Superconductivity in the two-dimensional Hubbard model close to the metal-insulator transition: A strong-coupling description

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We discuss the problem of phonon-induced superconductivity in the two-dimensional Hubbard model close to the metal-insulator transition. The Coulomb correlations have been taken into account within the Hubbard I approximation, whereas superconductivity is treated by the Eliashberg scheme. The superconducting transition temperature has been evaluated for the anisotropic s-wave and d-wave channels. Results support the view that the gap function is of mixed, $d+s$ wave, symmetry but with a dominating d-wave component. [S0163-1829(98)09717-3]

The actual symmetry of the order parameter in high-temperature superconductors is still unsettled. There is experimental evidence for d-wave symmetry.[1–4] However, one cannot exclude admixture of components with s-like symmetry.[5,6] In particular, there is a new class of Josephson tunneling experiments that provide convincing arguments for mixed d- and s-wave pairing, at least in YBCO.[7] On one hand, in systems under consideration, superconductivity occurs in the vicinity of the metal-insulator transition. On the other hand, there is evidence for strong electron-phonon interactions that can contribute to the formation of a superconducting state and modify phononic properties below the transition temperature.[8–10] Therefore, one may expect that the symmetry of the gap function can be related both to Coulomb correlations and the electron-phonon interaction. The problem that arises is, how to consider the metal-insulator transition within the strong-coupling theory of superconductivity (see Ref. 11 for the Eliashberg formalism).

This can partially be taken into account within the mean-field approximation for the slave-boson fields[12] of the two-dimensional Hubbard model. Using this scheme we find that d-wave symmetry dominates for small doping.[13,14] However, this approach does not allow us to reproduce the formation of the insulating gap in the density of states at half filling. The same refers to the more refined perturbative treatment of Coulomb correlations.[15] The simplest approach that allows us to mimic the metal-insulator transition is the Hubbard I approximation.[16] One should be aware that this approximation neither reproduces the Hartree-Fock solution for small values of the Coulomb repulsion U nor fulfills the Luttinger theorem. These drawbacks are certainly important when considering superconductivity within the bare Hubbard model. However, in the case of phonon induced pairing this approach can be useful to discuss pairing in the vicinity of the metal-insulator transition, even if this approximation overestimates the magnitude of the insulating gap as a function of U. This is the problem we address in this paper.

The Hamiltonian is of the form

$$H=H_0+H_1, \tag{1}$$

where

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

and

$$H_1=\sum_{\mathbf{k},\mathbf{q}} g_{\mathbf{k}\mathbf{k}+\mathbf{q}}\Psi^+_{\mathbf{k}+\mathbf{q}}\tau_3\Psi_{\mathbf{k}}(B^+_{-\mathbf{q}}+B_{\mathbf{q}}), \tag{3}$$

with the Nambu notation.[11,13–15] $\tau_0 \ldots \tau_3$ stand for the Pauli matrices. The band energy is $\varepsilon_{\mathbf{k}}=-t\gamma(\mathbf{k})$, where $\gamma(\mathbf{k})=2(\cos k_x a+\cos k_y a)$ for the nearest-neighbor hopping t; μ is the chemical potential. In the systems under consideration one deals with highly ionic layers close to the metallic sheets. The ionic contribution dominates in the electron-phonon interaction. Therefore, it is justified to model phonons by an Einstein oscillator of frequency ω_0. The electron-phonon interaction given by H_1 will be considered within the Eliashberg scheme[11,13–15] and we assume t as an energy unit. It can be proved[17] (also for multiband models[18,19]) that to account for local Coulomb repulsion in the Hubbard I approximation[16] one has to renormalize the electron propagator in the Dyson equation

$$\Sigma_{\mathbf{k}}(i\omega_l)=G^{-1}_{0\mathbf{k}}(i\omega_l)-G^{-1}_{\mathbf{k}}(i\omega_l), \tag{4}$$

which corresponds to the substitution

$$G^{-1}_{0\mathbf{k}}(i\omega_l)=\begin{pmatrix} G^{-1}_{at}(i\omega_l)-\varepsilon_{\mathbf{k}} & 0 \\ 0 & -G^{-1}_{at}(-i\omega_l)+\varepsilon_{\mathbf{k}} \end{pmatrix}, \tag{5}$$

with

$$G^{-1}_{at}(i\omega_l)=\frac{(i\omega_l+\mu)(i\omega_l+\mu-U)}{(i\omega_l+\mu)-U(1-n/2)}. \tag{6}$$

