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PHONON-INDUCED AND PHONON-FREE SUPERCONDUCTIVITY IN CORRELATED SYSTEMS: ELIASHBERG EQUATIONS FOR THE TWO-DIMENSIONAL HUBBARD MODEL* **

Marcin Mierzejewski, Janusz Zieliński

Institute of Physics, University of Silesia
Bankowa 14, 40-007 Katowice, Poland

and Peter Entel

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

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The problem of phonon-induced and phonon-free superconductivity in the two-dimensional Hubbard model has been addressed. We have generalized the Eliashberg equations to account for both on-site and intersite pairing and consider the electron–electron and electron-phonon channels on an equal footing. This approach allows for the discussion of pairing and depairing properties of the local repulsive interaction. We demonstrate the possibility of cooperation between electron-phonon and electron–electron interaction in the stabilization of the d-wave superconductivity, in particular close to the experimental value of optimal doping ($\delta \simeq 0.15$). We have also discussed the problem of phonon-induced superconductivity in the two-dimensional Hubbard model close to the metal-insulator transition. Here, the Coulomb correlations have been incorporated within the Hubbard I approximation whereas the superconductivity is treated by the Eliashberg scheme. The results support the view that a d-wave component dominates in the gap function.

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1. Introduction

In spite of active experimental and theoretical investigations the origin of pairing correlations responsible for high-temperature superconductivity is still the matter at issue. On one hand, the proximity of the superconducting and antiferromagnetic phase suggests that Coulomb correlations may give rise to the formation of superconducting phase at low doping. Here, the antiferromagnetic spin fluctuations [1-8] can be considered as a phonon-free mechanism of d-wave superconductivity. This scenario is supported by increasing experimental evidence for $d_{x^2-y^2}$ symmetry of the superconducting order parameter [9–13] but one can not exclude admixture of components with s-like symmetry. In particular, the Monte Carlo calculations [4–6] suggest the dominating role of d-wave pairing. The Monte Carlo scheme works for temperatures which are by far too high to be identified with superconducting transition temperature T_c. However, the dominating role of d-wave symmetry in the two-dimensional Hubbard model has been proved within the second order self-consistent perturbation theory [14]. One should bear in mind that in strictly two dimensions (2d), d-wave superconductivity is absent, even at zero temperature [15]. Therefore, model calculations for the 2d-Hubbard model always assume that there is some effective coupling to the third dimension.

On the other hand, modification of phononic properties below T_c [16–18] remains in agreement with the expectation of strong electron-phonon coupling [19, 20]. Generally, there are arguments that phonon-induced superconductivity can survive in the presence of strong Coulomb correlations [21–27] which may even lead to an enhancement of the electron–phonon coupling [28, 29]. In particular, the inclusion of vertex corrections to the electron–phonon interaction gives rise to the pronounced reduction of the isotope shift exponent α at optimal doping [30]. There are experimental indications that in the copper oxides α is inversely correlated with T_c [31–33]. Therefore, this result supports the view that small values of α do not eliminate electron–phonon interaction as a possible pairing mechanism in high-temperature superconductors. In order to explain small values of α one has not to assume that the non-phononic mechanism is plugged in (and starts to play the dominating role in superconducting pairing) when approaching optimal doping. This picture may emerge within the electron–phonon mechanism due to multiphonon processes contained in corrections to the bare electron–phonon vertex. Phonons can also contribute to the interlayer coupling. It has been argued that momentum conserving interlayer tunnelling can play a substantial role in the formation of the superconducting state [34, 35]. Phonon assisted transitions between intra- and interlayer states result in the c-axis two-phonon-mediated interlayer coupling which

gives an important contribution to the transportation of Cooper pairs between adjacent copper–oxygen sheets [36, 37].

Often, when considering phonon-mediated superconductivity [21–25, 27, 30], the Coulomb correlations have been taken into account by using auxiliary boson fields in the $U \to \infty$ limit [38]. In Refs [24, 27, 39] fluctuations of auxiliary boson fields over the mean-field value have been considered to allow for the phonon-free pairing mechanism. It has been found that the phonon-mediated and correlation-mediated pairing mechanism cooperate in the stabilization of d-wave superconductivity for physically interesting concentrations of holes. This approach partially accounts for the many body effects responsible for the exchange-like origin of superconductivity similarly to superconductivity based on the electron-phonon interaction. However, the relative significance of correlation-mediated and phonon-mediated contributions to the formation of superconducting state is still an open problem. In order to see the actual role of Coulomb correlations, one has to consider the electron–electron and electron–phonon channel on an equal footing. We will outline a generalization of Eliashberg equations [40] which accounts for both channels and allows to consider pairing and depairing effects originating from the U-term in the Hubbard model. The impact of Coulomb correlations upon the magnitude of the isotope shift exponent α will also be discussed.

In high-temperature superconductors superconductivity occurs in the vicinity of the metal-insulator transition. Neither the slave boson technique nor perturbation theory can reproduce the formation of the insulating gap in the density of states at half filling. The fundamental problem is, how to consider the metal-insulator transition within the strong-coupling theory of superconductivity. We will mimic the metal–insulator transition by making use of the Hubbard I approximation [40] and renormalize propagators in the matrix Dyson equation. This approach allows to discuss pairing in the vicinity of the metal–insulator transition.

