1 - 2\langle n \rangle_0) e^{-\beta E_x} \\
&+ (\langle n \rangle_0^2 - 2\langle n \rangle_0) (e^{-\beta E_0} + e^{-\beta E_x}) \right] \\
&+ \frac{\beta^2}{\lambda(i\omega)} \left[ - (1 - 2\langle n \rangle_0) e^{-\beta E_x} \\
&+ (\langle n \rangle_0^2 - 2\langle n \rangle_0) (e^{-\beta E_0} + e^{-\beta E_x}) \right].
\end{align*}
\]
\[\text{(B12)}\]

For the case of half filling we have,
\[
Z_0 = 2(1 + e^{\beta \mu}), \quad \lambda(i\omega) = \omega + \mu,
\]
\[\begin{align*}
\bar{\lambda}(i\omega) &= i\omega - \mu, \\
G_0^0(i\omega) &= \frac{i\omega}{\omega^2 - \mu^2}.
\end{align*}\]
\[\text{(B13)}\]

\[
\psi_2(i\omega) = \delta_{\sigma,\sigma'} \left\{ - \frac{\beta i\omega}{(i\omega)^2 - \mu^2} + \frac{(i\omega)^2 + \mu^2}{[(i\omega)^2 - \mu^2]^2} \right\}
\]
\[\begin{align*}
&- \frac{\beta \mu}{(1 + e^{\beta \mu})[(i\omega)^2 - \mu^2]} \\
&\psi_3(i\omega) = \frac{2\beta}{(1 + e^{\beta \mu})} \left\{ - \frac{4i\omega}{(i\omega)^2 + \mu^2} + \frac{(i\omega)^2 + \mu^2}{[(i\omega)^2 - \mu^2]^2} \right\}
\end{align*}\]
\[\begin{align*}
&+ \frac{4\beta[(i\omega)^2 + \mu^2] e^{\beta \mu}}{[(i\omega)^2 - \mu^2]^2} + \frac{4\beta[(i\omega)^2 + \mu^2 + 2i\omega \mu]}{[(i\omega)^2 - \mu^2]^2} \\
&- \frac{2i\omega^2 e^{\beta \mu}}{(i\omega)^2 - \mu^2} + \frac{4\beta^2(i\omega + \mu)}{(i\omega)^2 - \mu^2}.
\end{align*}\]
\[\text{(B14)}\]

The corresponding analytical continuation \(i\omega \rightarrow E + i0^+\) for \(E = 0\) gives to,
\[
\psi_2(0) = \frac{\delta_{\sigma,\sigma'} \beta \mu}{\mu^2} \left( \frac{1}{1 + e^{\beta \mu}} \right),
\]
\[\text{(B16a)}\]
\[
\psi_3(0) = \frac{\delta_{\sigma,\sigma'} 2\beta \mu}{\mu^2} \left( \frac{1}{1 + e^{\beta \mu}} \right),
\]
\[\text{(B16b)}\]
\[
G_0^0(0) = 0.
\]
\[\text{(B16c)}\]

In this case the \(\Gamma\) function is of particular simple form,
\[
\Gamma_\sigma(0) = \frac{\delta_{\sigma,\sigma'} \beta \mu}{\mu^2} \left( \frac{1}{1 + e^{\beta \mu}} \right)[1 - \langle n \rangle_0].
\]
\[\text{(B17)}\]

**APPENDIX C: THE CRITICAL TEMPERATURE**

With help of the Poisson summation formula,
\[
\frac{1}{\beta} \sum_{\omega_n} f(i\omega_n) = \frac{1}{4\pi i} \int_C dz \tanh \left[ 2\beta z f(z) \right],
\]
\[\text{(C1)}\]

where \(C\) is the usual counterclockwise contour of the imaginary axis, we obtain for case that the parameters in Eq. 123 obey \(\gamma^4 > (c^2 - d^2)^2/4\),
\[
I_1 = \frac{1}{\beta} \sum_{\omega_n} Q_1(i\omega) = - \frac{1}{\sqrt{4\gamma^4 - (c^2 - d^2)^2}} \times \text{Im} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right),
\]
\[\text{(C2a)}\]
\[
I_2 = - \frac{c^2 - d^2}{2\gamma^4} I_1 - \frac{\tanh \frac{1}{2} \beta \gamma}{2\gamma^4} + \frac{1}{2\gamma^4} \times \text{Re} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right),
\]
\[\text{(C2b)}\]
\[
I_3 = - \frac{c^2 - d^2}{2\gamma^4} I_1 - \frac{\tanh \frac{1}{2} \beta d}{2d\gamma^4} + \frac{1}{2d\gamma^4} \times \text{Re} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right),
\]
\[\text{(C2c)}\]

with
\[
\alpha_1 = \frac{1}{\sqrt{2}} \left( \frac{\gamma^4 + c^2d^2 \pm (c^2 - d^2)^2}{2} \right)^{1/2},
\]
\[\text{(C3)}\]

and
\[
\begin{align*}
&\text{Re} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right) \\
&\quad = \frac{\alpha_1 \sinh \beta \alpha_1 + \alpha_2 \sin \beta \alpha_2}{(\alpha_1^2 + \alpha_2^2) \cosh \beta \alpha_1 + \cos \beta \alpha_2}.
\end{align*}\]
\[\text{(C4)}\]

