PHYSICAL REVIEW B VOLUME 56, NUMBER 18 1 NOVEMBER 1997-II

Charge-density-wave and superconductivity d-wave gaps in the Hubbard model for underdoped high-T_c cuprates

T. Dahm,* D. Manske, and L. Tewordt
Abteilung für Theoretische Festkörperphysik, Universität Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

(Received 7 May 1997)

We present a general theory of coexisting charge-density-wave (CDW) and superconductivity d-wave gaps for the two-dimensional (2D) Hubbard model. This motivates the description of the normal state of the underdoped cuprates by the previous fluctuation-exchange equations with a phenomenological CDW d-wave gap. The resulting neutron-scattering intensity, spin-lattice relaxation rate $1/T_1$, magnetic susceptibility, resistivity, and photoemission intensity are in qualitative agreement with the data on underdoped high-T_c cuprates. The T_c decreases and the crossover temperature T_* for $1/T_1T$ increases with increasing amplitude of the CDW gap. [S0163-1829(97)51342-7]

A normal-state pseudogap has been inferred from neutron-scattering,[1] nuclear magnetic resonance (NMR),[2] heat capacity,[3] and resistivity[4] data on underdoped $YBa_2Cu_3O_{7-\delta}$ and $YBa_2Cu_4O_8$. Angle-resolved photoemission (ARPES) measurements[5] on underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi 2212) indicate the presence of a gap with $d_{x^2-y^2}$-wave symmetry above T_c in the charge excitation spectrum. Recently it has been shown[6] that both the normal-state and superconducting NMR Knight-shift data of several underdoped high-T_c cuprates can be described in terms of a BCS-like pseudogap with d-wave symmetry. The resulting phase diagram has a strong similarity to that of competing charge-density-wave and superconductivity gaps.[7]

We follow here the idea of competing charge-density-wave (CDW) and superconductivity (SC) gaps which are caused by the same interaction.[7] The attractive electron-phonon interaction yielding s-wave pairing is replaced by the repulsive interaction due to exchange of nearly antiferromagnetic spin fluctuations, which leads to CDW and SC gaps having $d_{x^2-y^2}$-wave symmetry. The aim is to describe a number of different physical quantities in the normal state of the underdoped cuprates by the calculated physical quantities for a two-dimensional (2D) Hubbard model in the regime where the CDW gap (the pseudogap) is different from zero and the SC gap is zero. We formulate the fluctuation-exchange approximation for the 2D Hubbard model[8] in this CDW regime. In the fluctuation-exchange approximation the exchange of spin-fluctuations is treated according to the strong-coupling theory of superconductivity in a self-consistent and conserving manner. This yields the following equations for the quasiparticle self-energies Σ_{ij} in terms of the Green's functions G_{ij} and the spin-fluctuation interaction P_s:

$$\Sigma_{ij}(k)=\sum_{k'} P_s(k-k')G_{ij}(k') \quad [k\equiv(\mathbf{k},i\omega_n)]\ ; \tag{1}$$

$$\Sigma_{ii}=i\omega_n(1-Z_i)+\xi_i, \quad (i=1,2)\ ; \quad \Sigma_{12}=\phi_c; \tag{2}$$

$$G_{11}=(i\omega_n Z_2-\epsilon_2-\xi_2)/D, \tag{3}$$

$$G_{22}=(i\omega_n Z_1-\epsilon_1-\xi_1)/D, \quad G_{12}=\phi_c/D\ ;$$

$$D=(i\omega_n Z_1-\epsilon_1-\xi_1)(i\omega_n Z_2-\epsilon_2-\xi_2)-\phi_c^2;$$

$$(1\equiv(\mathbf{k},i\omega_n),2\equiv(\mathbf{k}+\mathbf{Q},i\omega_n)). \tag{4}$$

Here, Z_i is the effective mass function, ϵ_i the bare tight-binding band, ξ_i the energy shift function, and ϕ_c the CDW order parameter proportional to $\langle c^\dagger_{k+Q,\sigma}c_{k,\sigma}\rangle$. The subscript 1 refers to the main band with variables $1\equiv(\mathbf{k},i\omega_n)$, and the subscript 2 refers to the ''shadow'' band with variables $2\equiv(\mathbf{k}+\mathbf{Q},i\omega_n)$ and $\mathbf{Q}=(\pi,\pi)$. The interaction has the random-phase approximation (RPA) form, $P_s=(3/2)U^2\chi_s$, where $\chi_s=\chi_0(1-U\chi_0)^{-1}$ is the dynamical spin susceptibility. The irreducible susceptibility χ_0 is calculated self-consistently from the quasiparticle spectral functions $-\mathrm{Im}G_{ij}/\pi$ by taking into account the renormalization by the self-energies Σ_{ij} (see Ref. 8).