ω_l is the Matsubara frequency $\omega_l=(\pi/\beta)(2l+1)$, $\beta=(k_BT)^{-1}$. In the present notation the usual ansatz for $\Sigma_{\mathbf{k}}(\omega_l)$ is of the form[11,13]

$$\Sigma_{\mathbf{k}}(i\omega_l)=[1-Z_{\mathbf{k}}(i\omega_l)]i\omega_l\tau_0+\phi_{\mathbf{k}}(i\omega_l)\tau_1+\chi_{\mathbf{k}}(i\omega_l)\tau_3, \tag{7}$$

where $Z_{\mathbf{k}}(i\omega_l)$ stands for the wave-function renormalization factor that can be considered as a momentum-independent quantity $Z_{\mathbf{k}}(i\omega_l)=Z(i\omega_l)$.[11] $\phi_{\mathbf{k}}(i\omega_l)$ denotes the momentum-dependent order parameter

$$\phi_{\mathbf{k}}(i\omega_l)=\phi_0(i\omega_l)+\gamma(\mathbf{k})\phi_\gamma(i\omega_l)+\eta(\mathbf{k})\phi_\eta(i\omega_l) \tag{8}$$

with $\eta(\mathbf{k})=2(\cos k_x a-\cos k_y a)$. Here, ϕ_0, ϕ_γ, ϕ_η denote the s-wave, extended s-wave, and d-wave amplitudes. ϕ_γ and ϕ_η originate from nearest-neighbor Cooper pairs. In what follows we will neglect the energy shift $\chi_{\mathbf{k}}$ and make use of the Kresin's method of introducing an average phonon frequency $\langle\Omega\rangle$ (Ref. 20)

$$\nu=\frac{\langle\Omega\rangle}{2\pi k_B T_c}, \tag{9}$$

corresponding to the frequency of an Einstein oscillator ω_0. We assume $\omega_0=0.1t$ throughout this paper.

At $T=T_c$ the s symmetry separates from the d symmetry and one gets the following system of Eliashberg equations:

$$Z(i\omega_l)=1+\frac{1}{\beta\omega_l}\sum_{\omega_n}\frac{\lambda\nu^2}{(l-n)^2+\nu^2}\,d_Z(i\omega_n), \tag{10}$$

$$\phi_\eta(i\omega_l)=\frac{1}{\beta}\sum_{\omega_n}\frac{\lambda_\gamma\nu^2}{(l-n)^2+\nu^2}\,d_{\eta^2}(i\omega_n)\phi_\eta(i\omega_n), \tag{11}$$

$$\phi_0(i\omega_l)=\frac{1}{\beta}\sum_{\omega_n}\frac{\lambda\nu^2}{(l-n)^2+\nu^2}\,[d_0(i\omega_n)\phi_0(i\omega_n)+d_\gamma(i\omega_n)\phi_\gamma(i\omega_n)], \tag{12}$$

$$\phi_\gamma(i\omega_l)=\frac{1}{\beta}\sum_{\omega_n}\frac{\lambda_\gamma\nu^2}{(l-n)^2+\nu^2}\left[d_\gamma(i\omega_n)\,\frac{\phi_0(i\omega_n)}{4}+d_{\gamma^2}(i\omega_n)\,\frac{\phi_\gamma(i\omega_n)}{4}\right], \tag{13}$$

where

$$d_Z(i\omega_n)=\frac{1}{N}\sum_{\mathbf{k}}d_{\mathbf{k}}(i\omega_n)\omega_n(2U(1-n/2)(U-2\mu)+\omega_n^2+\mu^2+[Z(i\omega_n)-1]\{\omega_n^2+[\mu-U(1-n/2)]^2\}), \tag{14}$$

$$\begin{pmatrix} d_0(i\omega_n)\\ d_\gamma(i\omega_n)\\ d_{\gamma^2}(i\omega_n)\\ d_{\eta^2}(i\omega_n)\end{pmatrix}=\frac{1}{N}\sum_{\mathbf{k}}d_{\mathbf{k}}(i\omega_n)\{\omega_n^2+[\mu-U(1-n/2)]^2\}\times\begin{pmatrix}1\\ \gamma(\mathbf{k})\\ \gamma^2(\mathbf{k})\\ \eta^2(\mathbf{k})\end{pmatrix}, \tag{15}$$

