STRONG INTERACTION OF CORRELATED ELECTRONS WITH PHONONS: A NEW APPROACH TO POLARON SUPERCONDUCTIVITY

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ABSTRACT

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

The aim of the present paper is to gain further insight into the mutual influence of strong on-site Coulomb repulsion and strong electron-phonon interaction by using the single-band Hubbard-Holstein model and a recently developed diagrammatic approach 1-4. For simplicity we consider coupling to dispersionless phonons only, although this might not be the most interesting case with respect to superconductivity. However, previous investigations 5-7 have shown that the Hubbard-Holstein model 8-9 constitutes a formidable problem of its own. Other authors have also intensively studied this model Hamiltonian 10-13.

Because the interactions between electrons and electrons and phonons are strong, we include the Coulomb repulsion in the zero-order Hamiltonian and apply the canonical transformation of Lang and Firsov 14 in order to eliminate the linear electron-phonon interaction. In the strong electron-phonon coupling limit the resulting Hamiltonian of hopping polarons (i.e., hopping electrons surrounded by clouds of phonons) can lead to an attractive interaction among electrons being mediated by the phonons. In this limit the chemical potential, on-site Coulomb energy as well as the frequency of the collective mode of phonon clouds (which is much larger than the bare frequency of the Einstein oscillators) are strongly renormalized 7,15,16 affecting the dynamical properties of the polarons and the character of the superconducting transition. This will be discussed by assuming that renormalized on-site Coulomb repulsion and attractive electron-electron interaction completely cancel each other. We suggest that the resulting superconducting state with polaronic Cooper pairs is mediated by the exchange of phonon clouds during the hopping processes of the electrons.

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

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

$$H_e = \sum_{ij\sigma} \left\{ t(j-i) + \varepsilon_0 \delta_{ij} \right\} a^+_{j\sigma} a_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

$$H^0_{ph} = \sum_i \hbar\omega_0 \left(b^+_i b_i + \frac{1}{2} \right), \qquad H_{e-ph} = g \sum_i n_i q_i, \tag{3}$$

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

Here $a^+_{i\sigma}(a_{i\sigma})$ and $b^+_{i\sigma}(b_{i\sigma})$ are creation (annihilation) operators of electrons and phonons, respectively; i refers to the lattice site and σ to the spin; q_i is the phonon coordinate and g the electron-phonon interaction constant;
$\varepsilon_0 = \bar{\varepsilon}_0 - \mu$ with local energy $\bar{\varepsilon}_0$ and chemical potential μ; U the on-site Coulomb repulsion; $t(j-i)$ is the two-center transfer integral. The Fourier representation of $t(j-i)$ is connected to the tight-binding dispersion $\varepsilon(k)$ of the bare electrons, with band width.

After applying the Lang-Firsov transformation[14]

$$H_p = e^s H e^{-s}, \qquad c_{i\sigma} = e^S a_{i\sigma} e^{-S}, \qquad c^+_{i\sigma} = e^S a_{i\sigma} e^{-S}, \tag{5}$$

with

$$S = -i\bar{g}\sum_i n_i p_i, \qquad \bar{g} = \frac{g}{\hbar\omega_0}, \qquad p_i = \frac{i}{\sqrt{2}}\left(b_i^+ - b_i\right), \tag{6}$$

where p_i is the phonon momentum and $\bar{g}$ the dimensionless interaction constant, the polaron Hamiltonian has been obtained. The polaron Hamiltonian is by nature a polaron-phonon operator, i.e., the creation operator $c^+_{i\sigma}$ and destruction operator $c_{i\sigma}$ in H_p

$$c^+_{i\sigma} = a^+_{i\sigma} e^{-i\bar{g}p_i}, \quad c_{i\sigma} = a_{i\sigma} e^{i\bar{g}p_i},$$

should be interpreted as creation and destruction operators of polarons (electrons dressed with the displacements of the ions) which couple dynamically to the momentum of the optical phonon. In zero-order approximation polarons and phonons are localized with strongly renormalized chemical potential $\bar{\mu}$ and on-site Coulomb interaction $\bar{U}$:

$$\bar{\mu} = \mu + \alpha\hbar\omega_0, \; \bar{U} = U - 2\alpha\hbar\omega_0, \; \alpha = \frac{1}{2}\bar{g}^2.$$

The problem is now to deal properly with the impact of electronic correlations and tunneling on the polaron problem. This can be done best by using Green's functions provided one finds a key to deal with the spin and charge degrees of freedom.