We consider here a tight-binding band $\epsilon_1\equiv\epsilon(\mathbf{k})$ whose Fermi line approximates those of the Y-Ba-Cu-O and Bi 2212 compounds. Then the ''hot spots'' where the Fermi lines $\epsilon(\mathbf{k})+\xi(\mathbf{k})=0$ and $\epsilon(\mathbf{k}+\mathbf{Q})+\xi(\mathbf{k}+\mathbf{Q})=0$ in the first quadrant of the Brillouin zone cross each other lie in the vicinity of the points $\mathbf{k}=(\pi,0)$ and $\mathbf{k}=(0,\pi)$. One recognizes from Eqs. (1)–(4) that at the hot spots $(\epsilon_2+\xi_2=-\epsilon_1-\xi_1,\ Z_2=Z_1)$ these equations reduce to the fluctuation-exchange equations for the superconducting regime[8] where the SC gap function ϕ_s is replaced by the CDW gap function ϕ_c.

In analogy to Ref. 7 we have developed also the general theory of coexisting CDW and SC d-wave gaps due to spin-fluctuation pairing interaction. In order to save space we present here only the gap equation for the superconducting (SC) gap in the weak-coupling BCS form (Δ_s is the SC gap and Δ_c is the CDW gap):

$$\Delta_s(\mathbf{k})=-\sum_{\mathbf{k}'} P_s(\mathbf{k}-\mathbf{k}')\Delta_s(\mathbf{k}')\tfrac{1}{2}(\,[1-2f(E'_+)]/2E'_+ +[1-2f(E'_-)]/2E'_- +(\epsilon'_1-\epsilon'_2)\times[(\epsilon'_1-\epsilon'_2)^2+4\Delta_c^2]^{-1/2}\times\{[1-2f(E'_+)]/2E'_+ -[1-2f(E'_-)]/2E'_-\}); \tag{5}$$

$$E_\pm^2=\{\tfrac{1}{2}(\epsilon_1+\epsilon_2)\pm\tfrac{1}{2}[(\epsilon_1-\epsilon_2)^2+4\Delta_c^2]^{1/2}\}^2+\Delta_s^2,$$

$$\epsilon_1=\epsilon(\mathbf{k}),\quad \epsilon_2=\epsilon(\mathbf{k}+\mathbf{Q})\ ,\quad \Delta_s=\Delta_s(\mathbf{k}),\quad \Delta_c=\Delta_c(\mathbf{k}). \tag{6}$$

One notices again that at the hot spots with $\epsilon_1+\epsilon_2=0$ the quasiparticle energies $E_\pm$ in Eq. (6) take on the BCS form with a total squared gap energy equal to $\Delta_s^2(\mathbf{k})+\Delta_c^2(\mathbf{k})$. Since the repulsive spin-fluctuation interaction $P_s(k-k')$ has a large peak at $\mathbf{k}-\mathbf{k}'=\mathbf{Q}'=(-\pi,\pi)$, the CDW gap [see Eqs. (1)–(4) for ϕ_c] as well as the SC gap [see Eqs. (5) and (6) for Δ_s] both have $d_{x^2-y^2}$-wave symmetry. The form of $E_\pm$ at the hot spots with $\epsilon_1+\epsilon_2=0$ in Eq. (6) may justify the expression for the quasiparticle energy which has been used by Loram *et al.*[3] and Williams *et al.*[6] to fit the heat capacity and Knight-shift data in both the normal and superconducting states in the underdoped cuprates.

