Phase diagram of underdoped cuprate superconductors:
effect of Cooper-pair phase fluctuations

C. Timm, D. Manske, and K. H. Bennemann
Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany
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In underdoped cuprates fluctuations of the phase of the superconducting order parameter play a role due to the small superfluid density. We consider the effects of phase fluctuations assuming the exchange of spin fluctuations to be the predominant pairing interaction. Spin fluctuations are treated in the fluctuation-exchange approximation, while phase fluctuations are included by Berezinskii-Kosterlitz-Thouless theory. We calculate the stiffness against phase fluctuations, \( n_s(\omega)/m^* \), as a function of doping, temperature, and frequency, taking its renormalization by phase fluctuations into account. The results are compared with recent measurements of the high-frequency conductivity. Furthermore, we obtain the temperature \( T^* \), where the density of states at the Fermi energy starts to be suppressed, the temperature \( T_c^* \), where Cooper pairs form, and the superconducting transition temperature \( T_c \), where their phase becomes coherent. We find a crossover from a phase-fluctuation-dominated regime with \( T_c \propto n_s \) for underdoped cuprates to a BCS-like regime for overdoped materials.

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I. INTRODUCTION

For about fifteen years cuprate high-temperature superconductors (HTSC’s) have stimulated significant advances in the theory of highly correlated systems as well as in soft condensed matter theory. Nevertheless, we still do not fully understand the various phases of these materials. Of particular interest is the underdoped regime of hole-doped cuprates, in which the hole density (doping) \( x \) in the CuO\(_2\) planes is lower than required for the maximum superconducting transition temperature \( T_c \). In this regime the superfluid density \( n_s \) decreases with decreasing doping and is found to be proportional to \( T_c \). Above \( T_c \), one finds a strong suppression of the electronic density of states close to the Fermi energy, \( i.e., \) a pseudogap, which appears to have the same symmetry as the superconducting gap. Furthermore, there may be fluctuating charge and spin fluctuations (stripes).

It has been recognized early on that the small superfluid density \( n_s \) leads to a reduced stiffness against fluctuations of the phase of the superconducting order parameter. Phase fluctuations are additionally enhanced because they are canonically conjugate to charge density fluctuations, which are believed to be suppressed. Furthermore, the cuprates consist of weakly coupled two-dimensional (2D) CuO\(_2\) planes so that fluctuations are enhanced by the reduced dimensionality. Phase fluctuations might destroy the long-range superconducting order, although there is still a condensate of preformed Cooper pairs. In conventional, bulk superconductors this mechanism is not relevant, since the large superfluid density leads to a typical energy scale of phase fluctuations much higher than the superconducting energy gap \( \Delta \), which governs the thermal breaking of Cooper pairs. Thus in conventional superconductors the transition is due to the destruction of the Cooper pairs and \( T_c \) is proportional to \( \Delta \). On the other hand, the observation that \( T_c \propto n_s \) in underdoped cuprates indicates that the phase fluctuations drive the transition in this regime. The Cooper pairs only break up at a crossover around \( T_c^* > T_c \). If the feedback of phase fluctuations on the local formation of Cooper pairs is small, \( T_c^* \) is approximately given by the transition temperature one would obtain without phase fluctuations. Between \( T_c \) and \( T_c^* \) Cooper pairs exist but the order parameter is not phase coherent any more. Recent thermal expansion experiments strongly support this picture. However, there is no close relation between our \( T_c^* \) and the mean-field transition temperature of Ref. \( \cite{10} \), which is determined by extrapolation from the low-\( T \) behavior of the expansivity.

There is a third temperature scale \( T^* \) with \( T^* > T_c^* \), below which a pseudogap starts to open up as seen in nuclear magnetic resonance, tunneling, and transport experiments. It seems unlikely that the pseudogap at these temperatures is due to local superconductivity. Rather, it is thought to be caused by spin fluctuations or the onset of stripe inhomogeneities. Recent experiments on the Hall effect in GdBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) film\( s \) also support the existence of two crossover temperatures \( T_c^* \) and \( T^* \). In this work we are mostly concerned with the strong pseudogap regime \( T_c < T < T_c^* \).