2. Phonon-induced and phonon-free superconductivity in the two-dimensional Hubbard model

Our starting point is the two-dimensional Hubbard model with electron–phonon interaction. In Nambu notation [40] the Hamiltonian is of the form

$$H \;=\; H_0 + H_U + H_{E-PH}\,, \tag{1}$$

where

$$H_0 \;=\; \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu)\, \Psi^{+}_{\boldsymbol{k}} \tau_3 \Psi_{\boldsymbol{k}} \;+\; \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} B^{+}_{\boldsymbol{q}} B_{\boldsymbol{q}}\,, \tag{2}$$

$$H_U \;=\; \frac{U}{N}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \Psi^{+}_{\boldsymbol{k}}\tau_{+}\Psi_{-\boldsymbol{k}'}\Psi^{+}_{-\boldsymbol{k}'-\boldsymbol{q}}\tau_{-}\Psi_{\boldsymbol{k}-\boldsymbol{q}}\,, \tag{3}$$

$$H_{E-PH} \;=\; \sum_{\boldsymbol{k},\boldsymbol{q}} g_{\boldsymbol{k}\boldsymbol{k}+\boldsymbol{q}}\Psi^{+}_{\boldsymbol{k}+\boldsymbol{q}}\tau_3\Psi_{\boldsymbol{k}}\left(B^{+}_{-\boldsymbol{q}}+B_{\boldsymbol{q}}\right). \tag{4}$$

Here, $\Psi^{+}_{\boldsymbol{k}}=\left(c^{+}_{\boldsymbol{k}\uparrow}\; c_{-\boldsymbol{k}\downarrow}\right)$, where $c_{\boldsymbol{k}\sigma}\left(c^{+}_{\boldsymbol{k}\sigma}\right)$ denotes the annihilation (creation) operator for an electron in a Bloch state with momentum $\boldsymbol{k}$ and spin σ; $\tau_0,\ldots,\tau_3$ denote the Pauli matrices and $\tau_{\pm}=\frac{1}{2}\left(\tau_1\pm i\tau_2\right)$. The band energy is $\varepsilon_{\boldsymbol{k}}=-t\gamma\left(\boldsymbol{k}\right)$ where $\gamma\left(\boldsymbol{k}\right)=2\left(\cos k_x+\cos k_y\right)$ for the nearest-neighbor hopping t which will be taken as energy unit throughout the paper. The energy U is the on-site Coulomb repulsion and μ stands for the chemical potential. $g_{\boldsymbol{k}\boldsymbol{k}+\boldsymbol{q}}$ is the electron–phonon interaction. For the sake of simplicity phonons will be modelled by an Einstein oscillator with frequency ω_0.

The self-energy can be derived from the matrix Dyson equation

$$\Sigma_{\boldsymbol{k}}\left(i\omega_l\right) \;=\; G^{-1}_{0\boldsymbol{k}}\left(i\omega_l\right)-G^{-1}_{\boldsymbol{k}}\left(i\omega_l\right), \tag{5}$$

where $G_{\boldsymbol{k}}\left(i\omega_l\right)=\left\langle\left\langle\Psi_{\boldsymbol{k}}\mid\Psi^{+}_{\boldsymbol{k}}\right\rangle\right\rangle$ stands for the Matsubara Green's function and $G_{0\boldsymbol{k}}\left(i\omega_l\right)$ denotes the unperturbed propagator ($U=0$ and $g_{\boldsymbol{k}\boldsymbol{k}+\boldsymbol{q}}=0$); ω_l is the Matsubara frequency $\omega_l=\left(2l+1\right)\pi/\beta$, $\beta=\left(kT\right)^{-1}$. Within second-order perturbation theory there is no direct mixing between electron–phonon and electron–electron contributions to $\Sigma_{\boldsymbol{k}}\left(i\omega_l\right)$:

$$\Sigma_{\boldsymbol{k}}\left(i\omega_l\right)=\Sigma^{PH}_{\boldsymbol{k}}\left(i\omega_l\right)+\Sigma^{U}_{\boldsymbol{k}}\left(i\omega_l\right), \tag{6}$$

where $\Sigma^{PH}_{\boldsymbol{k}}\left(i\omega_l\right)$ originates from the electron–phonon interaction and $\Sigma^{U}_{\boldsymbol{k}}\left(i\omega_l\right)$ comes from the Coulomb term. Figure 1 shows the diagrammatic representation of both these contributions to the self-energy. The usual ansatz for $\Sigma_{\boldsymbol{k}}\left(i\omega_l\right)$ is of the form [39]

$$\Sigma_{\boldsymbol{k}}\left(i\omega_l\right)=\left[1-Z_{\boldsymbol{k}}\left(i\omega_l\right)\right]i\omega_l\tau_0\;+\;\phi_{\boldsymbol{k}}\left(i\omega_l\right)\tau_1\;+\;\chi_{\boldsymbol{k}}\left(i\omega_l\right)\tau_3. \tag{7}$$

$Z_{\boldsymbol{k}}\left(i\omega_l\right)$ denotes the wave function renormalization factor which will be considered within the local approximation [39,41] ($Z_{\boldsymbol{k}}\left(i\omega_l\right)\to Z\left(i\omega_l\right)$). We will neglect the energy shift $\chi_{\boldsymbol{k}}\left(i\omega_l\right)$ which is usually considered to be a small quantity in the electron–phonon problem and can be incorporated in the chemical potential. For the case of local and nearest-neighbor Cooper pairs we can express the momentum dependence of the superconducting order parameter

$$\phi_{\boldsymbol{k}}\left(i\omega_l\right)=\phi_0\left(i\omega_l\right)\;+\;\gamma\left(\boldsymbol{k}\right)\phi_{\gamma}\left(i\omega_l\right)\;+\;\eta\left(\boldsymbol{k}\right)\phi_{\eta}\left(i\omega_l\right), \tag{8}$$

with the help of form-factors like $\gamma(\boldsymbol{k}) = 2(\cos k_x + \cos k_y)$ and $\eta(\boldsymbol{k}) = 2(\cos k_x - \cos k_y)$. In our notation, $\phi_0(i\omega_l)$, $\phi_\gamma(i\omega_l)$, $\phi_\eta(i\omega_l)$ corresponds to the s-wave, extended s-wave, and d-wave component of the superconducting state, respectively.

