Correlation-renormalized electron-phonon interaction in the two-dimensional Hubbard model

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(Received 26 April 1999; revised manuscript received 18 June 1999)

We have addressed the problem of the influence of Coulomb correlations on the electron-phonon interaction in the two-dimensional Hubbard model. Both the energy and momentum dependence of the renormalization factor have been taken into account. We find that the superconducting properties of the system depend strongly on the phononic momentum and energy transfer values. This dependence is related to the symmetry of the superconducting order parameter. On one hand, the renormalization of the electron-phonon coupling function acts to the detriment of superconductivity in the *s*-wave channel. On the other hand, an enhancement of pairing correlations for anisotropic extended *s*-wave and *d*-wave superconductivity is observed.
[S0163-1829(99)03738-8]

I. INTRODUCTION

The proximity of the superconducting and antiferromagnetic phase in high-temperature superconductors suggests that Coulomb correlations may be responsible for the superconducting state at low doping. There is increasing experimental evidence for $d_{x^2-y^2}$ symmetry of the superconducting order parameter (see Ref. 1 for recent results) with antiferromagnetic spin fluctuations[2] as a possible phonon-free pairing mechanism. However, one can also invoke phonon-mediated pairing because of modification of phononic properties below the superconducting transition temperature T_c (Refs. 3 and 4) due to strong electron-phonon coupling.[5] In order to discuss superconductivity originating from strong electron-phonon interaction, one has to go beyond mean-field theory by using an Eliashberg-type of approach.[6] The problem that arises is how to develop the strong-coupling theory in systems with Coulomb correlations that are responsible for narrow quasiparticle bands, lifetime effects of one-particle states close to the Fermi energy, and opening of the insulating gap close to half-filling. Usually one considers phonon-mediated superconductivity, whereby Coulomb correlations are taken into account by using auxiliary boson fields[7] in the $U\rightarrow\infty$ limit of the two-dimensional (2D) Hubbard model.[8–14] The case of *d*-wave pairing has been considered in Refs. 10–14. In Ref. 14 an extension of the Eliashberg formalism has been presented and vertex corrections have been taken into account. In particular, the inclusion of vertex corrections to the electron-phonon interaction gives rise to a pronounced reduction of the exponent of the isotope shift α at optimal doping. As there are experimental indications that in the copper oxides α is inversely correlated with T_c,[15] this result supports the view that small values of α do not eliminate the electron-phonon mechanism because multiphonon processes contained in corrections to the bare electron-phonon vertex are important. The scheme of auxiliary boson fields does not allow us to reproduce the formation of the insulating gap in the density of states at half-filling. One can mimic this effect when renormalizing normal Green functions in the Eliashberg equations with propagators evaluated within the Hubbard I approximation.[16]

The relative significance of correlation-mediated and phonon-mediated contributions to the formation of the superconducting state within the framework of the Hubbard model is still an open problem. One has to consider the electron-electron and electron-phonon channel on an equal footing. We have generalized the Eliashberg equations for the Coulomb channel and shown the dominating role of *d*-wave superconductivity within the second-order self-consistent perturbation theory.[17] This approach allows for a discussion of pairing and depairing properties of the local repulsive interaction and leads to rather small values of T_c. A combination of electron-electron and electron-phonon contributions to the pairing kernels allows us to investigate their impact on *d*-wave superconductivity, in particular for the case of optimal doping.[18] There is an indirect and rather weak coupling between the electron-electron and electron-phonon channel brought about by the chemical potential and the wave-function renormalization factor *Z*. The self-consistent calculation shows that the difference between $Z(U)$ and $Z(U=0)$ is more pronounced in the underdoped region, close to half-filling, when spin fluctuations, which are to some extent contained in the Coulomb contribution, lead to a more effective modification of the normal state properties. Generally the change of T_c, when including the Coulomb channel in the Eliashberg equations, is of minor importance.[18] This may originate from the fact that within this approach there is no renormalization of the electron-phonon coupling due to the presence of Coulomb correlations.

