Phase diagram of hole-doped high-T_c superconductors: Effects of Cooper-pair phase fluctuations within fluctuation-exchange theory

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Using the Hubbard model Hamiltonian we study spin-fluctuation exchange-induced superconductivity of d-wave symmetry. Results are presented for the characteristic temperature T^* at which a gap appears in the spectral density, for T_c^* at which Cooper-pairs are formed, for T_c at which Cooper pairs become phase coherent, and for the superfluid density n_s. We find that, with increasing doping, for $x>0.15$ the phase coherence energy becomes larger than the Cooper-pair condensation energy. Accordingly, one has $T_c \propto n_s$ for $x<0.15$ and $T_c \propto \Delta$ for the overdoped cuprates. We use our results to discuss dynamics and recent dynamical conductivity and ultrafast nonequilibrium measurements.

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I. INTRODUCTION

For several decades spin-fluctuation (or paramagnon) theories have been quite successful in describing superfluidity in the nearly ferromagnetic liquid ^{3}He (Ref. 1–4) and unconventional superconductivity in nearly antiferromagnetic liquids—for example, the high-temperature superconductors.[5–15] In the latter system, the occurrence of a d-wave instability, the description of inelastic neutron scattering data, nuclear magnetic resonance (NMR) relaxation rates, and Knight-shift measurements, as well as tunneling, angular-resolved photoemission spectroscopy (ARPES), the isotope exponent, and many other important physical properties can be described qualitatively within the Hubbard model. However, existing microscopic theories have serious problems in explaining the underdoped regime of the cuprates and instead many phenomenological approaches have been used.[16–19] These problems are, in particular, the existence of a so-called weak pseudogap up to room temperature,[20,21] the occurrence of a strong pseudogap close to T_c,[17] and, finally, a decreasing T_c in the underdoped regime. Furthermore, Uemura *et al.*[24,25] have found experimentally that T_c is proportional to the superfluid density at $T=0$ divided by the effective mass, $n_s(T=0)/m$, and, in addition, indications of a nonzero phase stiffness $\propto n_s$ for $T_c<T<T_c^*$ on short length and time scales have been reported by Orenstein and co-workers.[26,27]

Rather than using phenomenological models we calculate various properties of hole-doped high-T_c superconductors with the help of the Hubbard Hamiltonian, yielding spin-fluctuation exchange-induced Cooper pairing of d-wave symmetry.[7–10,12,15] Since presently the origin of high-T_c superconductivity is still being debated, it is important to see how far such an explicit electronic model can explain various basic properties of the cuprate superconductors.

Thus, in this paper we use an electronic theory and the Hubbard Hamiltonian in which Cooper pairs are formed due to spin-fluctuation exchange. Recently, we have shown that this approach can also explain the important feedback of superconductivity on the pairing potential.[28] Studies of amplitude fluctuations of the superconducting order parameter with this approximation did not give a satisfactory pseudogap behavior.[29] Here we focus on phase fluctuations. We determine the doping dependence of the relevant temperatures of the phase diagram, namely, $T_c^*(x)$, $T_c(x)$, and also T^* at which a gap appears in the spectral density. Below T_c^* we find incoherent Cooper pairs (''preformed pairs'') which become phase coherent only below the critical temperature T_c of the bulk. We will show that phase fluctuations contributing ΔF_{phase} to the free energy lead to a decreasing critical temperature in the underdoped regime and thus to the appearance of an optimal doping x_{opt}. It is shown that this result is due to the small superfluid density $n_s(T)$ in the system. Most importantly we calculate that $\Delta F_{cond} > \Delta F_{phase}$ (ΔF_{cond} denotes the contribution to the free energy due to Cooper-pair formation, and ΔF_{phase} refers to the contribution due to phase fluctuations of the Cooper pairs, respectively) for doping $x<x_{opt}$ and vice versa for $x>x_{opt}$. We show that the temperature range where preformed Cooper pairs occur, $(T_c^*-T_c)$, as well as the structure in the density of states, depends on the dispersion $\epsilon_{\mathbf{k}}$ and thus on the appearance of a pseudogap for underdoped cuprates. Furthermore, we show how the dynamical conductivity $\sigma(\omega)$ reflects T_c and T_c^* for $\omega\tau \ll 1$ and $\omega\tau \gg 1$, respectively. Here, τ refers to the phase-fluctuation lifetime. We also discuss the relaxation dynamics in pump-probe spectroscopy.

This paper is organized as follows: within the next section we present our theory for the self-consistent description of the quasiparticles (dressed holes) and the pairing interaction [extended fluctuation-exchange (FLEX) approximation]. These results are used in order to calculate the current-current correlation function and thus the superfluid density n_s and the optical conductivity $\sigma(\omega)$ with the help of standard many-body theory. Then, we use these results as a microscopical input for the calculation of the free-energy contributions ΔF_{cond} and ΔF_{phase} and compare our results with the XY model and Kosterlitz-Thouless theory. These results are presented in Sec. III and a summary is given in Sec. IV.