Instead of solving the full set of Eqs. (1)–(4) for the CDW state (the ''normal''state with respect to the SC state) we approximate here these equations by the simpler form which they acquire at the hot spots with $\epsilon_2+\xi_2=-\epsilon_1-\xi_1$. This seems to be a reasonable approximation because the hot spots yield the dominant contribution to the right-hand side of Eq. (1): first, the denominator D of $G_{ij}(k')$ becomes small, and second, the interaction $P_s(k-k')$ for scattering of quasiparticles from one hot spot to the other becomes large because $\mathbf{k}-\mathbf{k}'$ is of the order of $\mathbf{Q}'=(-\pi,\pi)$. This treatment of the CDW is somewhat similar to the work by Rice and Scott,[9] although in our case the hot spots do not coincide with the saddle points. Furthermore we assume that the CDW gap ϕ_c has the simple form of a BCS d-wave gap like that introduced in Ref. 6:

$$\phi_c(\mathbf{k})\equiv\Delta_c(\mathbf{k})=E_g(\,\cos k_x-\,\cos k_y)\ . \tag{7}$$

Then Eqs. (1)–(4) for Σ_{11} take on the form of the previous fluctuation-exchange equations[8] where the SC gap ϕ_s occurring in the quasiparticle spectral functions A_0, A_3, and A_1 is replaced by ϕ_c given in Eq. (7). The T_c for superconductivity is given by $\lambda_d(T_c)=1$ where the eigenvalues $\lambda_d(T)$ are determined now by the linearized gap equation for ϕ_s containing the kernel A_1/ϕ_c. We remark that the gap equation for ϕ_s below T_c contains the squared order parameter $\phi_c^2+\phi_s^2$ in the denominator of A_1/ϕ_c. This equation corresponds to the weak-coupling gap equation in Eq. (5) for $\epsilon_1+\epsilon_2=0$.

We have solved the fluctuation-exchange equations with the CDW gap in Eq. (7) for a bare tight-binding band $\epsilon(\mathbf{k})$ with first- and second-nearest-neighbor hopping, an effective on-site repulsion $J(\mathbf{q})$ having a maximum $U=3.6t$ at $\mathbf{q}=\mathbf{Q}$ (t is the nearest-neighbor hopping energy),[10] and a renormalized band filling $n=0.91$. From the results for the spectral functions of the dynamical spin susceptibility and the quasiparticles we can calculate a large number of physical quantities for which the expressions are given elsewhere.[8] First we consider the NMR and neutron-scattering intensity which are calculated from the spectral density of the dynamical spin susceptibility, $\mathrm{Im}\chi_s(\mathbf{q},\omega)$. This function has a broad peak as a function of $\mathbf{q}$ which is centered at $\mathbf{Q}$, and it exhibits a peak as a function of ω at the antiparamagnon energy ω_s. The slope of this function at $\omega=0$ first increases with decreasing T down a crossover temperature called T_*, and then it decreases with further decrease of T. At the same time the peak at $\omega_s\sim E_g$ narrows and increases with decreasing T. In Fig. 1 we have plotted the nuclear spin-lattice relaxation rate divided by T, $1/T_1T$, versus T. One recognizes that this quantity first increases with decreasing T, then acquires a maximum at about the crossover temperature T_*, and then it decreases rapidly as T tends to T_c. This behavior is plausible from the behavior of $\mathrm{Im}\chi_s(\mathbf{Q},\omega)$ because $1/T_1T$ is essentially given by the slope of this function at $\omega=0$. The occurrence of a maximum of $1/T_1T$ (see Fig. 1) is in agreement with the NMR data in the underdoped regime.[2] In the overdoped regime of the cuprates $1/T_1T$ increases monotonically with decreasing T.