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

$$G\left(x,\sigma,\tau \middle| x',\sigma',\tau'\right) = -\left\langle T c_{x\sigma}(\tau)\bar{c}_{x'\sigma'}(\tau')U(\beta)\right\rangle_0^c, \tag{7}$$

with

$$c_{x\sigma}(\tau) = e^{H^0\tau} c_{x\sigma} e^{-H^0\tau}, \quad \bar{c}_{x\sigma}(\tau) = e^{H^0\tau} c^+_{x\sigma} e^{-H^0\tau},$$

with $H^0 = H^0_p + H^0_{ph}$ and $U(\beta)$ evolution operator and where **x**, **x**' are the site indices and τ, τ' stand for the imaginary time with $0 < \tau < \beta$; T is the time ordering operator and β the inverse temperature. The upper index c in above equation means that only connected diagrams must be taken into account. A detailed inspection of the equations will only be undertaken for the special case $\bar{U} = 0$.

Wick's theorem of weak-coupling quantum field theory can be used when evaluating statistical averages of phonon operators like, for example, the propagator for the phonon cloud,

$$\Phi\left(\tau_1|\tau_2\right) = \Phi\left(\tau_1 - \tau_2\right) \equiv \left\langle T \exp\left\{i\bar{g}\left[p(\tau_1) - p(\tau_2)\right]\right\}\right\rangle_0 = \tag{8}$$

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

where

$$\sigma(|\tau_1-\tau_2|)=\bar{g}^2\langle Tp(\tau_1)p(\tau_2)\rangle_0=\alpha\,\frac{\cosh\left(\hbar\omega_0\left\{\frac{\beta}{2}-|\tau_1-\tau_2|\right\}\right)}{\sinh\left(\frac{\beta\hbar\omega_0}{2}\right)}. \qquad (9)$$

In order to facilitate the investigation we have evaluated the propagator of the phonon cloud in the strong-coupling limit $\alpha >> 1$, [5,6,16]

$$\Phi(\tau)=\frac{1}{\beta}\sum_{\Omega_n}e^{-i\Omega_n(\tau)}\overline{\Phi}(i\Omega_n), \qquad (10)$$

$$\overline{\Phi}(i\Omega_n)=\frac{e^{-\sigma(\beta)}}{2}\int_{-\beta}^{\beta}d\tau e^{i\Omega_n\tau+\sigma(|\tau|)}, \qquad (11)$$

with $\Omega_n=2n\pi/\beta$. In order to find $\overline{\Phi}(i\Omega_n)$ we use the Laplace approximation[17] for the integral which contains an exponential function with the parameter α. In the strong-coupling limit $\alpha >> 1$ we have obtained

$$\overline{\Phi}(i\Omega_n)\approx\frac{2\omega_c}{\Omega_n^2+\omega_c^2}, \qquad \omega_c=\hbar\alpha\omega_0=\frac{g^2}{2\hbar\omega_0}. \qquad (12)$$

This term is the harmonic propagator of the collective mode of phonons belonging to the polaron clouds. In our theory the sum of all strongly connected diagrams containing all kinds of irreducible Green's functions in the perturbation expansion of the evolution operator, defines the special function $Z(x|x')$ (for details see Ref. [1,2]). This function contains all contributions from charge and spin fluctuations. It allows us, together with the mass operator which is in our case the hopping matrix element, to formulate a Dyson-type of equation for the one-polaron Green's function [1-4],

$$G(x|x')=\Lambda(x|x')+\sum_{1,2}\Lambda(x|1)t(1-2)G(2|x'), \qquad (13)$$

where

$$\Lambda(x|x')=G_p^{(0)}(x|x')+Z(x|x'). \qquad (14)$$

This method can be used also in our case of polarons with cancelled resulting local interaction $\overline{U}=0$, because of the complex structure of polarons (as electrons surrounded by phonon clouds). For complex particles the irreducible Green's functions, or Kubo cumulants, are different from zero and under such circumstances out diagram technique is actual.

In the following we check whether the polaronic system may have a superconducting instability in the absence of a direct attractive interaction for the polarons, i.e., for $\overline{U}=0$. In this case the attraction is only brought about dynamically by polarons exchanging phonon clouds. With respect to superconductivity we need in addition to the normal state Green's function the anomalous propagators[18]. For simplicity we limit the discussion to s-wave superconductivity as in previous investigations of superconducting instabilities in the Hubbard model[3,4] and Hubbard-Holstein model in the strong-coupling limit, $\alpha >> 1$ [16].