II. THEORY

Extending previous studies using FLEX theory and the two-dimensional (2D) Hubbard Hamiltonian for a CuO_2 plane,[10,12]

$$H=-\sum_{\langle ij\rangle\,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

where $c^\dagger_{i\sigma}$ creates an electron with spin σ on site i, U denotes the on-site Coulomb interaction, and t_{ij} is the hopping integral. We calculate various properties like the dynamical spin susceptibility $\chi(q,\omega,x,T)$, the superfluid density $n_s(q,\omega,x,T)$, and the superconducting gap function $\Delta(q,\omega,x,T)$. We take $t=250$ meV and $U=4t$ yielding a tight-binding energy dispersion.[30]

Within a conserving approximation, the one-electron self-energy is given by the functional derivation of generating functional Φ, related to the free energy,[7] with respect to the Green's function $\mathcal{G}$. From H and the functional differentiation of the generating functional Φ with respect to $\mathcal{G}$, $\delta\Phi\{H\}/\delta\mathcal{G}=\Sigma$, one obtains with the help of the Dyson equation the Green's function and the self-energies. Note that this gives coupled equations for the amplitude and phase $\phi(\mathbf{r})$ of $\mathcal{G}$ (see Ref. 31) and in accordance with the Ginzburg-Landau (Wannier) type treatment an energy gain due to phase coherence of Cooper pairs and due to Cooper-pair condensation.[31,16,17,19,32] Below we will show how to solve these equations. Then, we will calculate the current-current correlation function which is used as a microscopical input for the Ginzburg-Landau functional. In the Ginzburg-Landau functional the prefactor of $\nabla\phi(\mathbf{r})$ is n_s/m (m is the effective mass), i.e., the stiffness against phase fluctuations. Thus, the energy scale of Cooper-pair phase fluctuations is determined by n_s. In the underdoped regime of high-T_c superconductors n_s is small and, therefore, phase fluctuations do not cost much energy and the superconducting transition is expected to be due to disordering of the phase. In such a case where n_s/m is the only relevant energy scale one finds $T_c\propto n_s/m$. In other words, if the phase coherence energy gain $\Delta E_{phase}\propto n_s$ is the smallest, one gets from the estimate $\Delta E_{phase}(T=0)=k_BT_c$ the superconducting transition temperature $T_c\propto n_s(0)$.[33] This seems to be the case for the underdoped cuprates, because this scaling is observed experimentally.[24]

In the FLEX, (Refs. 7–12,14, and 15) or T-matrix[34] approximation the dressed one-electron Green's functions are used to calculate the charge and spin susceptibilities. These susceptibilities are used in order to construct a Berk-Schrieffer-like[35] pairing interaction describing the exchange of charge and spin fluctuations. A self-consistent description is essential and is required because the electrons do not only condense into Cooper pairs but also provide the pairing interaction. The quasiparticle self-energy components X_ν ($\nu=0,3,1$) with respect to the Pauli matrices τ_ν in the Nambu representation,[36,37] i.e., $X_0=\omega(1-Z)$ (renormalization), $X_3=\xi$ (energy shift), and $X_1=\phi$ (gap parameter), are given by

$$X_\nu(\mathbf{k},\omega)=N^{-1}\sum_{\mathbf{k}'}\int_0^\infty d\Omega[P_s(\mathbf{k}-\mathbf{k}',\Omega)\pm P_c(\mathbf{k}-\mathbf{k}',\Omega)] \times\int_{-\infty}^{\infty}d\omega'\, I(\omega,\Omega,\omega')A_\nu(\mathbf{k}',\omega'). \quad (2)$$

Here, the plus sign holds for X_0 and X_3 and the minus sign for X_1. The kernel I and the spectral functions A_ν are given by[39]

$$I(\omega,\Omega,\omega')=\frac{f(-\omega')+b(\Omega)}{\omega+i\delta-\Omega-\omega'}+\frac{f(\omega')+b(\Omega)}{\omega+i\delta+\Omega-\omega'}, \quad (3)$$

$$A_\nu(\mathbf{k},\omega)=-\pi^{-1}\,\mathrm{Im}[a_\nu(\mathbf{k},\omega)/D(\mathbf{k},\omega)]$$

and

$$D=[\omega Z]^2-[\epsilon(\mathbf{k})+\xi]^2-\phi^2,$$

$$a_0=\omega Z,\quad a_3=\epsilon(\mathbf{k})+\xi,\quad a_1=\phi. \quad (4)$$

Here, f and b are the Fermi and Bose distribution function, respectively. For the bare tight-binding dispersion relation one has $\epsilon(\mathbf{k})=2t[2-\cos(k_x)-\cos(k_y)-\mu]$. The band filling $n=1/N\Sigma_{\mathbf{k}}n_{\mathbf{k}}$ is determined with the help of the $\mathbf{k}$-dependent occupation number $n_{\mathbf{k}}=2\int_{-\infty}^{\infty}d\omega f(\omega)A(\mathbf{k},\omega)$ which is calculated self-consistently. $n=1$ corresponds to half filling. The spin and charge fluctuation interactions are given by $P_s=(2\pi)^{-1}U^2\,\mathrm{Im}(3\chi_s-\chi_{s0})$ with $\chi_s=\chi_{s0}(1-U\chi_{s0})^{-1}$ and $P_c=(2\pi)^{-1}U^2\,\mathrm{Im}(3\chi_c-\chi_{c0})$ and $\chi_s=\chi_{c0}(1+U\chi_{c0})^{-1}$, where

$$\mathrm{Im}\chi_{s0,c0}(\mathbf{q},\omega)=\frac{\pi}{N}\int_{-\infty}^{\infty}d\omega'\,[f(\omega')-f(\omega'+\omega)] \times\sum_{\mathbf{k}}[A(\mathbf{k}+\mathbf{q},\omega'+\omega)A(\mathbf{k},\omega') \pm A_1(\mathbf{k}+\mathbf{q},\omega'+\omega)A_1(\mathbf{k},\omega')]\ . \quad (5)$$

Here, $A(\mathbf{k},\omega)=A_0(\mathbf{k},\omega)+A_3(\mathbf{k},\omega)$, and the real parts are calculated with the help of the Kramers-Kronig relation. The subtracted terms in P_s and P_c remove a double counting that occurs in second order.