Inserting the results in Eq. (C2) into Eq. (123) allows us to obtain expressions for the parameters \(\eta_{11}, \eta_{12}\) and \(\eta_{12}\). Furthermore, this allows to decompose the \(T_c\) equation with the help of the following abbreviations,
\[
A = \left( 1 - \frac{U^2}{(2\mu - U)^2} \right) \frac{1}{Z_0^2} \left( \frac{e^{\beta \mu} + e^{\beta(2\mu - U)}}{1 + e^{\beta \mu}} \right)
\]
\[\begin{align*}
&\quad \times (\eta_{11}\eta_{12} - \eta_{12}^2) \\
&\quad = \left( 1 - \frac{U^2}{(2\mu - U)^2} \right) \frac{1}{Z_0^2} \left( \frac{e^{\beta \mu} + e^{\beta(2\mu - U)}}{1 + e^{\beta \mu}} \right)
\end{align*}\]
\[\begin{align*}
&\quad \times (U \phi \kappa)^2 \left( \frac{c^2 - d^2}{d^2} \right)^2 \left\{ \left( \frac{\tanh \frac{1}{2} \beta c}{c} + \frac{\tanh \frac{1}{2} \beta d}{d} \right) \right\}
\end{align*}\]
\[\begin{align*}
&\quad \times \text{Re} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right) - \frac{\tanh \frac{1}{2} \beta \cosh \frac{1}{2} \beta c}{c} \\
&\quad - \left( \frac{\tanh \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right)^2 + \frac{2c^2 - (c^2 - d^2)^2}{\alpha_1 + i\alpha_2} \\
&\quad \times \text{Im} \left( \frac{\tan \frac{1}{2} \beta (\alpha_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right) \left( \frac{\tanh \frac{1}{2} \beta d}{d} - \frac{\tanh \frac{1}{2} \beta c}{c} \right)
\end{align*}\]
\[\begin{align*}
&\quad \times \frac{1}{c^2 - d^2}.
\end{align*}\]
\[\text{(C6)}\]
and

\[ B = \left( 1 + \frac{U}{2\mu - U} \right) \frac{1 + e^{\beta \mu}}{Z_0} \eta_1 + \left( 1 - \frac{U}{2\mu - U} \right) e^{\beta (2\mu - U)} \eta_2 \]

\[ = \frac{\eta_1}{2\eta_2} \left\{ \left[ 2z^4 - (z^2 - d)^2 \right] \left( 1 + \frac{U(1 - e^{\beta (2\mu - U)})}{Z_0 (2\mu - U)} \right) I_1 + \text{Im} \left( \frac{\tan \frac{\beta}{2} (a_1 + i\alpha_2)}{\alpha_1 + i\alpha_2} \right) \times \left( U + \frac{U(2\mu - U)(1 - e^{\beta (2\mu - U)})}{Z_0} \right) \right. \]

\[ + 2U \left( \frac{\mu - U}{d} \tan \frac{\beta}{2} e^{\beta \mu} + e^{\beta (2\mu - U)} \right) \]

\[ - \frac{\mu - c}{d} e^{\beta \mu} \right\} \right) I_1, \quad (C7) \]

where the value of \( I_1 \) is determined by Eq. (C2a). Equation (105), which determines \( T_c \), can then be written as

\[ 1 + Bf_c + Af_c^2 = 0, \quad (C8) \]

where the quantity \( f_c \) is given by Eq. (96). Equation (C7) would allow to investigate in detail the interplay of the different parameters and renormalized quantities obtained after eliminating the electron-phonon interaction by the Lang-Firsov transformation. The influence of these parameters on \( T_c \) can however only be obtained by numerical work, which has yet to be undertaken. The simplified discussion in the main text shows that \( T_c \) is proportional to the typical energy scale involved, which is the renormalized chemical potential and not the bare quantities of the original model. This means that due to the Lang-Firsov transformation the proportionality of \( T_c \) to a typical phonon frequency as in BCS theory or in the Eliashberg formulation is lost. This is an interesting observation but must be tested numerically by analyzing the more complex expressions of this paper. In order to find out whether the proportionality \( T_c \propto |\mu| \), i.e., \( T_c \) proportional to a renormalized electronic energy scale and not proportional to an average phonon frequency, \( \langle \hbar \omega_k \rangle \), is an intrinsic property of the model, we will perform investigations in infinite dimensions. This is nowadays much at debate by using other approaches like the dynamical mean field theory, which allows to evaluate more or less accurate materials properties if combined with density functional theory.31-34. We believe that our approach allows for similar accurate description of materials including superconducting properties. This is left for future work.

Finally we would like to stress that the present approach, to start from the exact local (atomic) description and to take into account the properties of the correlated tight-binding electrons on a lattice by perturbation theory in the transfer integral, has conceptually some advantages compared to other theories.