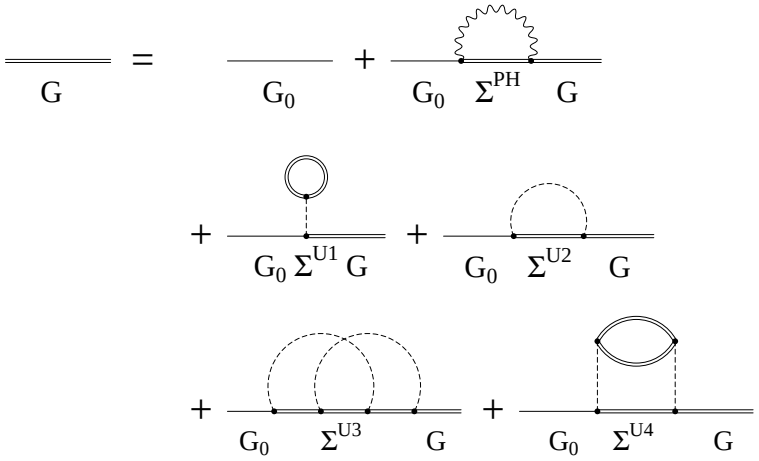

Fig. 1. Diagrammatic representation of contributions to the self-energy. Σ^{PH} originates from the electron–phonon coupling, whereas Σ^{U1}, Σ^{U2}, Σ^{U3}, and Σ^{U4} correspond to contributions from the electron–electron interaction.

In order to derive the system of Eliashberg equations which determine the wave function renormalization factor $Z_{\boldsymbol{k}}(i\omega_l)$ and components of the order parameter one has to combine Eqs (5)–(7) with $\Sigma^{PH}_{\boldsymbol{k}}(i\omega_l)$ and $\Sigma^{U}_{\boldsymbol{k}}(i\omega_l)$ which are both represented diagrammatically in figure 1. Then electron–phonon and electron–electron interactions are considered on an equal footing within the self-consistent second-order perturbation theory. The details of the two-dimensional band structure will be explicitly taken into account. For $T \to T_c$ the Eliashberg equations take on the form

$$Z(i\omega_l) = 1 + \frac{1}{\beta\omega_l}\sum_n \left[U^2 K^I_U(i\omega_l + i\omega_n) + \lambda K_{PH}(l-n)\right] \times \frac{1}{N}\sum_{\boldsymbol{k}} Z(i\omega_n)\,\omega_n D^{-1}_{\boldsymbol{k}}(i\omega_n), \tag{9}$$

$$\phi_0(i\omega_l) = \frac{1}{\beta}\sum_n \left[-U + U^2 K^I_U(i\omega_l + i\omega_n) + \lambda K_{PH}(l-n)\right] \times \frac{1}{N}\sum_{\boldsymbol{k}} \left(\phi_0(i\omega_n) + \gamma(\boldsymbol{k})\,\phi_\gamma(i\omega_n)\right) D^{-1}_{\boldsymbol{k}}(i\omega_n), \tag{10}$$

$$\phi_\gamma(i\omega_l) = \frac{1}{4\beta}\sum_n \left[U^2 K_U^A(i\omega_l + i\omega_n) + \lambda_\gamma K_{PH}(l-n)\right] \times \frac{1}{N}\sum_{\boldsymbol{k}} \left(\gamma(\boldsymbol{k})\phi_0(i\omega_n) + \gamma^2(\boldsymbol{k})\phi_\gamma(i\omega_n)\right) D_{\boldsymbol{k}}^{-1}(i\omega_n), \quad (11)$$

$$\phi_\eta(i\omega_l) = \frac{1}{4\beta}\sum_n \left[U^2 K_U^A(i\omega_l + i\omega_n) + \lambda_\gamma K_{PH}(l-n)\right] \times \frac{1}{N}\sum_{\boldsymbol{k}} \eta^2(\boldsymbol{k})\phi_\eta(i\omega_n) D_{\boldsymbol{k}}^{-1}(i\omega_n), \quad (12)$$

where

$$K_{PH}(l-n) = \frac{\nu^2}{(l-n)^2 + \nu^2}, \quad (13)$$

$$K_U^{I(A)}(i\omega_l + i\omega_n) = \frac{1}{\beta}\sum_m \Big[d_{Z(Z\gamma)}(i\omega_l + i\omega_n - i\omega_m) d_{Z(Z\gamma)}(i\omega_m) + d_{\varepsilon(\varepsilon\gamma)}(i\omega_l + i\omega_n - i\omega_m) d_{\varepsilon(\varepsilon\gamma)}(i\omega_m)\Big], \quad (14)$$

and

$$\begin{pmatrix} d_Z(i\omega_n) \\ d_{Z\gamma}(i\omega_n) \\ d_\varepsilon(i\omega_n) \\ d_{\varepsilon\gamma}(i\omega_n) \end{pmatrix} = \frac{1}{N}\sum_{\boldsymbol{k}} D_{\boldsymbol{k}}^{-1}(i\omega_n) \begin{pmatrix} Z(i\omega_n)\omega_n \\ \frac{1}{4}Z(i\omega_n)\omega_n\gamma(\boldsymbol{k}) \\ \bar{\varepsilon}_{\boldsymbol{k}} \\ \frac{1}{4}\bar{\varepsilon}_{\boldsymbol{k}}\gamma(\boldsymbol{k}) \end{pmatrix}, \quad (15)$$

$$D_{\boldsymbol{k}}(i\omega_n) = [Z(i\omega_n)\omega_n]^2 + (\bar{\varepsilon}_{\boldsymbol{k}})^2. \quad (16)$$