Our numerical calculations are performed on a square lattice with 256×256 points in the Brillouin zone and with 200 points on the real ω axis up to $16t$ with an almost logarithmic mesh. The full momentum and frequency dependence of the quantities is kept. The convolutions in $\mathbf{k}$ space are carried out with fast Fourier transforms.[40] Note that T_c^* is determined from the linearized gap equation and the superconducting state is found to have $d_{x^2-y^2}$-wave symmetry.[10]

The bulk transition temperature T_c at which phase coherence of the Cooper pairs occur is determined by the Ginzburg-Landau free-energy functional $\Delta F\{n_s,\Delta\}$ where the superfluid density $n_s(x,T)/m$ is calculated self-consistently from the current-current correlation function and from

$$\frac{n_s}{m} = \frac{2t}{\hbar^2}(S_N - S_S), \qquad (6)$$

where we have introduced for convenience the oscillator strength

$$S_N = \frac{\hbar^2 c}{2\pi e^2 t}\int_{0^+}^{\infty} \sigma_1(\omega)\, d\omega. \qquad (7)$$

S_S is the value of Eq. (7) in the superconducting state. Here, we utilize the f-sum rule for the real part of the conductivity $\sigma_1(\omega)$, i.e., $\int_0^\infty \sigma_1(\omega)\, d\omega = \pi e^2 n/2m$, where n is the 3D electron density and m denotes the effective band mass for the tight-binding band considered. $\sigma(\omega)$ is calculated in the normal and superconducting states using the Kubo formula[38,39]

$$\sigma(\omega) = \frac{2e^2}{\hbar c}\frac{\pi}{\omega}\int_{-\infty}^{\infty} d\omega' [f(\omega') - f(\omega'+\omega)] \times \frac{1}{N}\sum_{\mathbf{k}} [v_{k,x}^2 + v_{k,y}^2][A(\mathbf{k},\omega'+\omega)A(\mathbf{k},\omega') + A_1(\mathbf{k},\omega'+\omega)A_1(\mathbf{k},\omega')], \qquad (8)$$

where $v_{k,i} = \partial\epsilon_k/\partial k_i$ are the calculated band velocities within the CuO_2 plane and c is the c-axis lattice constant. Vertex corrections have been neglected. Physically speaking, we are looking for the loss of spectral weight of the Drude peak at $\omega = 0$ that corresponds to excited quasiparticles above the superconducting condensate for temperatures $T < T_c^*$. Furthermore, the penetration depth $\lambda(x,T)$ is calculated within the London theory through $\lambda^{-2} \propto n_s$.[41]

Most importantly, using our results for $n_s(x,T)$, we calculate the doping dependence of the Ginzburg-Landau-like free-energy change $\Delta F \equiv F_S - F_N$,[10,12]

$$\Delta F = \Delta F_{cond} + \Delta F_{phase}, \qquad (9)$$

where $\Delta F_{cond} \simeq \alpha\{n_s/m\}\Delta_0(x)$ is the condensation energy due to Cooper pairing and $\Delta F_{phase} \simeq \hbar^2 n_s/2m$ the loss in energy due to phase incoherence of the Cooper pairs. α describes the available phase space for Cooper pairs (normalized per unit volume) and can be estimated in the strongly overdoped regime. In the BCS limit one finds $\alpha \simeq 1/400$. Δ_0 is the superconducting order parameter at $T=0$. Within standard (time-dependent) Ginzburg-Landau theory[33] the superfluid density n_s can be calculated via $\langle n_s \rangle = n_s^0 \langle \nabla\phi(\mathbf{r},t)\nabla\phi(0)\rangle$, where $\nabla\phi(\mathbf{r},t)$ reflects the changes of the spatial and time dependence of the Cooper-pair wave function. n_s^0 the static mean-field value of the superfluid density for a given temperature calculated with our extended FLEX approximation.

As suggested by Chakraverty *et al.*[16] and by Emery and Kivelson[17] and also by Schmalian *et al.*[15] one expects that for underdoped cuprates $0.15 > x \to 0$, phase fluctuations become stronger and thus $\Delta F_{phase} < \Delta F_{cond}$.[31] Using Eq. (9) we will show that, in agreement with the experimental observation by Uemura and co-workers,[24] one has for the superconducting transition temperature $T_c \propto n_s$ for $x < 0.15$, but $T_c \propto \Delta_0(x)$ for the overdoped cuprates with $x > 0.15$. Note that T_c and in particular $T_c \propto n_s$ follow also from $\langle n_s \rangle = 0$, where one averages over the phase fluctuation time.