The problem that we address in this paper is to consider the influence of correlations on the electron-phonon interaction in the 2D Hubbard model. On one hand, this problem has been considered in the $U\rightarrow\infty$ limit within the $1/N$ expansion.[19] It has been found that the electron-phonon interaction responsible for transport is pronouncedly suppressed, whereas the superconducting pairing is affected only in a minor way.[19] On the other hand, the application of the generalized random-phase approximation shows that, when

accounting for a finite band-width, the electron-phonon coupling function decreases almost linearly with the increase of Coulomb correlations up to values of U for which the perturbation theory is not applicable any more.[20] This indicates that the dominating contributions to the mixed electron-phonon channel are of the order of g^2U. Therefore, we restrict ourselves only to the lowest-order contributions $(\sim g^2U)$. In our treatment the phononic momentum, the energy transfer, and the two-dimensional density of states are explicitly taken into account. The modification of the electron-phonon coupling functions, which enter Eliashberg equations, is also discussed.

II. RENORMALIZATION OF THE ELECTRON-PHONON INTERACTION ANALYTICAL RESULTS

We consider the 2D Hubbard model coupled to phonons,

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

where

$$H_0=\sum_{\mathbf{k},\sigma}\bar{\varepsilon}_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{\mathbf{q}}\omega_{\mathbf{q}}b^{\dagger}_{\mathbf{q}}b_{\mathbf{q}}, \tag{2}$$

$$H_{E\text{-}PH}=\sum_{\mathbf{k},\mathbf{q},\sigma}g(\mathbf{q})c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}(b^{\dagger}_{-\mathbf{q}}+b_{\mathbf{q}}), \tag{3}$$

$$H_U=\frac{U}{N}\sum_{\mathbf{k},\mathbf{q},\mathbf{p}}c^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}-\mathbf{q}\uparrow}c^{\dagger}_{\mathbf{p}\downarrow}c_{\mathbf{p}+\mathbf{q}\downarrow}. \tag{4}$$

Here, $\bar{\varepsilon}_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\mu$, where $\varepsilon_{\mathbf{k}}=-t\gamma(\mathbf{k})$ with $\gamma(\mathbf{k})=2(\cos k_x a+\cos k_y a)$; t is the nearest-neighbor hopping integral; μ stands for the chemical potential; $H_{E\text{-}PH}$ represents the ionic part of the electron-phonon interaction; H_U is the on-site Coulomb repulsion written in the Bloch representation.

We consider $\langle\langle c_{\mathbf{k}\sigma}|c^{\dagger}_{\mathbf{k}\sigma}\rangle\rangle\equiv G_{\mathbf{k}}(i\omega_n)$, where ω_n is the fermionic Matsubara frequency $\omega_n=\pi/\beta(2n+1)$, $\beta=(k_BT)^{-1}$. Making use of the equations of motion[21] one obtains after some algebra,

$$G_{\mathbf{k}}(i\omega_n)=G_{0\mathbf{k}}(i\omega_n)+G_{0\mathbf{k}}(i\omega_n)\Big[U\langle n_{-\sigma}\rangle+\sum_{A_{\mathbf{k}},B_{\mathbf{k}}}\langle\langle A_{\mathbf{k}}|B^{\dagger}_{\mathbf{k}}\rangle\rangle\Big]G_{0\mathbf{k}}(i\omega_n), \tag{5}$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ stand for the two operators

$$X_{\mathbf{k}}=\sum_{\mathbf{q}}g(\mathbf{q})c_{\mathbf{k}-\mathbf{q}\sigma}\Phi_{\mathbf{q}}, \tag{6}$$

$$Y_{\mathbf{k}}=\frac{U}{N}\sum_{\mathbf{p},\mathbf{q}}c_{\mathbf{k}-\mathbf{q}\sigma}c^{\dagger}_{\mathbf{p}-\sigma}c_{\mathbf{p}+\mathbf{q}-\sigma}. \tag{7}$$