The band energy $\bar{\varepsilon}_{\boldsymbol{k}} = -t\gamma(\boldsymbol{k}) - \mu + nU/2$ is renormalized by the Hartree–Fock contribution; n stands for the average number of electrons per site. In addition one has the equation for the chemical potential

$$n = 1 - \frac{4}{\beta}\sum_{n\geq 0}\frac{1}{N}\sum_{\boldsymbol{k}}\frac{-t\gamma(\boldsymbol{k}) - \mu + Un/2}{[Z(i\omega_n)\omega_n]^2 + [-t\gamma(\boldsymbol{k}) - \mu + Un/2]^2}. \quad (17)$$

Here we distinguish between two types of kernels: K_{PH} corresponds to the electron–phonon interaction, whereas $K_U^{I(A)}$ represents the result of the second-order perturbative treatment of the local Coulomb repulsion U. K_U^I determines the magnitude of the wave function renormalization factor Z and contains correlations leading to the formation of local Cooper pairs (s-wave). K_U^A is responsible for anisotropic superconductivity (extended s-wave and d-wave). Note that when accounting for nearest-neighbor Cooper pairs, one obtains two different electron–phonon coupling functions λ and

λ_γ [24, 25, 27]. $\lambda_{(\gamma)}$ is derived with the help of Fermi-surface averaged Eliashberg function

$$\lambda \;=\; 2\int\limits_0^\infty \frac{\mathrm{d}\Omega}{\Omega}\left\langle -\frac{1}{\pi}\, g_{\boldsymbol{pk}}\, g_{\boldsymbol{kp}}\, \mathrm{Im}\, D_{\boldsymbol{k}-\boldsymbol{p}}\left(\Omega + i\delta\right)\right\rangle_{\boldsymbol{k},\boldsymbol{p}}, \tag{18}$$

$$\lambda_\gamma \;=\; 2\int\limits_0^\infty \frac{\mathrm{d}\Omega}{\Omega}\frac{1}{N}\sum_{\boldsymbol{q}}\frac{1}{4}\gamma\left(\boldsymbol{q}\right)\left\langle -\frac{1}{\pi}\, g_{\boldsymbol{kk}-\boldsymbol{q}}\, g_{\boldsymbol{k}-\boldsymbol{q}\boldsymbol{k}}\, \mathrm{Im}\, D_{\boldsymbol{q}}\left(\Omega + i\delta\right)\right\rangle_{\boldsymbol{k}}, \tag{19}$$

with $D_{\boldsymbol{q}}\left(\Omega\right)$ being the phonon propagator. The quantity λ_γ determines the amplitudes of extended s-wave and d-wave components of the superconducting order parameter, whereas λ determines the magnitude of s-wave component and wave function renormalization factor. Generally, λ and λ_γ depend on the occupation number [27], however, in order to simplify our model calculations, we consider them as parameters [24, 25]. Equations (9)–(13) and (17) represent a self-consistent system which allows for a thorough comparison between electron–electron and electron–phonon contributions to the superconducting state in the two-dimensional Hubbard model. For numerical purposes we have used Kresin's method of introducing an average phonon frequency $\langle\Omega\rangle$ [43]

$$\nu = \frac{\langle\Omega\rangle}{2\pi k T_c}, \tag{20}$$

which corresponds to the frequency ω_0 of an Einstein oscillator ($\omega_0 = 0.1t$ has been used throughout this paper). In the electron–phonon problem the phonon-frequency is related to a cut-off energy. Note, that there is no cut-off energy in the Coulomb channel. This implies that in order to solve the system of Eliashberg equations one has to carry out the summation over a much larger number of Matsubara frequencies than in the usual electron–phonon problem. We have carried out a summation over 400 Matsubara frequencies.

Figure 2 shows the modification of the wave function renormalization factor due to the on-site repulsion. We have plotted $Z\left(i\omega_m\right)$ for the lowest Matsubara frequency ($Z_{m=0} = Z\left(i\pi kT\right)$) as a function of the occupation number. For relatively large concentration of holes $\delta = 1 - n \simeq 0.3$ the difference $Z(U) - Z(U=0)$ (calculated with and without Coulomb repulsion) hardly depends on the magnitude of the electron–phonon coupling. Therefore, electron–phonon and electron–electron contributions to $Z\left(i\omega_l\right)$ can be considered as almost independent quantities in the overdoped region. The difference between $Z\left(U\right)$ and $Z\left(0\right)$ becomes more pronounced in the underdoped region, close to half filling. One may say that spin fluctuations, which are to some extent contained in the U^2-contribution, lead to a more