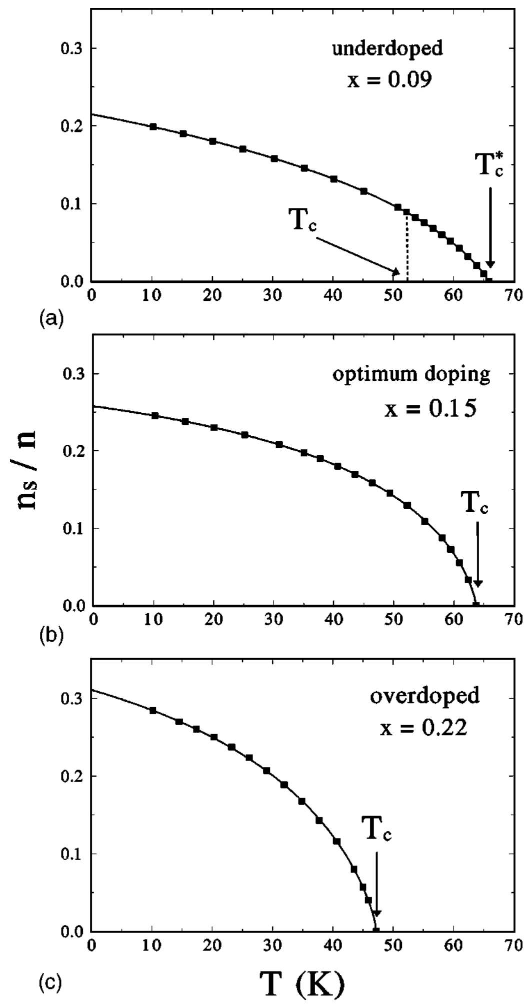

FIG. 1. Temperature dependence of the superfluid density $n_s(x,T)$ calculated with the help of Eqs. (1)– (8) for various hole doping concentrations x. We extrapolate the results to $T \to 0$. The dashed curve in (a) illustrates the effect of Cooper-pair phase fluctuations according to the (static) Kosterlitz-Thouless theory. In Ginzburg-Landau theory the superfluid density can be described as $\langle n_s \rangle = n_s^0 \langle \nabla\phi(r)\nabla\phi(0)\rangle$. Here, $\phi(r)$ denotes the spatial dependence of the Cooper-pair wave function and n_s^0 the static mean-field value of the superfluid density for a given temperature calculated with the FLEX approximation. At $T_c < T < T_c^*$, where Cooper pairs get phase incoherent, $n_s^0 \to 0$ (see Fig. 3).

III. RESULTS AND DISCUSSION

Our results for $n_s(x,T)$ (normalized by n) for different doping concentration x are shown in Fig. 1. For low temperatures we find a linear behavior of the superfluid density due to the nodes in the d-wave order parameter.[7–10,12] Note that we find $n_s(T=0)/n \ll 1$ due to strong-coupling quasiparticle lifetime effects and the observed characteristic change of the nearly linear decrease of n_s for underdoped superconductors

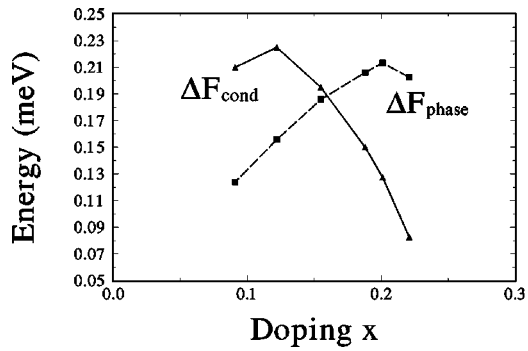

FIG. 2. Calculated crossover of the phase-stiffness energy. We find $\Delta F_{phase} \propto n_s/m^*$ whereas the condensation energy $\Delta F_{cond} \simeq \alpha\{n_s/m\}\Delta_0(x)$. Here, we estimate $\alpha \simeq 1/400$. Note that $\Delta F_{phase} < \Delta F_{cond}$ implies the two characteristic temperatures T_c^*, where Cooper pairs are formed at $T_c \sim \Delta_0$, and $T_c \approx \Delta F_{phase} \propto n_s$, where Cooper pairs become phase coherent.

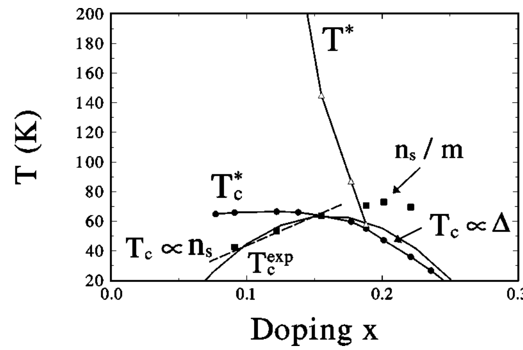

FIG. 3. Phase diagram for high-T_c superconductors resulting from a spin-fluctuation-induced Cooper pairing including their phase fluctuations. The calculated values for $n_s(0)/m$ are in good agreement with muon-spin rotation (Ref. 50). T_c^* denotes the temperature below which Cooper pairs are formed. The dashed curve gives $T_c \propto n_s(T=0,x)$. Below T^* we get a gap structure in the spectral density.

to a more rounded decrease for the overdoped case for increasing temperature and $T \rightarrow T_c$. This is a signature of the opening of the superconducting gap $\Delta(\omega)$ which is itself dependent on the quasiparticle scattering rate below T_c. Both effects are treated self-consistently in our FLEX theory and no further parameter is introduced. Therefore, the important feedback effect of superconductivity on the calculated response functions of the systems is taken into account. We have recently shown that this feedback is needed in order to explain inelastic neutron scattering and tunneling data.[28] Furthermore, this behavior of $n_s(x,T)$ gives results for the London-penetration depth,[41,15]

$$\lambda^2(x,T) \propto n_s^{-1}, \quad (10)$$

in fair agreement with experimental results as discussed later in more detail. For a comparison with the calculated phase diagram for hole-doped cuprates (which is shown later) we have calculated for underdoped cuprates the superconducting bulk transition temperature T_c using $n_s(T)/m$ also calculated from Eq. (6) and $(a=2/\pi)$[31,42–44] using Kosterlitz-Thouless[45] theory,

$$k_B T_c(x) = \frac{1}{a}\frac{\hbar^2}{4m} n_s(T_c), \quad (11)$$

which is shown as a dashed line in Fig. 1(a). Thus, in the underdoped regime one indeed finds a difference between T_c and T_c^*. A finite value of $n_s(T_c<T<T_c^*)$ can be interpreted in terms of local Cooper pairs with a strongly fluctuating phase. In the case of $YBa_2Cu_3O_{6+x}$ (YBCO) this has been recently confirmed by experiment.[46] Physically speaking, for temperatures $T_c<T<T_c^*$ we find preformed pairs without long-range phase coherence in the underdoped regime. In a simple model the origin of the Cooper-pair phase fluctuations is due to the occurrence of vortices which we simply treat within Kosterlitz-Thouless theory. It is remarkable that we get the characteristic temperature dependence of $n_s(x)/n$ for overdoped and underdoped superconductors as seen in experiment.