Due to the layered structure of the cuprates, they behave like the 2D XY model except in a narrow critical range around \( T_c \), where they show three-dimensional (3D) XY critical behavior. The standard theory for the 2D XY model, the Berezinskii-Kosterlitz-Thouless (BKT) renormalization group theory, should thus describe these materials outside of the narrow critical range. Also, recent transport measurements for a gate-doped cuprate with only a single superconducting CuO\(_2\) plane show essentially the same doping dependence of \( T_c \) as found for bulk materials. BKT theory predicts a transition at a temperature \( T_c < \)
\[ T^*_c, \text{ due to the unbinding of fluctuating vortex-antivortex} \]

pairs in the superconducting order parameter. Gaussian phase fluctuations are less important, since they do not shift \( T_c \). In addition, the coupling of the phase to the electromagnetic field causes them to be gapped at the plasma frequency \( \omega_p \) whereas the BKT picture of vortex unbinding remains basically unchanged.

In the early days of HTSC’s, BKT theory was invoked to interpret a number of experiments on bulk samples. \[ \text{Recently, two experiments have lent strong additional support to the BKT description: First, Corson et al. have measured the complex conductivity of underdoped Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8+\delta \text{ and extracted the frequency-dependent phase stiffness from the data. The authors interpret the data in terms of dynamical vortex-pair fluctuations and conclude that vortices—} \]

and thus a local superconducting condensate—exist up to at least 100 K. We discuss this assertion in Sec. III. Second, Xu et al. have found signs of vortices at temperatures much higher than \( T_c \) in underdoped La\(_2-\delta\)Sr\(_\delta\)CuO\(_4\) in measurements of the Nernst effect. A recent reanalysis of the data yields an onset temperature of vortex effects of 40 K for an extremely underdoped sample \( x = 0.05 \) and of 90 K for \( x = 0.07 \).

So far, we have not said anything about the superconducting pairing mechanism. There is increasing evidence that pairing is mainly due to the exchange of spin fluctuations. The conserving fluctuation-exchange (FLEX) approximation \[ \text{based on this mechanism describes optimally doped and overdoped cuprates rather well. In particular, the correct doping dependence and order of magnitude of } T_c \text{ are obtained in this regime. On the other hand, the FLEX approximation does not include phase fluctuations and we believe this to be the main reason why it fails to predict the downturn of } T_c \text{ in the underdoped regime. Instead, } T_c \text{ is found to approxi-}

mately saturate for small doping } x \text{. However, the FLEX approximation is able to reproduce two other salient features of underdoped cuprates, namely the decrease of } n_s \text{ and the opening of a weak pseudogap at } T^*, \text{ as we show below.} \]

This encourages us to apply the following description. We employ the FLEX approximation to obtain the dynamical phase stiffness \( n_s(\omega)/m^* \), where \( n_s(\omega) \) is the generalization of the superfluid density for finite frequencies. The static density \( n_s(0) \) starts to deviate from zero at the temperature where Cooper pairs start to form and which we identify with \( T^*_c \). Then, phase fluctuations are incorporated by using the phase stiffness from FLEX as the input for BKT theory, which leads to a renormalized \( n_s^R < n_s \) and predicts a reduced \( T_c \). Then, we consider the dynamical case \( \omega > 0 \) and use dynamical BKT theory \[ \text{to find the renormalized phase stiffness } n_s^* = n_s^R(\omega)/m^* \text{ and compare the results with experiments.} \]

**II. STATIC CASE**

Transport measurements for a gate-doped cuprate \[ \text{show that the superconducting properties are determined by a single CuO}_2 \text{ plane. The simplest model believed to contain the relevant strong correlations is the 2D one-band Hubbard model.} \]

We here start from the Hamiltonian

\[ H = - \sum_{\langle ij \rangle} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \]

Here, \( c_{i\sigma}^\dagger \) creates an electron with spin \( \sigma \) on site \( i \), \( U \) denotes the on-site Coulomb interaction, and \( t_{ij} \) is the hopping integral. Within a conserving approximation, the one-electron self-energy is given by the functional derivative of a generating functional \( \Phi \), which is related to the free energy, with respect to the dressed one-electron Green function \( \tilde{G}_0 \) of the kinetic part of \( H \) alone. These equations determine the dressed Green function \[ \text{in terms of the unperturbed Green function } G_0 \text{.} \]

The \( T \)-matrix or FLEX approximation is distinguished by the choice of a particular infinite subset of ladder and bubble diagrams for the generating functional \( \Phi \). The dressed Green functions are used to calculate the charge and spin susceptibilities. From these a Bork-Schrieffer-type pairing interaction is contructed, describing the exchange of charge and spin fluctuations. In a purely electronic pairing theory a self-consistent description is required because the electrons do not only form Cooper pairs but also mediate the pairing interaction. The quasiparticle self-energy components \( \Sigma_\nu \) \[ \text{with respect to the Pauli matrices } \tau_v \in \text{ the Nambu representation } \text{i.e., } X_\nu = \omega(1 - Z) \text{ (renormalization), } X_3 = \xi \text{ (energy shift), and } X_1 = \phi \text{ (gap parameter) are given by} \]

\[ X_\nu(k, \omega) = \frac{1}{N} \sum_{k'} \int_0^\infty d\Omega \left\{ P_\nu(k-k', \Omega) \pm P_\nu(k-k', -\Omega) \right\} \times \int_{-\infty}^{\infty} d\omega' I(\omega, \omega') A_\nu(k', \omega'). \]