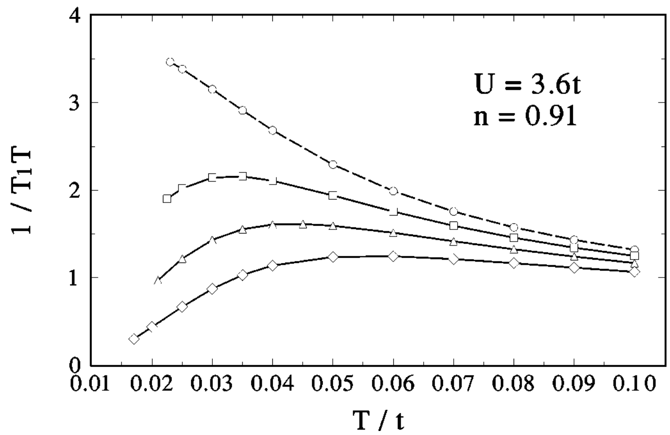

FIG. 1. The spin-lattice relaxation rate divided by T, $1/T_1T$, versus T, for amplitudes of the CDW gap $E_g=0$ (dashed line) and $E_g=0.05$, 0.075, 0.1t (solid lines from top to bottom). The parameters are $J(\mathbf{Q})=U=3.6t$ (t is the next-nearest-neighbor hopping energy), $n=0.91$ for the Y-Ba-Cu-O-like band. The lower ends of the curves refer to $T_c=0.023$, 0.022, 0.021, and 0.016t (from top to bottom).

The temperature behavior of $\mathrm{Im}\chi_s(\mathbf{Q},\omega)$ is also in agreement with the temperature dependence of the neutron-scattering intensity at fixed small energy ω. This neutron-scattering intensity first increases with decreasing T up to a maximum at about T_*, and then it decreases.[1] This behavior has been interpreted as a signature of the opening of a spin pseudogap in the spin excitation spectrum.[1]

In Fig. 1 we show $1/T_1T$ for three different values of the amplitude E_g of the CDW gap in Eq. (7): $E_g=0.1t$, 0.075t, and 0.05t. One recognizes that for this sequence of E_g values the position of the maximum at T_* decreases from about $T_*=0.06t$ to 0.045t, and to 0.035t, and that the T_c (lower ends of the curves) increases from about $T_c=0.016$ to 0.0206, and to 0.0223. For $E_g=0$ the $1/T_1T$ increases monotonically with decreasing T down to $T_{c0}\simeq0.023t$. The de-

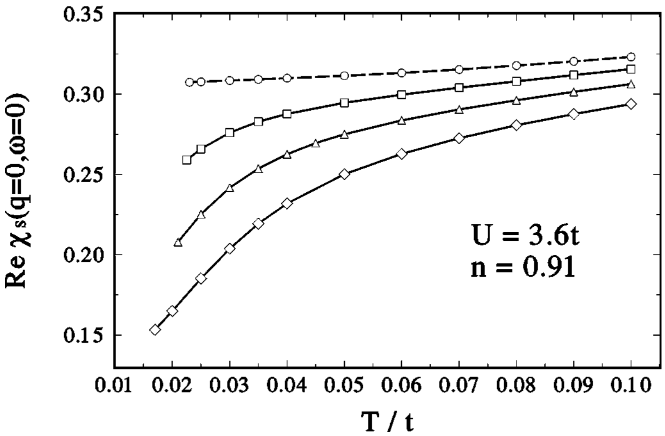

FIG. 2. The static and uniform spin susceptibility $\chi_s(\mathbf{q}=0,\omega=0)$ versus T for gap amplitudes $E_g=0$, 0.05, 0.075, and $0.1t$ (curves in this sequence from top to bottom). The notation is given in Fig. 1.

crease of T_c and the increase of T_* with increasing gap amplitude E_g is in qualitative agreement with the phase diagram of the Knight shift, magnetic susceptibility, and resistivity data in the underdoped regime.[6,4] Here we assume implicitly that E_g increases as the doping away from half filling, $x=1-n$, decreases.