$\langle n_\sigma\rangle$ is the average number of electrons per site and spin direction; $\Phi_{\mathbf{q}}=b_{\mathbf{q}}+b^{\dagger}_{-\mathbf{q}}$;

$$G_{0\mathbf{k}}(i\omega_n)=(i\omega_n-\bar{\varepsilon}_{\mathbf{k}})^{-1} \tag{8}$$

is the unperturbed Green's function. The correlation function $\langle\langle X_{\mathbf{k}}|X^{\dagger}_{\mathbf{k}}\rangle\rangle\sim g^2$ corresponds to the second-order self-energy in the electron-phonon channel and $\langle\langle Y_{\mathbf{k}}|Y^{\dagger}_{\mathbf{k}}\rangle\rangle\sim U^2$ represents the second-order self-energy in the Coulomb channel. Equation (5) can be generalized for the case of the matrix Green's function containing anomalous components. The matrix counterpart of the sum of $\langle\langle X_{\mathbf{k}}|X^{\dagger}_{\mathbf{k}}\rangle\rangle+\langle\langle Y_{\mathbf{k}}|Y^{\dagger}_{\mathbf{k}}\rangle\rangle$ has been considered in Ref. 18.

As mentioned in the Introduction, we restrict ourselves only to the lowest-order contributions $(\sim g^2U)$ to the mixed electron-phonon channel. In our formulation this is $\langle\langle X_{\mathbf{k}}|Y^{\dagger}_{\mathbf{k}}\rangle\rangle$ and $\langle\langle Y_{\mathbf{k}}|X^{\dagger}_{\mathbf{k}}\rangle\rangle$, which are linear in U. Our aim is to investigate these terms with respect to their momentum, Matsubara frequency, and occupation number dependence. Making use of Wick's theorem,[22] we decouple $\langle\langle X_{\mathbf{k}}|Y^{\dagger}_{\mathbf{k}}\rangle\rangle$ in the following way:

$$\langle\langle X_{\mathbf{k}}|Y^{\dagger}_{\mathbf{k}}\rangle\rangle_{i\omega_n}\simeq-\frac{1}{\beta}\frac{U}{N}\sum_{m}\sum_{\mathbf{p},\mathbf{q},\mathbf{q}'}g(\mathbf{q})\langle\langle c_{\mathbf{k}-\mathbf{q}\sigma}|c^{\dagger}_{\mathbf{k}-\mathbf{q}'\sigma}\rangle\rangle_{i\omega_m}\times\langle\langle\Phi_{\mathbf{q}}|c^{\dagger}_{\mathbf{p}+\mathbf{q}'-\sigma}c_{\mathbf{p}-\sigma}\rangle\rangle_{i\omega_n-i\omega_m}, \tag{9}$$

which is reasonable to do for the normal state. Since our aim is to investigate the terms $\sim g^2U$, we evaluate $\langle\langle\Phi_{\mathbf{q}}|c^{\dagger}_{\mathbf{p}+\mathbf{q}'-\sigma}c_{\mathbf{p}-\sigma}\rangle\rangle$ only with $H_0+H_{E\text{-}PH}$. This leads to

$$\begin{aligned}(i\omega_n-i\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}+\varepsilon_{\mathbf{p}})\langle\langle\Phi_{\mathbf{q}}|c^{\dagger}_{\mathbf{p}+\mathbf{q}\sigma}c_{\mathbf{p}\sigma}\rangle\rangle&=\sum_{\mathbf{k},\mathbf{q}'}g^{*}(\mathbf{q}')(\delta_{\mathbf{k}\mathbf{p}+\mathbf{q}-\mathbf{q}'}\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}'}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{p}\sigma}\rangle\rangle\\&\quad-\delta_{\mathbf{k}\mathbf{p}}\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}'}c^{\dagger}_{\mathbf{p}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}'\sigma}\rangle\rangle).\end{aligned} \tag{10}$$

