Theoretical analysis of Cooper-pair phase fluctuations in underdoped cuprates: a spin-fluctuation exchange study

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We study Cooper-pair phase fluctuations in cuprate superconductors for a spin fluctuation pairing interaction. Using an electronic theory we calculate in particular for the underdoped cuprate superconductors the superfluid density \( n_s(T) \), the superconducting transition temperature \( T_c(x) \propto n_s \) below which phase coherent Cooper-pairs occur, and \( T_c^*(x) \) where the phase incoherent Cooper-pairs disappear. Also we present results for the penetration depth \( \lambda(x, T) \) and for the weak pseudogap temperature \( T^*(x) \) at which a gap structure occurs in the spectral density. A Meißner effect is obtained only for \( T < T_c \). We find that phase fluctuations become increasingly important in the underdoped regime and lead to a reduction of \( T_c \) in good agreement with the experimental situation.

In accordance with the experimental observation for underdoped cuprate superconductors that the superconducting transition temperature is related to the superfluid density \( n_s \) and behaves as \( T_c \propto n_s(0) \), in contrast to the overdoped case [1], we use an electronic theory which takes into account phase fluctuations of the Cooper-pairs. From this one expects a phase diagram with \( T_c^* \) at which phase incoherent Cooper-pairs occur and a lower transition temperature \( T_c \propto n_s \) at which these Cooper-pairs become phase coherent. Such a physical picture for the underdoped cuprates has been treated phenomenologically before by Chakraverty et al. [2], more recently by Emery and Kivelson [3], and also by Schmalian et al. [4].

Close to \( T_c \) one gets as in Ginzburg-Landau (GL) theory the free energy (without external field)

\[
\Delta F = F_S - F_N = \Delta F_{BCS} + \Delta F_{phase}
\]

where \( \Delta F_{BCS} = \frac{1}{2} N(E_F) \Delta \omega_s^2 \) and \( \Delta F_{phase} = \frac{\partial^2}{\partial n^2} n_s \) with \( n_s = n_s(\nabla \Phi(r) \nabla \Phi(0)) \). Here, we assume only a spatial dependence of the phase \( \Phi(r) \) of the superconducting order parameter. This implies a superconducting transition at \( k_B T_c = \Delta F_{BCS} \), when \( \Delta F_{BCS} < \Delta F_{phase} \) and Cooper-pairs are formed and \( k_B T_c = \Delta F_{phase} \propto n_s(0) \), when \( \Delta F_{phase} < \Delta F_{BCS} \) and Cooper-pairs become phase coherent. This neglects 2d effects. In this letter we use an electronic theory in order to calculate the doping dependence of \( N(E_F), \Delta(0) \), and \( n_s(x) \) and thus the two contributions to \( \Delta F \) and the two doping regimes for non-BCS and BCS behavior of the superconducting transition temperature. Based on a spin fluctuation exchange mechanism we determine the doping dependence of the phase diagram with \( T_c^*(x) \), \( T_c(x) \), and also \( T^* \) at which far above \( T_c \) a gap appears in the spectral density. In accordance with Eq. [1] we find from our microscopic calculation that phase fluctuations of the Cooper-pairs are significant for the underdoped cuprates. For the overdoped superconductors we obtain a mean-field behavior and \( T_c^{exp} \sim T_c^* \). Our results suggest (see also Kosterlitz-
It follows from Eq. (3) that the quasiparticle self-energy components $X_\nu$ ($\nu = 0, 1, 2$) with respect to the Pauli matrices $\tau_\nu$ in the Nambu representation are given by

$$X_\nu(k, \omega) = N^{-1} \sum_{k'} \int_{-\infty}^{\infty} d\Omega \left[ P_{s}(k - k', \Omega) \pm P_{c}(k - k', \Omega) \right] \times \int_{-\infty}^{\infty} d\omega' I(\omega, \Omega, \omega') A_{\nu}(k', \omega') \ .$$

(3)