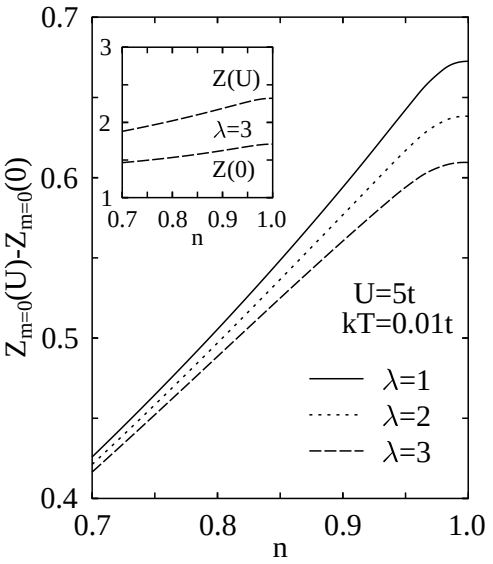

Fig. 2. Modification of the wave function renormalization factor due to Coulomb correlations plotted as a function of the occupation number; $Z_{m=0} = Z\,(i\pi kT)$ corresponds to the lowest Matsubara frequency; $Z_{m=0}\,(U)$ $(Z_{m=0}\,(0))$ denotes $Z\,(i\pi kT)$ calculated with (without) the Coulomb correlations. The inset shows the occupation number dependence of $Z\,(i\pi kT)$ for $U = 0$ and $U = 5t$.

effective modification of normal state properties close to the metal-insulator transition in the vicinity of the onset of an antiferromagnetic order. The inset illustrates the magnitude of $Z\,(i\pi kT)$ calculated with and without the on-site repulsion. For $U < t$ the wave function renormalization factor hardly depends on the magnitude of the on-site repulsion. This feature is related to the fact that only second- and higher-order contributions can lead to a modification of the band structure. With respect to the significance of the U-term for normal state properties one can infer from figure 3 that Coulomb correlations are much more important for larger values of the Matsubara frequencies. In the case of weak Coulomb correlations $Z\,(i\omega_n)$ differs significantly from unity only in the narrow region of ω_n around 0. Note that $Z\,(i\omega_n) = 1$ corresponds to the unperturbed propagator. However, already moderate values of the on-site repulsion U cause pronounced modification of the wave function renormalization factor for large values of ω_n. This feature originates from different structure of kernels corresponding to the electron–electron ($K_U^{I(A)}$) and electron–phonon (K_{PH}) interaction. On one hand, the Debye energy ω_0 which enters K_{PH} can be considered as an effective *cut-off* in summation over the Matsubara frequencies. On the other hand,

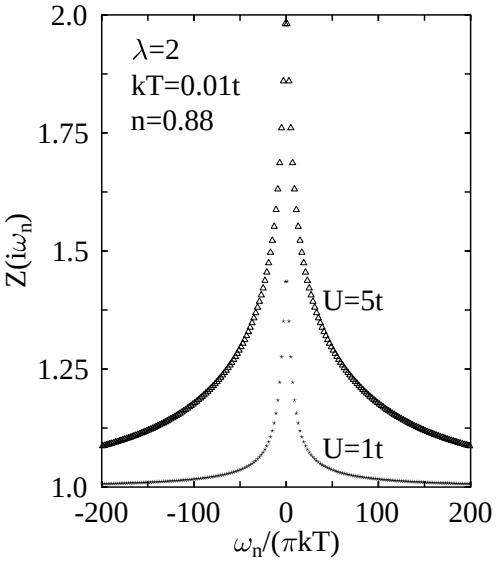

Fig. 3. The wave function renormalization factor $Z\,(i\omega_n)$ as a function of Matsubara frequencies. Note the pronounced modification of $Z\,(i\omega_n)$ due to the Coulomb correlations for large values of ω_n.

the band-width is the only quantity which can play the role of the *cut-off* when considering $K_U^{I(A)}$. Therefore, in order to proceed with the quantitative analysis of the electron–electron channel a few hundred of Matsubara frequencies have to be taken into account.

For $T \to T_c$ the s- and extended s-wave components separate from the d-wave component of the superconducting order parameter. Figure 4 shows the superconducting transition temperatures for both cases as a function of the on-site repulsion. One can see that even weak Coulomb correlations strongly reduce the role of the $s-$ and extended s-wave contributions. Keeping in mind that the wave function renormalization factor remains almost unchanged for small values of U one can attribute this behavior to the Hartree–Fock term which enters Eq. (10). This term is absent in Eq. (12) which causes that d-wave superconductivity can survive despite the presence of relatively strong on-site repulsion.

Figures 5 and 6 show interesting features connected with the presence of the Coulomb channel. We plot the relative change of the superconducting transition temperature due the on-site repulsion as a function of the occupation number. Here, $T_c\,(U)$ $(T_c\,(0))$ denotes the critical temperature calculated with (without) Coulomb correlations. Figures 5 and 6 explicitly show the possibility of a cooperation between the electron–phonon and

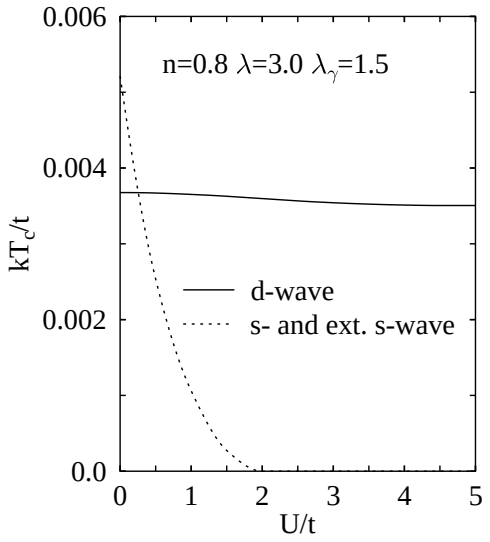

Fig. 4. The superconducting transition temperature corresponding to d-, s- and extended s-wave symmetry. At $T \to T_c$ a d-wave contribution separates from the s- and extended s-wave component of the superconducting order parameter.

electron–electron interaction in the formation of the superconducting phase. The on-site repulsion enters the Eliashberg equations in a highly non-trivial way. On one hand, the increase of the wave function renormalization factor with U leads to a reduction of the superconducting transition temperature. This mechanism plays the most important role for small values of λ. On the other hand, the electron–electron contribution to d-wave paring, as represented by the kernel K_U^A, leads to a significant increase of T_c, in particular when $\lambda_\gamma K_{PH}$ is sufficiently small. The relative role of these two mechanisms depends also on the concentration of holes, as can be inferred from the inset in figure 5. Therefore, the significance of the U^2-term for d-wave superconductivity is directly related to the occupation number and the ratio λ_γ/λ. It is remarkable, that stabilization of the d-wave superconductivity due to the on-site repulsion is mostly effective close to the experimental value of optimal doping ($\delta \simeq 0.15$).