For a description of the superconducting state we need the three irreducible functions $\Lambda_\sigma, \Upsilon_{\sigma,\sigma}$ and $\overline{\Upsilon}_{-\sigma,\sigma}$ which represent infinite sums of diagrams containing irreducible many-particle Green's functions. In order to obtain a close set of equations we will restrict ourselves to a class of rather simple contributions which, however, contain the most important charge, spin and pairing correlations; for details see Ref.[16]. This class of diagrams is obtained by neglecting contributions for which the Fourier representation of the superconducting order parameters, $\Upsilon_{\sigma,\sigma}$ and $\overline{\Upsilon}_{-\sigma,\sigma}$ depend on the polaron momentum **k.**

In order to gain further insight into the physics contained in our general equations we will linearize them in terms of the order parameter $\Upsilon_{\sigma,-\sigma}(i\omega)$ which will determine the critical temperature T_c. The resulting equation for the order parameter is of the form

$$\Upsilon_{\sigma,-\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{k,\omega_l}\frac{\varepsilon(k)\varepsilon(-k)\Upsilon_{\sigma,-\sigma}(i\omega_l)}{[1-\varepsilon(k)\Lambda_\sigma(i\omega_l)][1-\varepsilon(-k)\Lambda_{-\sigma}(-i\omega)]} \times \overline{G}_2^{(0)ir}(\sigma,i\omega;-\sigma,-i\omega|\sigma,i\omega_l;-\sigma,-i\omega_l). \quad (15)$$

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

$$\Lambda_\sigma(i\omega) = G_{p\sigma}^{(0)}(i\omega) - \frac{1}{\beta N}\sum_{k,\omega_l}\frac{\varepsilon^2(k)\Lambda_\sigma(i\omega_l)}{1-\varepsilon(k)\Lambda_\sigma(i\omega_l)}\overline{G}_2^{(0)ir}(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega)$$

$$-\frac{1}{\beta N}\sum_{k,\omega_l}\frac{\varepsilon^2(k)\Lambda_{-\sigma}(i\omega_l)}{1-\varepsilon(-k)\Lambda_{-\sigma}(i\omega_l)}\overline{G}_2^{(0)ir}(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega). \quad (16)$$

In order to determine T_c we must solve the equation for Λ_σ and insert the result in equation for $\Upsilon_{\sigma,-\sigma}(i\omega)$. The irreducible functions of these equations can be written as

$$\overline{G}_2^{(0)ir}(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega) = \frac{(\omega-\omega_l)^2}{\Delta^2\Delta_l^2}\{\, 2\omega_c^2(x+x_l)\tanh(\beta\varepsilon/2) - $$

$$-\frac{\coth(\beta\omega_c/2)}{\omega_c[(i\omega-i\omega_l)^2-4\omega_c^2]}[(xx_l+\omega_c^2)(\Delta\Delta_l+8\omega_c^4)-2\omega_c^2(\Delta+\Delta_l)(xx_l-\omega_c^2)]\,\}, \quad (17)$$

$$\overline{G}_2^{(0)ir}(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega) = -\frac{2\omega_c}{\Delta^2\Delta_l^2}\{\,\omega_c(x+x_l)(\Delta+\Delta_l)\tanh(\beta\varepsilon/2)$$

$$+\coth(\beta\omega_c/2)(x+x_l)^2(xx_l-\omega_c^2)\,\} + \frac{\coth(\beta\omega_c/2)(xx_l+3\omega_c^2)}{\omega_c\Delta\Delta_l}, \quad (18)$$

$$\overline{G}_2^{(0)ir}(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega) =$$

$$-\frac{2\varepsilon(2\omega_c)^2\,\mathrm{tangh}(\beta\varepsilon/2)[i\omega i\omega_l+\varepsilon^2-\omega_c^2]}{[\omega^2+(\varepsilon+\omega_c)^2][\omega^2+(\varepsilon-\omega_c)^2][\omega_l^2+(\varepsilon+\omega_c)^2][\omega_l^2+(\varepsilon+\omega_c)^2]}$$

$$+\frac{2\omega_c\coth(\beta\omega_c/2)[i\omega_l+2\omega_c(\varepsilon-\omega_c)-(\varepsilon-\omega_c)^2]}{[\omega^2+(\varepsilon-\omega_c)^2][\omega_l^2+(\varepsilon-\omega_c)^2][(\omega-\omega_l)^2+(2\omega_c)^2]}$$