Here, we used the $T$-matrix or fluctuation exchange (FLEX) approximation in which a Berk-Schrieffer-like pairing interaction is constructed with the dressed one-electron Green's functions. The spin fluctuation interaction is given by $P_{s} = (2\pi)^{-1} U^2 \text{Im} \left(3\chi_{s} - \chi_{s0}\right)$ with $\chi_{s} = \chi_{s0}(1 - U\chi_{s0})^{-1}$ and the charge fluctuation interaction is $P_{c} = (2\pi)^{-1} U^2 \text{Im} \left(3\chi_{c} - \chi_{c0}\right)$ with $\chi_{c} = \chi_{c0}(1 + U\chi_{s0})^{-1}$, where $\chi_{s0, c0}(q, \omega)$ is given in Ref. [12]. The subtracted terms in $P_{s}$ and $P_{c}$ remove a double counting that occurs in second order. In Eq. (3) the plus sign holds for $X_0$ (quasiparticle renormalization) and $X_3$ (energy shift), and the minus sign for $X_1$ (gap parameter). The kernel $I$ and the spectral functions $A_{\nu}$ are given in Ref. [12].

For the numerical evaluation we use a bare tight-binding dispersion relation $\epsilon(k) = 2t[2 - \cos(\pi x_1) - \cos(\pi x_2) - \mu]$ and $U/t = 4$. Then, the doping dependence $n = \frac{\pi}{h^2} \sum_{k} n_{k} = 1 - x$ is determined with the help of the $k$-dependent occupation number $n_{k} = 2 \int_{-\infty}^{\infty} d\omega f(\omega) N(k, \omega)$ that is calculated self-consistently, where $N(k, \omega) = A_{0}(k, \omega) + A_{3}(k, \omega)$. $n = 1$ corresponds to half filling. Our numerical calculations are performed on a square lattice with 256x256 points in $k$ space of the Brillouin zone and with 200 points on the real $\omega$ axis up to 16$t$ with an almost logarithmic mesh. The full momentum and frequency dependence of the quantities is kept [13]. Thus, our calculation includes pair breaking effects on the Cooper-pairs resulting from lifetime effects of the elementary excitations. $T_{c}^{*}$ is determined from the linearized gap equation and the superconducting state is found to have $d$-wave symmetry [12]. The transition temperature $T_{c}$ at which phase coherence occurs is determined by $T_{c} \propto n_{s}(x)$ where the superfluid density $n_{s}(x, T)/m$ is calculated self-consistently from

$$n_{s} = \frac{2t}{h^2} (S_{N} - S_{S}) \quad \text{with} \quad S_{N} = \frac{h^2 c}{2\pi e^2 t} \int_{0}^{\infty} \sigma_{1}(\omega) d\omega .$$

$S_{S}$ is the corresponding expression 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. $\sigma_{1}(\omega)$ is calculated in the normal and superconducting state using the standard Kubo formula [14]. 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 $T < T_{c}^{*}$. Finally, the penetration depth $\lambda(x, T)$ is calculated within the London theory through $n_{s} \propto \lambda^{-2}$ [13].