Because of $\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}'},\rangle\rangle\sim\delta_{\mathbf{q}\mathbf{q}'}$, we derive

$$\langle\langle\Phi_{\mathbf{q}}|c^{\dagger}_{\mathbf{p}+\mathbf{q}\sigma}c_{\mathbf{p}\sigma}\rangle\rangle=g^{*}(\mathbf{q})\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}}\rangle\rangle\times\frac{\langle n_{\mathbf{p}\sigma}\rangle-\langle n_{\mathbf{p}+\mathbf{q}\sigma}\rangle}{i\omega_n-i\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}+\varepsilon_{\mathbf{p}}}. \tag{11}$$

The same procedure can be applied to $\langle\langle Y_{\mathbf{k}}|X^{\dagger}_{\mathbf{k}}\rangle\rangle$. This leads to a renormalization of the electron-phonon interaction

$$|g(\mathbf{q})|^2\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}}\rangle\rangle_{i\omega_n-i\omega_m}\rightarrow|g(\mathbf{q})|^2\langle\langle\Phi_{\mathbf{q}}|\Phi^{\dagger}_{\mathbf{q}}\rangle\rangle_{i\omega_n-i\omega_m}\times[1+R_{\mathbf{q}}(i\omega_n-i\omega_m)], \tag{12}$$

where

$$R_{\mathbf{q}}(i\omega_n-i\omega_m)=\frac{2U}{N}\sum_{\mathbf{p}}\frac{\langle n_{\mathbf{p}\sigma}\rangle-\langle n_{\mathbf{p}+\mathbf{q}\sigma}\rangle}{i\omega_n-i\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}+\varepsilon_{\mathbf{p}}}. \tag{13}$$

This decoupling scheme corresponds to

$$R_{\mathbf{q}}(i\omega_n-i\omega_m)=\frac{2U}{\beta N}\sum_{l,\mathbf{p}}G_{0\mathbf{p}}(i\omega_l)G_{0\mathbf{p}+\mathbf{q}}(i\omega_n-i\omega_m+i\omega_l). \tag{14}$$

Here, the renormalization factor $R_{\mathbf{q}}$ is a dimensionless quantity that describes an enhancement (if $R_{\mathbf{q}}>0$) or reduction (if $R_{\mathbf{q}}<0$) of the effective electron-phonon coupling due to the local Coulomb repulsion. Evaluation of $R_{\mathbf{q}}$ allows one to

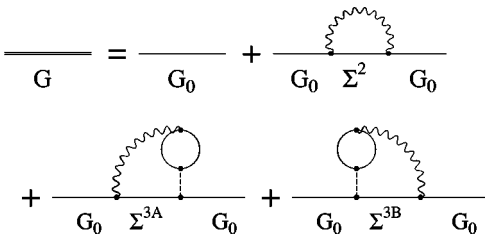

FIG. 1. Diagrammatic representation of the modification of Dyson's equation due to the renormalization of the electron-phonon interaction. Σ^{3A} corresponds to $\langle\langle X_{\mathbf{k}}|Y_{\mathbf{k}}^{\dagger}\rangle\rangle$ and Σ^{3B} to $\langle\langle Y_{\mathbf{k}}|X_{\mathbf{k}}^{\dagger}\rangle\rangle$, see Eq. (5).