There are experimental indications that for the copper oxides the isotope shift exponent α is inversely correlated with T_c and can take on values much smaller than the BCS value of 0.5 [30–32]. There are proposals to explain this feature within a purely phononic mechanism of superconductivity [21, 29]. In particular, the inclusion of vertex corrections can lead to a pronounced reduction of α at optimal doping [29]. Here, we demonstrate that such a reduction can also originate from the presence of Coulomb correlations

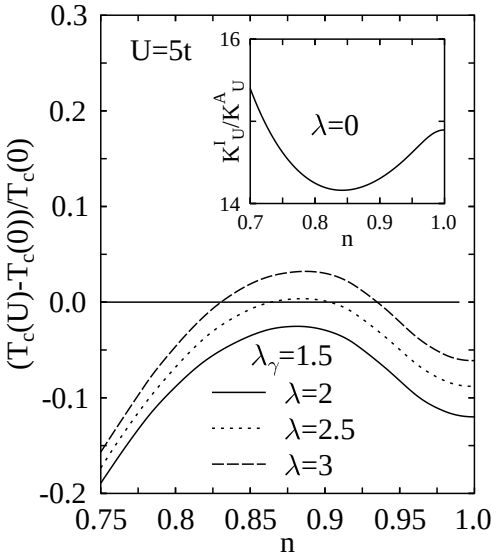

Fig. 5. The relative change of T_c (d-wave) due to the on-site repulsion plotted as a function of the occupation number. $T\,(U)$ $(T\,(O))$ denotes the critical temperature calculated with (without) the Coulomb correlations. The inset shows the ratio $K_U^I\,(i\omega_l + i\omega_n)\,/K_U^A\,(i\omega_l + i\omega_n)$ calculated for $i\omega_l + i\omega_n = 0$ and $\lambda = 0$.

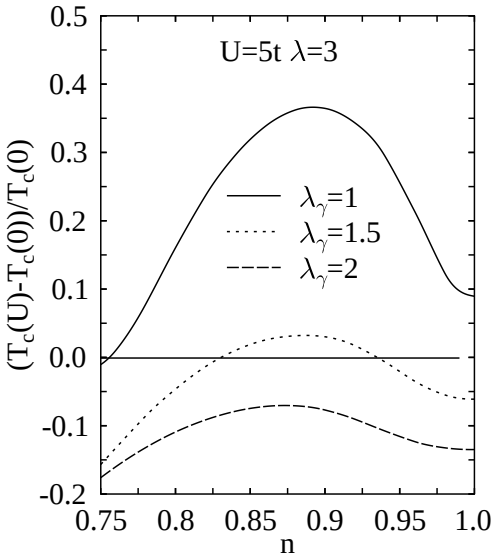

Fig. 6. The same as in Fig. 4 but for different values of the electron–phonon coupling functions.

which contribute to superconducting pairing. In order to evaluate α we assume that $\lambda_{(\gamma)}K_{PH}$ depends on M only through $\omega_0 \sim M^{-1/2}$, then

$$\alpha = \frac{\omega_0}{2\,T_c}\frac{\mathrm{d}T_c}{\mathrm{d}\omega_0}\,. \tag{21}$$

Numerical values of α are shown in figure 7. In the underdoped region U hardly affects α which can achieve values slightly higher than 0.5. For $n > 0.8$ the local repulsion leads to a fairly pronounced decrease of the isotope shift exponent. Close to the optimal doping this can be understood as a result of non-phononic contribution to the superconducting correlations (figures 6 and 7). However, the isotope shift exponent is inversely correlated with U also in the underdoped system despite the reduction of T_c due to Coulomb correlations (compare with results corresponding to $\lambda_\gamma = 1.5$ in figure 6). One should bear in mind that our perturbative formulation neither contains any direct pair-breaking mechanism for d-wave superconductivity nor accounts for the metal-insulator transition when approaching half filling. Therefore, one obtains a maximum T_c for $n \to 1$, simply due to the van Hove singularity. This drawback can be removed when accounting for the opening of an insulating gap for $n \to 1$. This simple approach to the problem will be discussed in the next section.

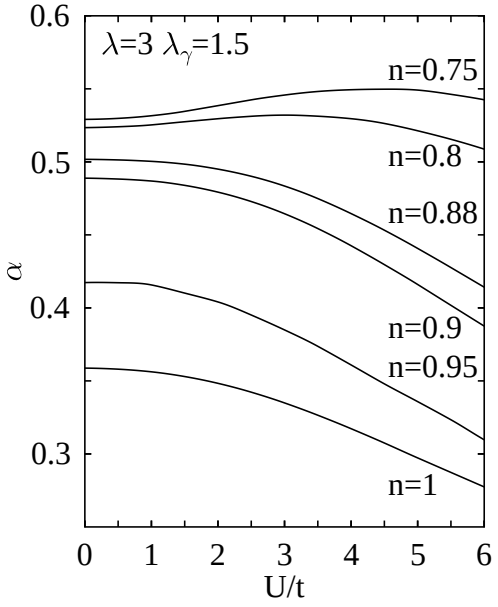

Fig. 7. The isotope shift exponent α as a function of the on-site repulsion for different concentrations of holes.