$$+\frac{2\omega_c\coth(\beta\omega_c/2)[i\omega_l-2\omega_c(\varepsilon+\omega_c)-(\varepsilon+\omega_c)^2]}{[\omega^2+(\varepsilon+\omega_c)^2][\omega_l^2+(\varepsilon+\omega_c)^2][(\omega-\omega_l)^2+(2\omega_c)^2]}, \quad (19)$$

where

$$x = i\omega - \varepsilon, \qquad \Delta = (i\omega - \varepsilon)^2 - \omega_c^2 \tag{20a}$$

$$x_l = i\omega_l - \varepsilon, \qquad \Delta_l = (i\omega_l - \varepsilon)^2 - \omega_c^2. \tag{20b}$$

Which allows to write the equation for the critical temperature T_c in the following form

$$\varepsilon^2 + \omega_c^2 - 2\varepsilon\omega_c \tanh(\beta\varepsilon/2) = \left(\omega_c^2 - \varepsilon^2\right)^2 (4/W)^2. \tag{21}$$

In this approximation T_c depends only on the local parameters; but we expect that close to half filling this should give an impression which of the local quantities is most important for superconductivity in the strong-coupling limit of the Hubbard-Holstein model. This equation has a lot of solutions for different values of the theory parameters. One of the main of them is the collective frequency ω_c. We shall suppose that the bare phonon frequency ω_0 is equal to 0.07 eV and consider two different values of dimensionless interaction constant $\bar{g}$. One of these values is equal to $\bar{g} = 3$ with α=4.5, and the second is $\bar{g} = 4$ with α=8. Two corresponding values of ω_c are 0.315 eV and 0.56 eV. By setting in our equation the values for T_c=100 K and $\omega_c = 0.315\, eV$ we shall obtain the many permitted values of other two parameters ε and W. Between them there are the following values : $\varepsilon = 0.10515$ eV and W=1.68057 eV; $\varepsilon = 0.20348$ eV and W=2.07393 eV; $\varepsilon = 0.30149$ eV and W=2.46594 eV.

In the case when T_c=200 K and the value of ω_c is the same we have obtained the following values of two other parameteres : $\varepsilon = 0.10515$ eV and W=1.67498 eV; $\varepsilon = 0.20349$ eV and W=2.07379 eV; $\varepsilon = 0.30149$ eV and W=2.46591 eV.

For the value of T_c =300 K and of $\omega_c = 0.315\, eV$ there are other examples of permitted ε and W parameters : $\varepsilon = 0.10516$ eV and W=1.63966 eV; $\varepsilon = 0.20349$ eV and W=2.09215 eV; $\varepsilon = 0.30149$ eV and\quad W=2.45757 eV.

If the value of ω_c is equal to 0.56 eV we have other three groups of examples. If T_c is equal to 100 K we have : $\varepsilon = 0.10497$ eV and W=2.65986 eV; $\varepsilon = 0.21003$ eV and W=3.08010 eV; $\varepsilon = 0.30252$ eV and W=3.45008 eV.

When T_c is equal to 200 K we have the following examples: $\varepsilon = 0.10497$ eV and W=2.65649 eV; $\varepsilon = 0.21003$ eV and W=3.08009 eV; $\varepsilon = 0.30252$ eV and W=3.45009 eV.

The last our examples are for T_c=300 K and the same value of $\omega_c = 0.56$ eV : $\varepsilon = 0.10498$ eV and W=2.63470 eV; $\varepsilon = 0.21004$eV and W=3.07839 eV; $\varepsilon = 0.30253$ eV and W=3.44996 eV.

We have discussed the occurrence of superconductivity for the Hubbard-Holstein model in the strong-coupling limit $(\alpha >> 1)$. For $\alpha >> 1$ we find a collective mode for the phonon clouds estimated by evaluating integrals in the Laplace approximation. Due to the absorption and emission of this mode by the polarons, the irreducible two-particle Green's functions are renormalized. Allowing for the exchange of polarons including their phonon clouds leads to a new irreducible Green's functions which have been used to study spin-singlet pairing of polarons. Analytical and numerical results for the superconducting phase have been obtained for the limiting case, for which the local repulsion of polarons is exactly cancelled by their attractive interaction. The resulting equation for the critical temperature has been obtained by assuming a large collective-mode frequency and a considerable deviation from half-filled band case. The parameters which determine T_c are ω_c, ε (ε=0 corresponds to half filling) and the band width W. In the strong-coupling limit we obtain a critical temperature which is of reasonable values for high-Tc superconductivity.

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