discuss the relative role of phonons with different momenta $\mathbf{q}$, whereas its average value corresponds to modification of the electron-phonon coupling function. Figure 1 shows the diagrams that have been taken into account for the normal state. Σ^2 is the usual contribution of order of g^2. Σ^{3A} corresponds to $\langle\langle X_{\mathbf{k}}|Y_{\mathbf{k}}^{\dagger}\rangle\rangle$ and Σ^{3B} to $\langle\langle Y_{\mathbf{k}}|X_{\mathbf{k}}^{\dagger}\rangle\rangle$, respectively. One can see that the decoupling of the equations of motion, as determined by Eq. (9), corresponds to the perturbation theory applied for calculation of terms $\sim g^2U$. Although these two methods give the same lowest-order contributions to the self-energy, the equations of motion enable more straightforward derivation of Eliashberg equations, which, due to their self-consistency, account for higher-order contributions. One should also note that in contradistinction to Ref. 20 the phononic momentum, dynamical effects and the two-dimensional band structure have explicitly been taken into account. It can be shown that $R_{\mathbf{q}}(i\omega_n - i\omega_m)$ fulfills the following relations: $\mathrm{Im}\,R_{\mathbf{q}}(i\omega_n - i\omega_m) = 0$; $R_{\mathbf{q}}(i\omega_n - i\omega_m) \leqslant 0$; for the half-filled band, $R_{\mathbf{q}=\mathbf{0}}(i\omega_n - i\omega_m) > R_{\mathbf{q}=(\pi,\pi)}(i\omega_n - i\omega_m)$; for $n \neq m$ we find $R_{\mathbf{q}=\mathbf{0}}(i\omega_n - i\omega_m) = 0$.

III. DISCUSSION OF NUMERICAL RESULTS

The momentum and frequency dependence of the renormalization factor $R_{\mathbf{q}}$ has been evaluated for different values of the occupation number (Figs. 2–6). The nearest-neighbor hoping intergral t has been taken as an energy unit. It is visible that the $\mathbf{q}=(0,0)$ phonons are not modified when changing the concentration of holes. This takes place for any temperature and energy values. Figures 2–4 show this feature for the concentration of holes close to optimal doping,

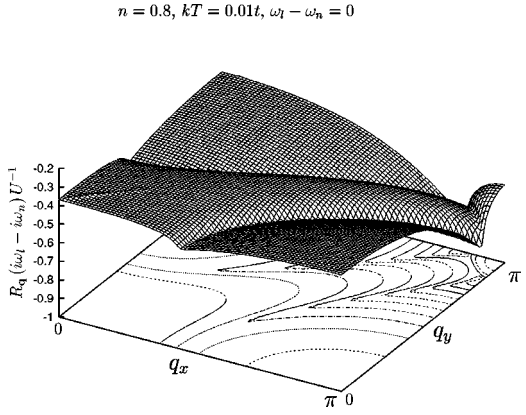

FIG. 2. The momentum dependence of the renormalization factor for the electron-phonon interaction $R_{\mathbf{q}}$.

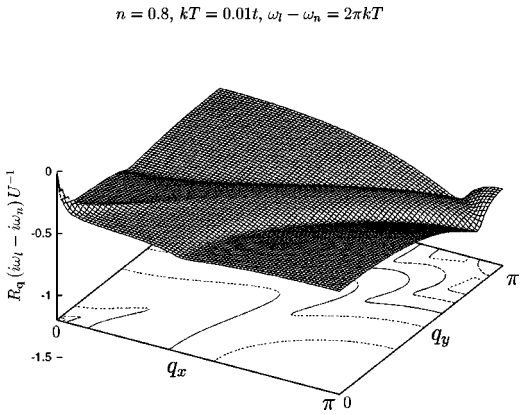

FIG. 3. The same as in Fig. 2 but for a different value of the Matsubara frequency.

whereas Fig. 5 and Fig. 6 show the influence of the occupation number on the behavior of $R_{\mathbf{q}}$. Note that these effects are caused by electronic correlations. This remains in agreement with an assumption of Pietronero and co-workers that phonons with small scattering momentum play the most important role for isotropic superconductivity[23]. This leads to an increase of the critical temperature due to vertex corrections for the uncorrelated electron-phonon system. It is remarkable that, when approaching half-filling, the (π,π) phonons are affected most of all. However, the (π,π) phonons come into the play only when increasing the concentration of holes. The increase of temperature (or, equivalently, the increase of Matsubara frequency) leads to a smearing of the renormalization of the electron-phonon vertex originating from Coulomb repulsion. Therefore, in the presence of Coulomb correlations, the dynamical effects become important.[23]