In Fig. 3 we show the phase diagram for the cuprate superconductors obtained from our electronic theory and compare with the generalized experimental phase diagram $T_{c}(x)$ that describes many superconductors as pointed out by Tallon [13]. We get $T_{c} \approx T_{c}^{*}$ for $x \sim x_{\text{opt}}$, whereas for the underdoped superconductors $T_{c} \propto n_{s}(T = 0)$ agrees much better with the experimental results than $T_{c}^{*}$. Note, for the overdoped cuprates one gets the superconducting transition at $T_{c}^{*}$, where phase coherent Cooper-pairing occurs since $\Delta_{\text{phase}}$ becomes largest. $T_{c}^{*}$ results from $\phi(x, T) = 0$, where $\phi(k, \omega) = Z(k, \omega)\Delta(k, \omega)$ is the strong-coupling superconducting order parameter and is a mean-field result in the sense that Cooper-pair phase fluctuations have been neglected. However, the AF fluctuations are treated well beyond the mean-field approximation. It is remarkable that we find approximately that $T_{c}$ varies linearly with $x$. This cannot be the case for $n_{s}(x \rightarrow 0)$. We also expect that an improved inclusion of the pseudogap behavior and reduction of the density of states (DOS) due to antiferromagnetic (AF) correlations will yield a faster decrease of $\Delta_{\text{phase}}$ for $x \rightarrow 0$. Also important is the fact that we find an optimal $T_{c}$ for $x \approx 0.15$ since for $x < x_{\text{opt}}$ we find $T_{c} \propto n_{s}(T = 0)$ and for $x > x_{\text{opt}}$ one has $T_{c} \propto \Delta(T = 0)$. Of interest are also the results for the pseudogap temperature $T^{*}$ at which a gap structure in the DOS in the normal state occurs. This has been discussed in Refs. [12,4]. Such a behavior is seen experimentally in various SIN tunneling data, reflectivity measurements as well as in the two-magnon response in Raman scattering [18,19]. Physically speaking, below $T^{*}$ the electrons are strongly coupled to the magnetic degrees of freedom which are generated due to paramagnon (spin fluctuation) excitations in the system. Finally, we would like to mention that at $x^{*} = 0.19$, $T^{*}$ and $T_{c}$ coincide. Furthermore, our results indicate that for $x > x^{*}$ the non-BCS behavior $T_{c} \propto n_{s}(T = 0)$ seems not valid anymore. In contrast to the underdoped regime, there the energy gain due to Cooper-pair formation is smaller than the energy to break up phase coherence. Thus, Cooper-pair phase fluctuations are unimportant in this regime. Note, $T_{c}$ may be viewed in analogy to the Curie temperature in Ferromagnets like Ni or Fe, where spin-disorder occurs.

In order to investigate different models used in the context of Cooper-pair phase fluctuations [2,4], we discuss now the superfluid density for finite temperatures. In Fig. 3(a) results are given for $n_{s}(T, x)/m$. To obtain $n_{s}(T = 0)$ we have used a polynomial fit up to third order [20]. For the doping values investigated here, we find a linear behavior of $n_{s}(0, x)$ except for the strongly
overdoped case, i.e. \( x \geq 0.22 \) where \( n_s(T=0) \) starts to decrease. This behavior indicates a crossover to the (BCS) weak-coupling limit where \( n_s = n \) for \( T = 0 \) is expected. This implies that \( \lambda(T=0,x) \) is asymmetric with respect to optimal doping as suggested from Fig. 1. Note that the energy \( \Delta F_{\text{phase}} \propto n_s(0) \) is still larger than the energy gain due to Cooper-pair condensation. Thus we conclude that Cooper-pair phase fluctuations are unimportant in the overdoped regime. Note, \( n_s(T,x) \rightarrow 0 \) for \( T \rightarrow T_c^* \), since Cooper-pairs disappear at \( T_c^* \). However, the phase coherence temperature \( T_c \) has to be determined by spatially averaging over the Cooper-pair phase fluctuations. In the presence of spatial phase fluctuations the average superfluid density \( \bar{n}_s \) will vanish at \( T_c \) so that as in KT theory no Meißner effect occurs above \( T_c \). Note, within KT theory \( T_c \) is given by

\[
\frac{1}{a} \frac{\pi}{h^2} \frac{n_s(T_c)}{4m} = k_B T_c \quad ,
\]