In a more complete picture one should not only use the XY-model or Kosterlitz-Thouless (KT) theory.[42–45,47–49] Instead, we calculate the doping dependence of the Ginzburg-Landau free energy F within the FLEX approximation directly. In order to avoid entropy effects on the free energy we extrapolate our calculations to $T=0$.

In Fig. 2 results are shown for $\Delta F(x)$. We find that ΔF_{cond} mainly follows the doping dependence of the mean-field transition temperature T_c^* which will be discussed in connection with Fig. 3. On the other hand, the doping dependence of $n_s(0)/m$ determines the doping dependence of ΔF_{phase}. Thus the energy costs due to phase fluctuations have the opposite behavior than the energy gain due to Cooper-pair condensation with respect to the doping concentration x. It is remarkable that we get from our electronic theory a crossing of the two energy contributions ΔF_{cond} and ΔF_{phase} at $x \simeq 0.15$ for which the largest T_c is observed. The consequence of this is that we find $T_c \propto n_s$ for underdoped cuprates and a nonmonotonic doping dependence of $T_c(x)$ with optimal doping at $x \simeq 0.15$. Physically speaking, in the overdoped regime we find a large ΔF_{phase} which means that Cooper-pair phase fluctuations are connected which a large amount of energy. Thus the system will undergo a mean-field transition according to a small condensation energy ΔF_{cond}. In the underdoped regime of cuprate superconductors the situation is the opposite: the energy gain due to the formation of Cooper pairs is not enough in order to reach the Meissner state of the bulk material. This is only possible at a smaller temperature, where the Cooper pairs become phase coherent which is determined by ΔF_{phase} and $\Delta F_{phase} < \Delta F_{cond}$.

In Fig. 3 we show the resulting doping dependence of $T_c(x)$. Our results for the doping dependence of $n_s(0)/m$, which are in good agreement with experimental results,[50,51] are also displayed. In particular, we find a maximum of $n_s(0)/m$ for a doping concentration $x=0.19$. Recent experiments have shown that this behavior is unique for hole-doped cuprates.[50] The curve T_c^{expt} describes many classes of cuprate materials and is taken from Loram and co-workers.[52,53] We would like to emphasize that for the un-

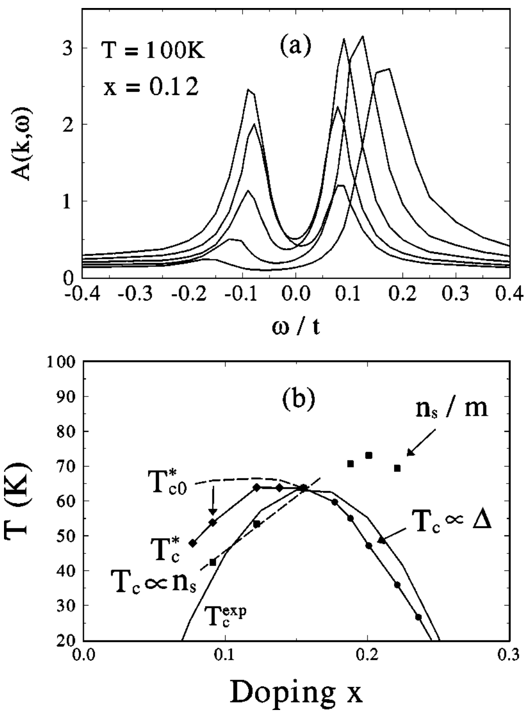

FIG. 4. (a)Results for the quasiparticle spectral function $A(\mathbf{k},\omega)$ ω for different vectors near the gap antinode: $\mathbf{k}=(0.14,1)$, (0.16,1), (0.17,1), (0.19,1), and (0.20,1) (in units of π). The Fermi wave vector is $\mathbf{k}_a=(0.18,1)\pi$. (b) Doping dependence of T_c^* and T_c using a dispersion relation $\tilde{\epsilon}(\mathbf{k})$ in accordance with ARPES data. For clarity, also $T_c^{exp}(x)$ and $n_s(0)/m$ are displayed. T_{c0}^* refers to a mean-field transition taking not into account the pseudogap in the tight-binding energy dispersion.

derdoped cuprates $T_c \propto n_s$ yields indeed better agreement with experimental results than T_c^* obtained from $\Delta(x,T)=0$ and marking the onset of Cooper pairing within our mean-field theory. As already mentioned in connection with Fig. 1 for temperatures $T_c<T<T_c^*$ one finds preformed Cooper pairs. Note that T_c^* depends on the dispersions $\epsilon(\mathbf{k})$ which will be discussed in Fig. 4. For the overdoped cuprates, i.e., $x>0.15$, we get largely BCS-type behavior, namely, $T_c \simeq T_c^* \propto \Delta$. Hence, our electronic theory yields in fair agreement with experiment the nonmonotonic doping dependence of $T_c(x)$. Note, we find similar results for the doping dependence of T_c from determining T_c using $n_s(x,T)=0$. Here, one must include the coupling between Cooper pairs and their phase fluctuations causing a reduction of $T_c^* \rightarrow T_c$ for the underdoped cuprates and $T_c \propto n_s$. Physically, $T_c(x)$ increases first for increasing x, since one has more holes for Cooper pairing [see $n_s(x,T)$ in Fig. 1], and then T_c decreases again, since the glue for the Cooper pairing, i.e., the antiferromagnetic spin fluctuations, mainly disappear.