The static and uniform spin susceptibility is given by $\chi_s(\mathbf{q}=0,\omega=0)=[1-J(\mathbf{q}=0)\chi_0]^{-1}\chi_0(\mathbf{q}=0,\omega=0)$. In Fig. 2 we have plotted our results for $\chi_s(0,0)$ versus T for $E_g=0.1$, 0.075, $0.05t$, and $E_g=0$. One sees that χ_s decreases with decreasing T, and that the overall reduction down to T_c increases with increasing gap amplitude E_g in qualitative agreement with the fits of the NMR Knight-shift data.[6] Here it should be pointed out that in our strong-coupling calculation the CDW gap in Eq. (7) is reduced by ReZ and is smeared out by the quasiparticle damping ω ImZ. The decrease of $\chi_s(0,0)$, or $\chi_0(0,0)$, for decreasing T is plausible because $\chi_0(0,0)$ is approximately given by the BCS expression $\chi_0=\int_{-\infty}^{\infty}d\omega\, N(\omega)[-\partial f(\omega)/\partial\omega]$, where the density of states $N(\omega)$ is shown in Fig. 3 for $E_g=0.1t$. One sees that $N(\omega)$ exhibits a typical d-wave gap where $N(\omega)$ is linear in ω for $\omega<E_g$. For decreasing T, $N(0)$ decreases rapidly and therefore χ_0 decreases with T.

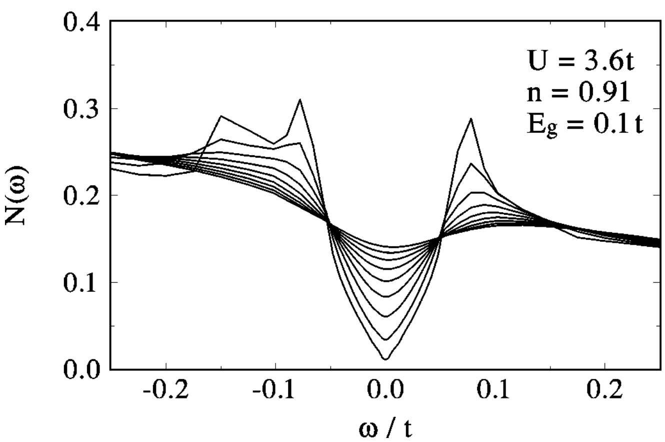

FIG. 3. Density of states $N(\omega)$ versus ω for $J(\mathbf{Q})=U=3.6t$, $n=0.91$, $E_g=0.1t$, and temperatures $T=0.1,0.09,\ldots,0.02t$ (curves in this sequence from top to bottom).