What one has to discuss is the influence of the renormalization of the electron-phonon coupling functions that enter the kernels of the Eliashberg equations. The presence of electronic correlations strongly reduces the isotropic component of the superconducting order parameter, and one is left with the anisotropic part being of predominantly *d*-wave character. One has to introduce two electron-phonon coupling functions λ and λ_γ.[13,12,16,18] λ leads to a modification of the normal state properties (wave-function renormalization factor and energy shift) and is responsible for the isotropic *s*-wave part of the superconducting order parameter. λ_γ en-

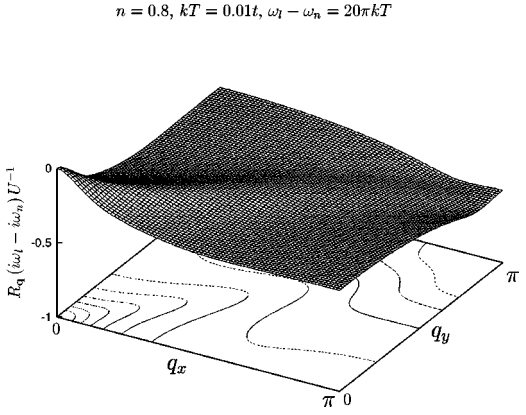

FIG. 4. The same as in Fig. 2 but for a different value of the Matsubara frequency.

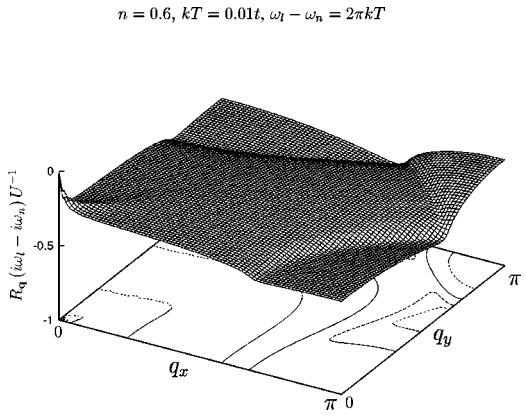

FIG. 5. The same as in Fig. 3 but for a different occupation number.

ters the kernels that account for anisotropic superconductivity. λ_γ differs from λ by the presence of the form factor $\gamma(\mathbf{q})$, which is related to nearest-neighbor pairing in the 2D lattice. In the presence of Coulomb correlations λ will be renormalized by $\Delta\lambda \sim \langle R_{\mathbf{q}} \rangle_{BZ}$, whereas the renormalization of λ_γ will be brought about by $\Delta\lambda_\gamma \sim \langle R_{\mathbf{q}} \gamma(\mathbf{q}) \rangle_{BZ}$. Note that the averaging is carried out with respect to the phononic momentum. Therefore, it can be carried out over the Brillouin zone instead of over a small slice around the Fermi surface. The strong momentum dependence of $\gamma(\mathbf{q})$ leads to a pronounced difference with respect to the relative significance of phonons with different momentum transfer $\mathbf{q}$ for isotropic and anisotropic superconductivity. In particular, even the negative values of $R_{\mathbf{q}}$ can lead to an enhancement of pairing correlations in the anisotropic channel. Figure 7 shows the numerical results.

On one hand, by inspecting the curve that corresponds to the averaging of $R_{\mathbf{q}}$ over the Brillouin zone, one can note the reduction of the isotropic electron-phonon coupling function λ. On the other hand, the positive contribution to the anisotropic pairing kernel ($\sim\lambda_\gamma$) occurs due to the presence of Coulomb repulsion. Our results show the important role of (π,π) phonons for the stabilization of the anisotropic superconducting state. One can see that in the underdoped region, these types of phonons are more important for anisotropic superconductivity, whereas for the overdoped case they are of minor importance. For isotropic superconductivity one