Also in Fig. 3 results are given for the characteristic temperature T^* at which a gap appears in the spectral density $A(\mathbf{k},\omega;T)$. Within our FLEX theory the occurrence of a pseudogap is due to inelastic electron-electron scattering which leads to a loss of spectral weight at the Fermi level. Agreement with experimental results is fair; however, the calculated magnitude of the gap itself is too small as compared with pseudogap measurements.[21,54] The reason for this is that the input dispersions $\epsilon(\mathbf{k})$ crossed the Fermi energy for $\mathbf{k}\simeq(\pi,0)$ in the Brillouin zone. Note that the result $T^*(x)\rightarrow T_c(x)$ for $x\simeq 0.19$ depends on the strength of the interaction between quasiparticles and the antiferromagnetic spin fluctuations. If we increase this coupling we will get for increasing x (and for the overdoped cuprates[55]) $T^*\rightarrow T_c$ and $T^*\approx T_c(x)$ as well as $T^*>T_c(x)$ for further increasing coupling.

As mentioned above we get the right doping dependence of the weak-pseudogap temperature T^* however, the calculated magnitude of the pseudogap is too small in comparison with experiment. In general, the magnitude of this pseudogap should also influence the mean-field transition temperature T_c^* and thus the temperature range where preformed Cooper pairs are formed, because less holes (or electrons) can pair if fewer states at the Fermi level are present. In order to investigate this question in detail we perform calculations with an appropriate energy dispersion $\tilde{\epsilon}(\mathbf{k})$ which exhibits, in accordance with recent photoemission data, d-wave symmetry. Furthermore, we choose $\tilde{\epsilon}(\mathbf{k})$ to be doping dependent in accordance with Refs. 21–23, 54, and 56.

In Fig. 4(a) we present results for the spectral density $A(\mathbf{k},\omega)$ calculated within our FLEX theory in the underdoped regime from the Green's function $G(\mathbf{k},\omega)$.[44] As an input we use for the underdoped superconductors the Fermi surface as observed by Marshall *et al.*[54] and a dispersion $\tilde{\epsilon}(\mathbf{k})=\sqrt{\epsilon^2(\mathbf{k})+\Delta^2(\mathbf{k})}$ including for $\mathbf{k}\simeq(\pi,0)$ the pseudogap structure.[44] The results show the interplay of pseudogaps and superconducting gap and the different features for under- and overdoped superconductors and should be compared with ARPES-data.[54] Of course, ARPES can only measure occupied states, i.e., the spectral density for $\omega<0$. As an example we show in Fig. 4(a) our calculated spectral function for a doping concentration of $x=0.12$ at $T=100$ K, where the magnitude of the pseudogap is $0.1t=25$ meV. One sees that the spectral function does not cross the Fermi level $(\omega=0)$. This has consequences for the Cooper pairing.

In Fig. 4(b) we present the corresponding results for $T_c^*(x)$ and $T_c(x)$ obtained by using as an input dispersions $\tilde{\epsilon}(\mathbf{k})$ which are for underdoped cuprates in accordance with recent angular-dependent photoemission results. To model the pseudogap behavior for $\mathbf{k}\simeq(\pi,0)$ we take $\Delta(\mathbf{k})=\Delta_0(\cos k_x-\cos k_y)/2$ for a fixed doping value. As expected, if for $\mathbf{k}\simeq(\pi,0)$, where pairing is most favorable, we take proper account of the observed pseudogaps[54] one obtains smaller values for T_c^* and T_c and for $(T_c^*-T_c)$ as well. The latter signals that the pseudogap decreases the reduction of $T_c^*\rightarrow T_c$ due to Cooper-pair phase fluctuations.[57,58]

Finally, note we may also estimate within Ginzburg-Landau theory and our FLEX theory the doping concentration $x_0 \gtrsim 0.06$ at which superconductivity begins. Our FLEX theory yields an attractive interaction essentially for two holes at nearest-neighbor sites. From this and the probability

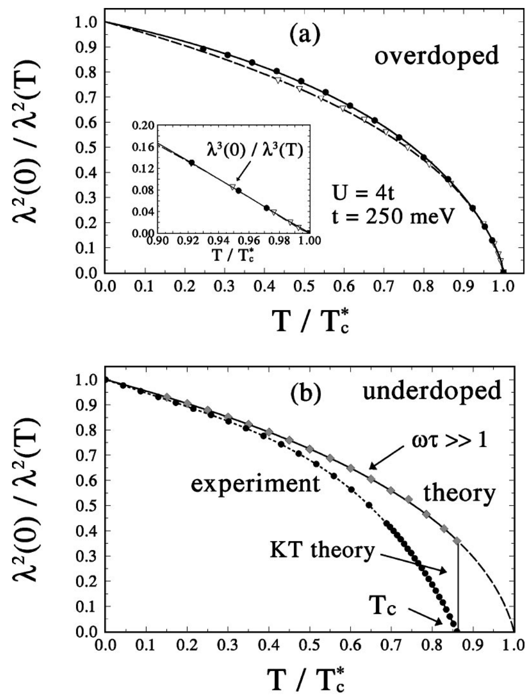

FIG. 5. Results for the penetration depth $\lambda(T,x)$ ($n_s \propto \lambda^{-2}$) for over- and underdoped cuprates. The inset in (a) shows a remarkable linear behavior for the overdoped superconductors of $\lambda^{-3}(T)$ for $T \simeq T_c^* \simeq T_c$ even without having included critical fluctuations. This is in good agreement with Ref. 59. In (b) we indicate the behavior expected for the Meissner effect occurring only for $n_s(\omega=0)>0$. Results derived from KT theory, where $n_s(T) \rightarrow 0$ at T_c are also shown. Theory refers to pure FLEX results neglecting Cooper-pair phase fluctuations for $T<T_c$. These should be compared with $n_s(\omega)$ results for $(\omega\tau) \rightarrow \infty$.