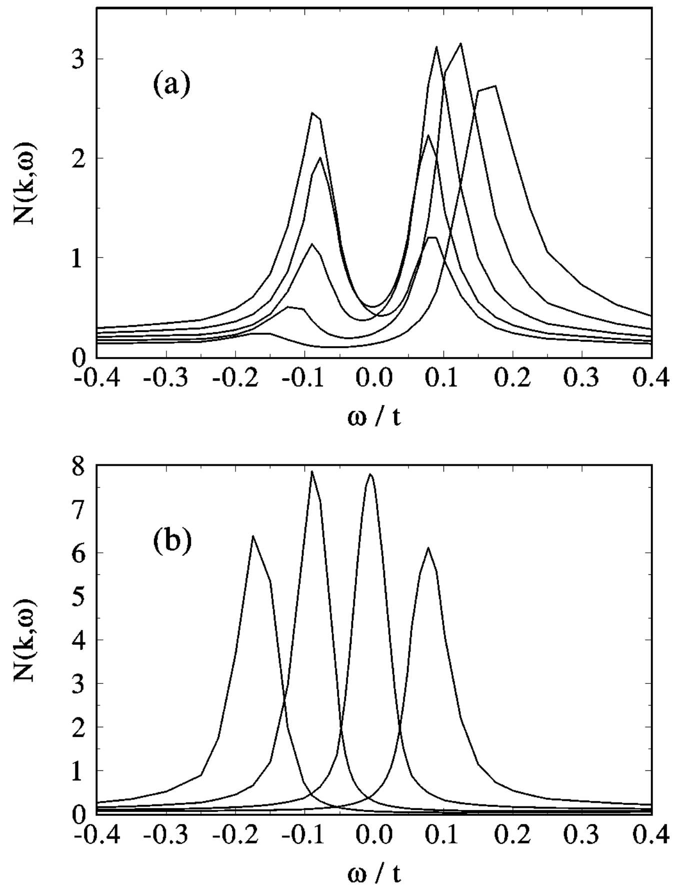

FIG. 4. Quasiparticle spectral function $N(\mathbf{k},\omega)$ versus ω for $E_g=0.1t$, $T=0.05t$, and different $\mathbf{k}$ vectors near the gap antinode (a) and node (b). (a) $\mathbf{k}=(0.14,1)$, $(0.16,1)$, $(0.17,1)$, $(0,19,1)$, and $(0,20,1)$ (in units of π) where the peaks below the Fermi energy $\omega=0$ decrease in this sequence of $\mathbf{k}$ vectors. The Fermi wave vector is $\mathbf{k}_a=(0.18,1)\pi$. (b) $\mathbf{k}=k(1,1)\pi$ with $k=0.38$, 0.39, 0.41, and 0.42 where the peaks go from left to right for this sequence of $\mathbf{k}$ vectors. The Fermi wave vector is about $\mathbf{k}_n=0.41(1,1)\pi$. The parameter values are the same as in Figs. 1 and 3.

In Fig. 4(a) we show the quasiparticle spectral function $N(\mathbf{k},\omega)$ versus ω for $E_g=0.1t$ and $T=0.05t$ and for different $\mathbf{k}$ vectors, i.e., $\mathbf{k}=(0.14,1)$, $(0.16,1)$, $(0.17,1)$, $(0.19,1)$, and $(0.20,1)$ (in units of π), where the peaks below the Fermi energy $\omega=0$ decrease in this sequence of $\mathbf{k}$ vectors. The Fermi wave vector is given by $\mathbf{k}_a=(0.18,1)\pi$. One sees that the right-hand side edge of the peak below the Fermi energy $\omega=0$ stays always a finite amount of energy (the gap energy) below the Fermi level and never crosses it as $\mathbf{k}$ moves along the direction from $(0,1)\pi$ to $(1,1)\pi$ through the Fermi line. This is in agreement with the ARPES data in the normal state on underdoped Bi 2212.[5] Notice that the photoemission intensity is given by $N(\mathbf{k},\omega)f(\omega)$ and that the Fermi function $f(\omega)$ cuts out the peaks for $\omega>0$ in Fig. 4(a). Along the node of the CDW gap in Eq. (7) we find that the quasiparticle peak of $N(\mathbf{k},\omega)$ moves through the Fermi energy $\omega=0$ as $\mathbf{k}$ moves along the direction from (0,0) to (π,π) through the Fermi line [see peaks in Fig. 4(b) from left to right for the sequence of $\mathbf{k}$ vectors $\mathbf{k}=0.38(1,1)$, $0.39(1,1)$, $0.41(1,1)$, and $0.42(1,1)$, in units of π]. Comparison with Fig. 4(a) shows that the peaks along the node of the gap are much larger than the peaks near the antinode of the gap.

We have calculated also the resistivity ρ versus T for gap amplitudes $E_g=0.1$, 0.075, 0.05t, and $E_g=0$. It turns out that ρ is nearly linear in T down to the lowest temperatures and that the curves for increasing E_g are shifted downwards and run almost parallel to that for $E_g=0$. According to the ARPES data on underdoped Bi 2212 the normal-state gap increases nearly linearly with decreasing T.[5] Thus, one can infer from these results that ρ bends downwards for decreasing T if the gap E_g is switched on slowly for decreasing T. However, the effect is too small in comparison to the data.[4] It is likely that the current contribution involving two order-parameter fluctuation propagators[11] yields a stronger bending downwards of ρ below T_*.