and

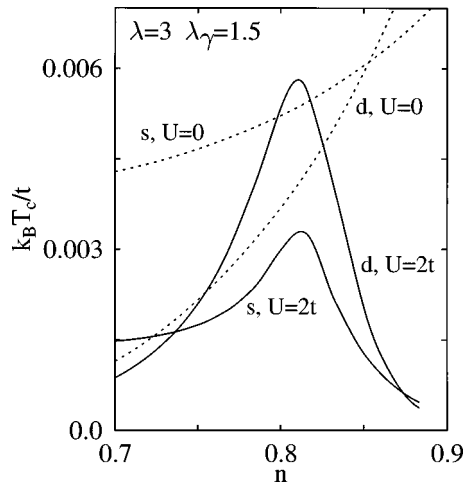

FIG. 1. The superconducting transition temperature as a function of band filling. Here, s refers to T_c for s-wave +extended s-wave channel whereas d corresponds to d-wave symmetry. The dashed curves represent the results for the uncorrelated case and solid curves have been obtained within the Hubbard I approximation ($U=2t$). λ and λ_γ are the electron-phonon coupling functions, where the first one determines the magnitude of the renormalization factor Z (and accounts for s-wave superconductivity) and the second one is responsible for anisotropic superconductivity.

$$d_{\mathbf{k}}^{-1}(i\omega_l)=(\omega_l^2+\mu^2)(\omega_l^2+(\mu-U)^2+2\{\omega_l^2[Z(i\omega_l)-1]-(\mu-U)\varepsilon_{\mathbf{k}}\})+2U(1-n/2)\{\omega_l^2[(Z(i\omega_l)-1]\times(U-2\mu)+\varepsilon_{\mathbf{k}}(\mu^2-\omega_l^2-U_\mu)\}+\{\omega_l^2+[\mu-U(1-n/2)]^2\}\times\{\omega_l^2+[Z(i\omega_l)-1]^2+\varepsilon_{\mathbf{k}}^2\}. \tag{16}$$

When considering superconductivity originating from nearest-neighbor Cooper pairs, one obtains two different electron-phonon coupling functions λ and λ_γ.[13–15,21] In general, λ and λ_γ depend on the occupation number,[21] however, in order to simplify the numerical calculations, we consider them as parameters.[13–15]

Figures 1 and 2 show the dependence of the supercon-

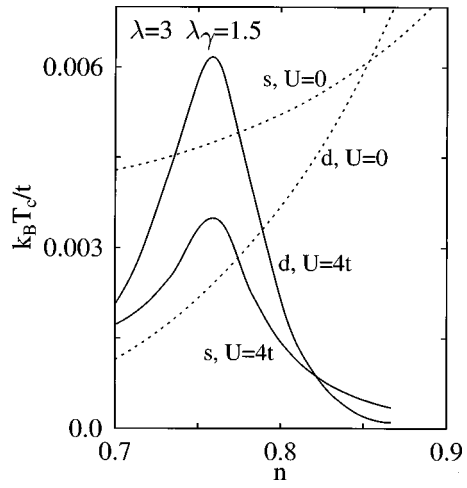

FIG. 2. The same as in Fig. 1 but for $U=4t$.

ducting transition temperature on the occupation number for different types of symmetry of the order parameter. *First:* One can note that the renormalization introduced within the Hubbard I approximation leads to results which correspond to the experimentally observed behavior. *Second:* The superconducting transition temperature for s- and d-wave superconductivity is of the same order of magnitude in the physically interesting region of concentration of holes. Both these features are related to the opening of the insulating gap. The insulating gap increases with U, which implies the shift in the position of maximal T_c-values in Figs. 1 and 2. A larger value of λ would imply a higher T_c value for the s-wave channel and larger values of λ_γ would imply higher T_c's for extended s-wave and d-wave symmetries. Due to the fact that the extended s-wave contribution becomes small because of the nesting of the Fermi surface for $n \rightarrow 1$, it is clear that it is the isotropic s-wave component that adds to the d-wave component. Previously we used the slave-boson method to deal with correlations (for mathematical simplicity in the $U \rightarrow \infty$ limit[13,14]). In the present work finite values of U have been considered and the results clearly show that s- and d-wave components can mix considerably. In addition, one can see that both types of pairing rapidly vanish when approaching the metal-insulator transition at half filling. Therefore, this simple description may partially account for the $d+s$-wave scenario of high-temperature superconductivity. One must be aware that the Hubbard I approximation does not reproduce the Hartree-Fock term that is of repulsive character and destroys local s-wave pairing in the purely electronic channel.[15] However, its role may be of minor importance when considering superconductivity originating from strong electron-phonon interactions in the vicinity of the metal-insulator transition. We expect that if we would use an improved treatment of correlation effects (like the two-pole approximation[22]) then qualitatively the result for the mixing of s- and d-wave pairing will not change.

We have not taken into account many-body effects that occur in the perturbative treatment of Coulomb correlations and contribute to d-wave pairing.[15] The incorporation of these effects in a strong-coupling theory of superconductivity with the inclusion of the metal-insulator transition could complete the actual picture of high-temperature superconductivity.

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