where \( 1/a = \pi/2 \). In the case of the similar 2D \( XY \) model one has \( 1/a = 0.9 \). Our construction used in Fig. 2 involves only the determination of \( n_s(T=T_c) \), but does not imply a jump in \( n_s \) at \( T_c \) which is true only for the 2D \( XY \)-model and KT theory. For a comparison with Ref. [23], we show also results for the 3D version of the \( XY \)-model. All these theories take into account phase and amplitude of the Cooper-pairs. We see that in the 2D (3D) version of the \( XY \)-model \( T_c \) is lower (higher) compared to the KT theory. Physically speaking, in the \( XY \)-model \( n_s \) (or the phase stiffness) is the only relevant energy scale. Thus one always has \( T_c \propto n_s \). In the KT theory one has two energy scales, namely the phase stiffness and also the vortex core energy. Nevertheless, all these theories yield within our microscopic treatment an optimal doping concentration. Note, we obtain \( n_s(x \rightarrow 0) \) due to pair breaking resulting from the decreasing lifetimes of the Cooper-pairs [22]. Improved calculations taking into account AF correlations leading to static antiferromagnetism cause a further decrease of \( n_s(x) \) for \( x \rightarrow 0 \) [26].

In Fig. 3 we show the mean field results for the penetration depth. In (a) the overdoped case is displayed: our results for \( \lambda^{-2}(T) \) agree qualitatively with the experimental data [22,23]. It is remarkable that we find a linear behavior of \( \lambda^{-3}(T) \) (see inset). In Ref. [22] at \( T = 0.9 T_c^* \) a value for \( \lambda^3(0)/\lambda^3(T) \) of 0.2 has been found. Instead, we find 0.16. Note that we did not include critical fluctuations. A closer inspection of our data leads to the conclusion that the rapid opening of the superconducting gap - which is calculated self-consistently - is the main reason for the reported behavior of the penetration depth [21,22]. Thus, we conclude that the existence of critical fluctuations is not necessary in order to understand the observed behavior of the penetration depth close to the critical temperature in the cuprates. This might shed some light on the significance of vertex corrections. However, very close to \( T_c \) we cannot present numerical results yet. For this range it remains unclear whether or not a change of the powerlaws from \( 1/3 \) to \( 1/2 \) occur. Fig. 3(b) indicates that for calculating \( \lambda(T,x) \) one must use the superfluid density \( n_s \) referring to phase coherence as is done in KT theory. Note, static KT theory predicts an universal jump in \( n_s \) at \( T = T_c \) as indicated, which is not observed experimentally [23,24]; the \( n_s \) results obtained from our electronic theory refer only to the Cooper-pair density \( n_s(x,T) \) but \( n_s = n_s \) at \( T < T_c \). As mentioned earlier, the spatially phase averaged \( \bar{n}_s(x,T) \) yields \( n_s(T_c,x) = 0 \) for incoherent Cooper-pairs. The comparison with experiment indicates that \( n_s < n_s \) already for \( T < T_c \). No Meißner effect is expected for \( T_c < T < T_c^* \). While our calculation of \( n_s(x,T) \) is expected to give the correct tendency for the behavior of the underdoped superconductors, stronger AF effects must be included for \( x \rightarrow 0 \). Also, quantum phase fluctuations are neglected. All this would cause a more rapid decrease
of $T_c \propto n_s(x)$ in Fig. 1.

In summary, it is interesting that our electronic theory using the model Hamiltonian $H$, Eq. (1), gives remarkable agreement with some basic experimental observations. In particular, we have shown within a microscopic theory based on a spin fluctuation pairing mechanism that Cooper-pair phase fluctuations become important for underdoped cuprates. This gives a microscopic justification for the phenomenological theories in Refs. 1-3. Of course, a fully self-consistent determination including the phase fluctuations of the Green’s functions and the electronic excitations should be performed [4]. Thus, one might get also an insight about the origin of the pseudogaps above $T_c$ and revealing asymmetric doping dependence of various properties with respect to $x_{opt}$.

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FIG. 3. Results for the penetration depth $\lambda(T, x)$ ($n_s \propto \lambda^{-2}$). The inset in (a) shows a remarkable linear behavior of $\lambda^{-3}(T)$ for $T \approx T_c^*$ even without having included critical fluctuations. In (b) we indicate the behavior expected for $\bar{n}_s$ and derived from KT theory, where $\bar{n}_s(T) \to 0$ at $T_c$.

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