x to find a hole one may easily get a rough estimate for the hole density necessary to get Cooper pairing.[25]

An important check on the validity of our results for the superfluid density $n_s(x,T)$ is provided by the analysis of the London-penetration depth λ_L. In agreement with experiment (see Ref. 59) we calculate λ for optimal doping and find a strong increase in $\lambda(T=0)$ for $0.15>x\rightarrow 0$. Clearly, the characteristic behavior of the superconductors regarding electromagnetism, the Meissner effect, requires phase coherence of the Cooper pairs,[33] $n_s(\omega=0)>0$. Hence, the Meissner effect occurs only for $T<T_c$, but not for $T_c<T<T_c^*$, where Cooper pairs are phase incoherent and $\langle n_s \rangle = n_s^0 \langle \nabla \phi(\mathbf{r}) \nabla \phi(0) \rangle \simeq 0$. Of course, on general grounds one expects still some phase correlations for $T \gtrsim T_c$ and $n_s < n_s(\omega\tau \rightarrow \infty)$ for $T \lesssim T_c$. Here, τ is the lifetime of the phase fluctuation and $n_s(\omega\tau)$ refers to a frequency-dependent measurement.

In Fig. 5 we present our calculated results for the penetration depth $\lambda(x,T)$. In (a) we demonstrate the remarkable agreement with experiment for the overdoped cuprates.[59] Furthermore, in the inset of (a) $\lambda^3(T,x)$ in the vicinity of T_c is displayed. We find a linear behavior which is indeed observed in the experiment.[59] It is interesting that we get this temperature dependence without critical fluctuations. In our FLEX theory this is due to strong-coupling lifetime effects which determine the opening of the superconducting gap $\Delta(\omega)$. However, at present it is not clear whether our FLEX calculations provide an explanation extremely close to T_c, because the numerical convergence of Eqs. (2)–(7) is very slow. Further calculations should clarify this interesting issue.

In Fig. 5(b) we present the FLEX results for underdoped superconductors. The effect of phase fluctuations can be seen from the discrepancy between experiment[59] and theory. One clearly sees that no Meissner effect results for $T>T_c$, since the phase correlation function $\langle \phi(\mathbf{r}) \phi(0) \rangle$ becomes zero. The results obtained using static Kosterlitz-Thouless theory (straight line) and the FLEX results (diamonds) for $n_s(x,T)$ are shown.[42] The pure FLEX results neglect phase fluctuations which is appropriate for $(\omega\tau) \rightarrow \infty$. Of course, in Kosterlitz-Thouless theory we get $\lambda^{-2} \rightarrow 0$ at T_c, while in our full FLEX calculations we have to use $\langle n_s \rangle = n_s^0 \langle \nabla \phi(\mathbf{r}) \nabla \phi(0) \rangle$ to get this. Note that for $T<T_c$ the discrepancy between experimental results and our FLEX calculations indicates the importance of Cooper-pair phase fluctuations below T_c.

Regarding the dynamical behavior of the underdoped cuprate superconductors we may conclude some interesting facts using the results shown in Fig. 5(b) and which may be related to the recent dynamical conductivity measurements by Corson *et al.*[26] In relation to the latter our theoretical pure FLEX results refer to the case of $\omega\tau \gg 1$ or $\tau \gg \omega^{-1}$ such that phase fluctuations are not effective and yield a "dynamical" Meissner effect $[n_s(\mathbf{q},\omega)>0]$ for $T_c<T<T_c^*$. Also, the difference $(\lambda_{theory}^{-2} - \lambda_{expt}^{-2})$ or, respectively, $[n_s(\omega\tau \gg 1) - n_s(\omega\tau \ll 1)]$ gives for a given temperature T the variation in λ^{-2}, n_s, or optical conductivity upon changing the frequency of the applied electromagnetic field. The lifetime τ of the phase fluctuations $\tau(x)$ may be calculated from our results for $n_s(x,T)$ using $\tau = (T/T_\theta^0 \Omega_0) \exp\{-2C\hbar^2 n_s(x)/m^* T\}$, where C and Ω_0 are constants and $T_\theta^0 \propto n_s/m$, see Corson *et al.*[26] Thus we get approximately 70.

Finally, we note that the frequency dependence does not stop at T_c, but for $T<T_c$; see the discrepancy between experimental and theoretical results in Fig. 5(b). This also is in fair agreement with experimental results by Corson *et al.* For example, $T_c = 33$ K where the frequency dependence stops at $T \simeq 15$ K.[26]

Concerning the dynamics of excited superconductors in general the phase diagram shown in Figs. 3 and 4(b) with characteristic temperatures T^* and T_c should imply various relaxation channels for electronic excitations in high-T_c superconductors due to photon absorption.[60,44] This is illustrated in Fig. 6. We estimate on general grounds that

$$\tau_1 \propto \Delta^{-1} \propto T_c^{-1}, \tag{12}$$

since the energy change involved in the excitation is of the order of $\langle \Delta e^{i\phi} \rangle$. Note that above T_c one has $\langle e^{i\phi} \rangle = 0$ due to phase-incoherent Cooper pairs. Hence, τ_1 describes dynamics only below T_c. Using data for $T_c(x)$ we estimate τ_1 to be of the order of picoseconds which is in agreement with Ref. 60. Furthermore, the energy involved in the gap structure of $A(\mathbf{k},\omega)$ and occurring at T^* and thus in the corresponding