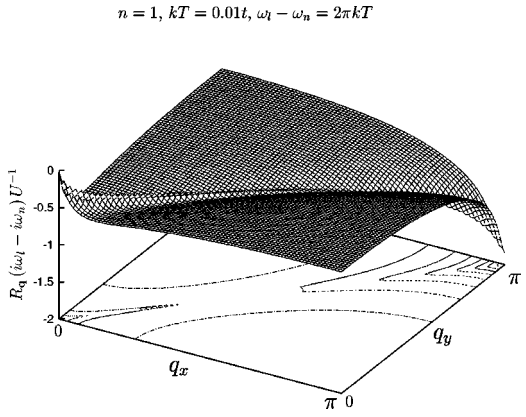

FIG. 6. The same as in Fig. 3 but for a different occupation number.

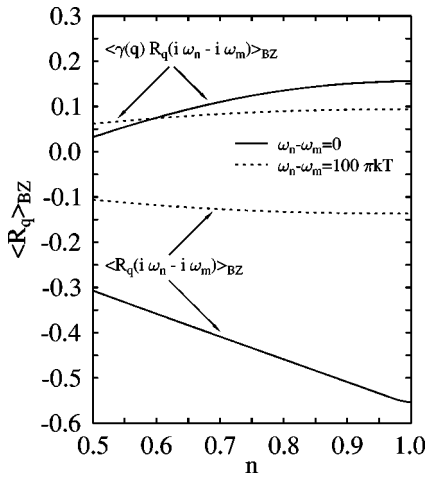

FIG. 7. The occupation number dependence of the Brillouin zone averaged electron-phonon interaction renormalization factor for $U=t$. The upper curves represent the contribution to the anisotropic electron-phonon coupling function $\Delta\lambda_\gamma \sim \langle R_{\mathbf{q}} \gamma(\mathbf{q}) \rangle_{BZ}$, whereas the lower ones show the reduction of the isotropic coupling function $\Delta\lambda \sim \langle R_{\mathbf{q}} \rangle_{BZ}$.

meets an opposite situation. The enhancement of the anisotropic electron-phonon coupling function is more pronounced in the underdoped region. Here, one may expect the antiferromagnetic fluctuations that contribute to the off-site pairing. In the case of isotropic superconductivity the local Coulomb repulsion always acts to the detriment of the on-site pairing. This shows up in the opposite behavior of anisotropic and isotropic coupling function with the variation of the occupation number.

IV. CONCLUDING REMARKS

We have considered the problem of renormalization of the electron-phonon interaction originating from the Coulomb interaction within the 2D Hubbard model. The energy- and momentum-dependent renormalization factor has been evaluated for different concentrations of holes. We have made use of the method of equations of motion for the thermodynamical Green's functions. It has been shown that the results of standard perturbation theory can be reproduced when making use of a reasonable decoupling scheme. We have found a strong momentum and occupation number dependence of the renormalization function. On one hand, the $\mathbf{q}=(0,0)$ phonons are hardly affected by Coulomb correlations. On the other hand, at least close to the half-filling, one can observe strong renormalization of (π,π) phonons. This results in a reduction of the electron-phonon coupling function for isotropic superconductivity and leads to a possible enhancement of the pairing interaction in the anisotropic channel. However, in the overdoped region one may expect that (π,π) phonons can significantly contribute to the stabilization of *s*-wave superconductivity. Therefore, the actual significance of phonons with different momenta is strongly related to the symmetry of the superconducting order parameter. The dynamical features have also been taken into account. In particular, one can note that the increase of the

energy transfer leads to a smearing of the negative renormalization in the *s*-wave channel.

We are aware of the fact that the opening of the insulting gap has not been taken into account when considering the renormalization of the electron-phonon interaction. This problem is under current investigation.

ACKNOWLEDGMENTS

This work has been supported by the Polish State Committee for Scientific Research, Grant No. 2 P03B 044 15. One of us (J.Z.) thanks the German Academic Exchange Service (DAAD) for financial help.

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