In summary, we have presented the general equations of the fluctuation-exchange approximation for coexisting charge-density-wave (CDW) and superconductivity (SC) d-wave gaps which are induced by exchange of spin fluctuations in the 2D Hubbard model. At the ''hot spots'' where the nesting condition $\epsilon(\mathbf{k})+\epsilon(\mathbf{k}+\mathbf{Q})=0$ is satisfied these equations reduce to the previous fluctuation-exchange equations[8] with a squared gap energy equal to $\Delta_c^2+\Delta_s^2$. We have solved the latter equations with a phenomenological CDW d-wave gap in analogy to the pseudogap which has been used to fit the heat capacity[3] and Knight-shift[6] data. Our strong-coupling calculation yields the full momentum and frequency dependence of the dynamical spin susceptibility and quasiparticle spectral function. For increasing E_g (corresponding to decreasing doping) the T_c for superconductivity decreases and the crossover temperature T_* for $1/T_1T$ increases (see Fig. 1). We remark that this behavior of $1/T_1T$ and the corresponding behavior of the neutron-scattering intensity can be described also by the effect of order-parameter fluctuations.[11] In the presence of a pseudogap E_g we find that the order-parameter fluctuations lead to a more rapid drop of $1/T_1T$ below T_*, which is in better agreement with experiment.[2] However, the order-parameter fluctuations fail to yield the other observed pseudogap properties in the normal state of the underdoped cuprates. The present theory can describe also the decrease of the static susceptibility χ_s with decreasing T (see Fig. 2) and the development of a d-wave gap in the density of states $N(\omega)$ (see Fig. 3) and in the photoemission intensity $N(\mathbf{k},\omega)f(\omega)$ for $\mathbf{k}$ vectors near the antinode of the gap (see Fig. 4).

In conclusion we can say the following. Our results for a number of physical quantities are consistent with the existence of a d-wave pseudogap in the normal state of the underdoped cuprates. Our strong-coupling calculations go far beyond the BCS calculations of Loram *et al.*[3] and Williams *et al.*[6] because we have taken into account self-consistently the effect of spin fluctuations on the quasiparticle self-energies, in particular, the quasiparticle damping (see Fig. 4). We did not consider dynamic effects of the CDW here like the ones discussed in Ref. 12, but as our results show, the experimental features in the pseudogap state can be understood consistently with a static CDW gap. The origin of the pseudogap is still unknown. It seems possible that it is a CDW gap because our Eqs. (1)–(4) for the fluctuation-exchange approximation of the one-band Hubbard model reduce at distinct points (the hot spots yielding the dominant contributions) to the fluctuation-exchange equations for d-wave superconductivity.[8] One might wonder whether a SDW instability could be more stable than a CDW. We found earlier, that the fluctuation-exchange equations do not give rise to a SDW instability, but approach it asymptotically.[8] Also, Eqs. (1)–(4) in this case do not reduce to the d-wave superconducting equations at the hot spots. A sign change of the CDW order parameter is crucial for this property and might also be supported by certain phonon modes.[13] Equations (1)–(4) have not been solved yet because they are much more complicated than the d-wave superconducting equations. It will be interesting to see whether or not the T_c for the d-wave CDW gap is higher than that for the d-wave superconductivity gap.

We acknowledge helpful discussions with D. Fay.

---

*Present address: Department of Physics, University of California, Santa Barbara, CA 93106-9530.

[1] For a review, see L. P. Regnault *et al.*, Physica B **213-214**, 48 (1995).

[2] For a review, see C. P. Slichter, in *Strongly Correlated Electronic Systems*, edited by K. S. Bedell *et al.* (Addison-Wesley, Reading, MA, 1994).

[3] J. Loram *et al.*, Phys. Rev. Lett. **71**, 1740 (1993); J. W. Loram *et al.*, J. Supercond. **7**, 243 (1994).

[4] B. Batlogg *et al.*, Physica C **235-240**, 130 (1994).

[5] D. S. Marshall *et al.*, Phys. Rev. Lett. **76**, 4841 (1996); J. M. Harris *et al.*, Phys. Rev. B **54**, R15 655 (1996).

[6] G. V. M. Williams *et al.*, Phys. Rev. Lett. **78**, 721 (1997).

[7] C. A. Balseiro and L. M. Falicov, Phys. Rev. B **20**, 4457 (1979).

[8] T. Dahm and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995); Phys. Rev. B **52**, 1297 (1995); Physica C **246**, 61 (1995).

[9] T. M. Rice and G. K. Scott, Phys. Rev. Lett. **35**, 120 (1975).

[10] L. Tewordt and T. Dahm, Physica C **265**, 67 (1996).

[11] T. Dahm, D. Manske, and L. Tewordt, Phys. Rev. B **55**, 15 274 (1997); Europhys. Lett. **39**, 201 (1997).

[12] P. B. Littlewood and C. M. Varma, Phys. Rev. Lett. **47**, 811 (1981).

[13] J. Song and J. F. Annett, Phys. Rev. B **51**, 3840 (1995).