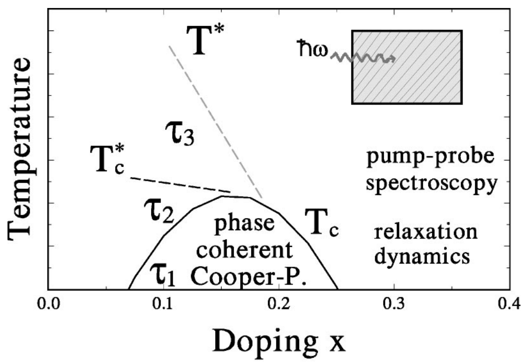

FIG. 6. Illustration of relaxation dynamics expected for excited electrons in cuprate superconductors. Time τ_1 refers to relaxation of excited electrons and time τ_3 to relaxation involving antiferromagnetic correlations characterized by T^*. If τ_1 refers to relaxation towards phase-coherent Cooper pairs it is only observed below T_c, since $\langle \Delta e^{i\phi}\rangle \to 0$ for $T > T_c$. The relaxation time τ_2 may refer to the dynamics of phase-incoherent Cooper pairs.

optically induced excitation, is mainly $E_{af} \sim T^*$. Then one may estimate a corresponding relaxation time with

$$\tau_3 \sim E_{af}^{-1} \sim (T^*)^{-1} \sim \left(\frac{T_c}{T^*}\right) \tau_1 . \tag{13}$$

Thus, $\tau_3(x)$ can be estimated to be of the order of a few hundred femtoseconds. Recently, by pump and probe spectroscopy such relaxations of the order of a few ps and 700 fs have been observed by Kaindl *et al.*[60]

It would be interesting to check the above analysis by further experiments, using different light frequencies and polarizations, and in particular the relaxation $\tau_3 \sim (T^*)^{-1}$. Note different dynamics is expected for $T^*(x) \to T_c$ at $x \simeq 0.15$ and $T^* \gtrsim T_c$ and $T^* > T_c$ for the overdoped cuprates. Of course, it might be also possible like in ARPES to detect excitations reflecting the energy $\Delta(\mathbf{k},\omega)$ and thus the *d*-wave symmetry of the pairing.

Circularly polarized light might also couple to magnetic excitations in the cuprates, but then spin-orbit coupling is involved and one gets much longer relaxation times.

Finally, we would like to mention that we have also investigated the quasiparticle spectral density below T_c. In standard FLEX theory we obtain the characteristic features in SIS conductance at approximately 3Δ and in SIN conductance at approximately $\pm 2\Delta$ and that these both disappear for $T \gtrsim T_c$.[61] Of course, it is of interest to see what happens for $T_c < T < T_c^*$. The fingerprint of phase incoherent Cooper pairs—for example, in SIS tunneling for $T > T_c$ for one superconductor and $T^* > T > T_c^*$ for the other one—depends on how much the measurement involves averaging of $\Delta e^{i\phi(\mathbf{r},t)}$. For example, a fluctuation phase can lead to a reduction of the measured gap amplitude through the coupling between amplitude and phase of a Cooper pair.[42–44] Thus phase fluctuations of Cooper pairs are indirectly observable even in slow or static experiments.

IV. SUMMARY

In summary, we have used as a model the Hubbard Hamiltonian and the self-consistent FLEX theory extended by including Cooper-pair phase fluctuations to calculate some basic properties of the hole-doped cuprate superconductors. We combined our results with standard many-body theory and used this as in input for the Ginzburg-Landau energy functional $\Delta F\{n_s,\Delta\}$. In particular, we have calculated the superfluid density n_s/n, n_s/m, and the critical temperature T_c as a function of the doping concentration. We found a phase diagram for hole-doped cuprates with two different regions: on the overdoped side we obtain a mean-field-like transition and $T_c \propto \Delta(T=0)$, whereas in the underdoped regime we find $T_c \propto n_s(T=0)$. The temperature region $T_c < T < T_c^*$ may be attributed to preformed Cooper pairs without long-range phase coherence. We show that an improved treatment of the weak pseudogap at room temperature narrows the range where preformed pairs may be found. The overall agreement with experiments is remarkably good and suggests spin-fluctuation exchange as the dominant pairing mechanism for superconductivity. We also investigated the time scale of Cooper-pair phase fluctuation and find fair agreement with experiments. We propose further time-resolved experimental studies in order to find the origin of the pseudogaps. Again, we would like to stress that we try to get various properties within a unified theoretical picture. An analysis of superconductivity in the cuprates can be performed mainly on the basis of $\chi(\mathbf{q},\omega)$ and the pronounced wave vectors $\mathbf{q}_i$ related to the peaks in Imχ and the topology of the Fermi surface. This sheds light on the general validity of our results. Also, it has been of central significance that we work within a conserving approximation and perform self-consistent calculations. We improve the numerical analysis for solving the Dyson equations for the full Green's functions[44] which contain an amplitude and a phase. As a further test, we apply our theory also to electron-doped superconductors and find superconductivity of mainly *d*-wave symmetry.[62,63] There might be general questions regarding the Hubbard model Hamiltonian and the validity of effective-second order perturbation theory treatment. However, the comparison of the results with experiments seem to support this handling of high-T_c superconductivity. Also note, FLEX theory corresponds to Eliashberg theory in the case of electron-phonon interactions and has the same transparency. The strength of the interaction to the spin fluctuations is presently posing a problem which needs further studies.

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