3. Phonon-induced superconductivity in the two-dimensional Hubbard model close to the metal-insulator transition

The simplest approach which can mimic the metal-insulator transition is the Hubbard I approximation [41, 44]. This approximation neither reproduces the Hartree–Fock solution for small values of the Coulomb repulsion U nor fulfils the Luttinger theorem. These deficiencies are important when discussing phonon-free superconductivity within the bare Hubbard model. In the case of phonon-induced superconductivity this approach can be useful to discuss pairing in the vicinity of the metal-insulator transition, even if the Hubbard I approximation overestimates the magnitude of the insulating gap which occurs for any finite value of U.

In order to account for local Coulomb repulsion in the Hubbard I approximation one has to renormalize the electron propagator in the Dyson equation [41, 44, 45]. This corresponds to the substitution

$$G_{0\boldsymbol{k}}^{-1}\left(i\omega_l\right) = \begin{pmatrix} G_{at}^{-1}\left(i\omega_l\right) - \varepsilon_{\boldsymbol{k}} & 0 \\ 0 & -G_{at}^{-1}\left(-i\omega_l\right) + \varepsilon_{\boldsymbol{k}} \end{pmatrix}, \tag{22}$$

with

$$G_{at}^{-1}\left(i\omega_l\right) = \frac{\left(i\omega_l + \mu\right)\left(i\omega_l + \mu - U\right)}{\left(i\omega_l + \mu\right) - U\left(1 - n/2\right)}. \tag{23}$$

At $T = T_c$ s- and d- wave symmetries separate and the Eliashberg equations take on the form [45]

$$Z\left(i\omega_l\right) = 1 + \frac{1}{\beta\omega_l}\sum_{\omega_n}\frac{\lambda\,\nu^2}{\left(l-n\right)^2+\nu^2}\,d_Z\left(i\omega_n\right), \tag{24}$$

$$\phi_0\left(i\omega_l\right) = \frac{1}{\beta}\sum_{\omega_n}\frac{\lambda\,\nu^2}{\left(l-n\right)^2+\nu^2}\,\left[d_0\left(i\omega_n\right)\phi_0\left(i\omega_n\right) + d_\gamma\left(i\omega_n\right)\phi_\gamma\left(i\omega_n\right)\right], \tag{25}$$

$$\phi_\gamma\left(i\omega_l\right) = \frac{1}{\beta}\sum_{\omega_n}\frac{\lambda_\gamma\,\nu^2}{\left(l-n\right)^2+\nu^2}\,\left[d_\gamma\left(i\omega_n\right)\frac{\phi_0\left(i\omega_n\right)}{4} + d_{\gamma^2}\left(i\omega_n\right)\frac{\phi_\gamma\left(i\omega_n\right)}{4}\right], \tag{26}$$

$$\phi_\eta\left(i\omega_l\right) = \frac{1}{\beta}\sum_{\omega_n}\frac{\lambda_\gamma\,\nu^2}{\left(l-n\right)^2+\nu^2}\,d_{\eta^2}\left(i\omega_n\right)\phi_\eta\left(i\omega_n\right), \tag{27}$$

where we have used

$$d_Z\left(i\omega_n\right) = \frac{1}{N}\sum_{\boldsymbol{k}} d_{\boldsymbol{k}}\left(i\omega_n\right)\,\omega_n\left\{2\,U\left(1-\frac{n}{2}\right)\left(U-2\mu\right)+\omega_n^2+\mu^2 + \left[Z\left(i\omega_n\right)-1\right]\left[\omega_n^2+\left(\mu-U\left(1-\frac{n}{2}\right)\right)^2\right]\right\}, \tag{28}$$

$$\begin{pmatrix} d_0\left(i\omega_n\right) \\ d_\gamma\left(i\omega_n\right) \\ d_{\gamma^2}\left(i\omega_n\right) \\ d_{\eta^2}\left(i\omega_n\right) \end{pmatrix} = \frac{1}{N}\sum_{\boldsymbol{k}} d_{\boldsymbol{k}}\left(i\omega_n\right)\left[\omega_n^2+\left(\mu-U\left(1-\frac{n}{2}\right)\right)^2\right]\begin{pmatrix} 1 \\ \gamma\left(\boldsymbol{k}\right) \\ \gamma^2\left(\boldsymbol{k}\right) \\ \eta^2\left(\boldsymbol{k}\right) \end{pmatrix}, \tag{29}$$

and

$$d_{\boldsymbol{k}}^{-1}\left(i\omega_l\right) = \left(\omega_l^2+\mu^2\right)\left\{\omega_l^2+\left(\mu-U\right)^2+2\left[\omega_l^2\left(Z\left(i\omega_l\right)-1\right)-\left(\mu-U\right)\varepsilon_{\boldsymbol{k}}\right]\right\} + 2\,U\left(1-\frac{n}{2}\right)\left\{\omega_l^2\left[\left(Z\left(i\omega_l\right)-1\right]\left(U-2\mu\right)+\varepsilon_{\boldsymbol{k}}\left(\mu^2-\omega_l^2-U\mu\right)\right\}\right. + \left\{\omega_l^2+\left[\mu-U\left(1-\frac{n}{2}\right)\right]^2\right\}\left\{\omega_l^2+\left[Z\left(i\omega_l\right)-1\right]^2+\varepsilon_{\boldsymbol{k}}^2\right\}. \tag{30}$$

Figure 8 shows the dependence of the superconducting transition temperature on the occupation number for different types of symmetry of the order parameter. It is remarkable that the renormalization introduced within the Hubbard I approximation, leads to a variation of T_c which corresponds to the experimentally observed behavior. One can also note that the superconducting transition temperature for s- and d-wave superconductivity is of comparable magnitude in the physically interesting region of concentration of holes. Due to the fact that the extended s-wave contribution becomes small because of the nesting of the Fermi surface for $n \to 1$, it is the isotropic s-wave component that adds to the d-wave component. Both types of pairing rapidly vanish when approaching the metal-insulator transition at half filling. Therefore, this simple approach may partially account for the d+s-wave scenario of high-temperature superconductivity [46,47]. However, one must be aware that the Hubbard I approximation does not reproduce the depairing role of the Hartree–Fock term in the purely electronic s-wave (isotropic) channel. May be, its role is of minor importance when considering superconductivity originating from strong electron–phonon interaction close to the metal-insulator transition.

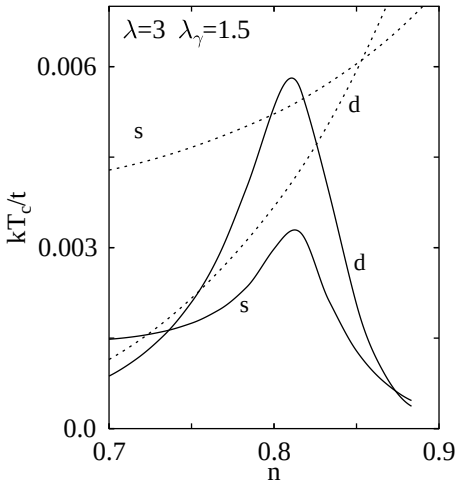

Fig. 8. The superconducting transition temperature as a function of the occupation number. Here, s refers to T_c for s-wave + extended s-wave symmetry, whereas d corresponds to d-wave symmetry. The dashed curves represent the uncorrelated case ($U = 0$) and solid curves have been obtained within the Hubbard I approximation ($U = 2t$). λ is the electron–phonon coupling function which determines the magnitude of the renormalization factor Z and accounts for s-wave (isotropic) superconductivity, whereas λ_γ is responsible for anisotropic superconductivity.

4. Concluding remarks

The two-dimensional Hubbard model coupled to phonons has been discussed in the context of isotropic and anisotropic superconductivity. Pairing correlations originating from the electron–phonon interaction and the on-site Coulomb repulsion have been considered on an equal footing within the self-consistent second-order perturbation theory. This scheme allows to account for both pairing and depairing features of the local Coulomb correlations. Our formulation leads to the generalization of the Eliashberg equations and is valid for moderate values of the on-site repulsion U. Numerical analysis has shown that the Coulomb repulsion pronouncedly enhances the frequency dependence of the wave function renormalization factor and leads to a serious increase in the magnitude of $Z(i\omega_n)$. When considering the symmetry of the superconducting state we have found that s- and extended s-wave components are eliminated already for small values of U. This is due to the presence of the Hartree–Fock contribution to the s-wave kernel in the Eliashberg equations. However, d-wave superconductivity can exist even in the presence of strong local repulsion. Our results demonstrate the possibility of cooperation between electron–phonon and electron–electron interactions

in the formation of d-wave superconducting state. It is remarkable that this cooperation is mostly effective around the experimental value of the optimal doping $\delta \simeq 0.15$. We have observed that the on-site repulsion may lead to a fairly pronounced reduction of the isotope shift exponent α. Therefore, even small values of α do not eliminate the electron–phonon interaction as a possible pairing mechanism in high-temperature superconductors. Small values of α may merely mean that Coulomb correlations contribute to the superconducting pairing in the d-wave channel.

The perturbative formulation is restricted to moderate values of U/t, in the sense that U does not exceed the band-width $8t$. On should bear in mind that the second-order perturbation theory does not account for all possible pairing correlations originating form the local Coulomb repulsion. Probably, this is the reason for which the Coulomb interaction alone cannot produce high superconducting transition temperature. Within the second-order perturbation theory the wave function renormalization factor remains finite independently on the occupations of holes. This implies the non-vanishing values of T_c when approaching the Mott-Hubbard transition for $n \to 1$, However, the simultaneous discussion of the interplay between superconductivity and antiferromagnetism including the metal-insulator transition is a difficult problem which needs a separate study. We have attempted to mimic the metal-insulator transition within the strong-coupling description making use of the Hubbard I approximation for the Coulomb term. This approach correctly describes the vanishing of superconductivity (predominantly of d-wave symmetry) with the opening of the insulating gap. We show that s- and d-wave component can mix considerably as seriously considered in the literature [46,47]. The drawback is that within the Hubbard I approximation one neglects pairing as well as depairing correlations originating from the Coulomb channel, the latter being related to the Hartree–Fock term in the perturbative series. This may be of minor importance when considering superconductivity originating from strong electron–phonon interaction in the vicinity of the metal-insulator transition. Therefore, the discussion of the role of Coulomb correlations for the formation and destruction of the superconducting state at low doping is still an open problem. Independently on the type of approximation it is d-wave superconductivity which plays a dominating role in the presence of local electron–electron interaction. may be that the renormalization of electron–phonon vertex originating from Coulomb correlations can complete the picture of superconductivity in strongly correlated systems. This is a challenge for future studies.

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