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 \( A_\nu \) are given by

\[ I(\omega, \Omega, \omega') = \frac{f(-\omega') + b(\Omega)}{\omega + i\delta - \Omega - \omega'} + \frac{f(\omega') + b(\Omega)}{\omega + i\delta + \Omega - \omega'}. \]

\[ A_\nu(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{a_\nu(k, \omega)}{D(k, \omega)}, \]

where \( a_0 = \omega Z, a_3 = \epsilon_k + \xi, a_1 = \phi \), and

\[ D = (\omega Z)^2 - |\epsilon_k + \xi|^2 - \phi^2. \]

Here, \( f \) and \( b \) are the Fermi and Bose distribution functions, respectively. We use the bare tight-binding dispersion relation for lattice constant \( a = b = 1 \),

\[ \epsilon_k = 2t \left( 2 - \cos k_x - \cos k_y - \mu \right). \]
The band filling \( n = 1/N \sum_{k} n_k \) is determined with the help of the \( k \)-dependent occupation number \( n_k = 2 \int_{-\infty}^{\infty} d\omega \, f(\omega) N(k, \omega) \) which is calculated self-consistently. \( n = 1 \) corresponds to half filling. The interactions due to spin and charge fluctuations are given by \( P_s = (2\pi)^{-1}U^2 \text{Im} (3\chi_e - \chi_{s0}) \) with \( \chi_s = \chi_{s0} (1 - U \chi_{s0})^{-1} \) and \( P_c = (2\pi)^{-1}U^2 \text{Im} (3\chi_e - \chi_{c0}) \) with \( \chi_c = \chi_{c0} (1 + U \chi_{c0})^{-1} \). In terms of spectral functions one has

\[
\text{Im} \chi_{s0,0}(q, \omega) = \frac{\pi}{N} \int_{-\infty}^{\infty} d\omega' \left[ f(\omega') - f(\omega' + \omega) \right]
\times \sum_{k} \left[ N(k + q, \omega' + \omega) N(k, \omega') + A_1(k + q, \omega' + \omega) A_1(k, \omega') \right].
\]

(7)

Here, \( N(k, \omega) = A_0(k, \omega) + A_2(k, \omega) \), and the real parts are calculated with the help of the Kramers-Kronig relation. The substracted terms in \( P_s \) and \( P_c \) remove double counting that occurs in second order. The spin fluctuations are found to dominate the pairing interaction. The numerical calculations are performed on a square lattice with 256 \( \times \) 256 points in 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. The convolutions in \( k \) space are carried out using fast Fourier transformation. The superconducting state is found to have \( d_{x^2-y^2} \)-wave symmetry. \( T^*_c \) is determined from the linearized gap equation.

A field-theoretical derivation of the effective action of phase fluctuations shows that the phase stiffness for frequency \( \omega = 0 \) is given by the 3D static superfluid density divided by the effective mass, \( n_s(x, T)/m^* \). This quantity is given by

\[
\frac{n_s}{m^*} = \frac{2}{\pi e^2} (I_N - I_S)
\]

(8)

with

\[
I_{N,S} = \int_{0}^{\infty} d\omega \, \sigma_{N,S}^{N,S}(\omega),
\]

(9)

where \( \sigma_N^N (\sigma_S^S) \) is the real part of the conductivity in the normal (superconducting) state. Here we utilize the \( f \)-sum rule \( \int_{0}^{\infty} d\omega \sigma_1(\omega) = \pi e^2n/2m^* \) where \( n \) is the 3D electron density. The interpretation of Eq. (8) is that the spectral weight missing from the quasi-particle background in \( \sigma(\omega) \) for \( T < T^*_c \) must be in the superconducting delta-function peak.

\( \sigma(\omega) \) is calculated in the normal and superconducting states using the Kubo formulæ:

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

(10)

where \( v_{k,i} = \partial \epsilon_k/\partial k_i \) are the band velocities within the CuO\(_2\) plane and \( c \) is the \( c \)-axis lattice constant. Vertex corrections are neglected.

The superfluid density (phase stiffness) \( n_s/m^* \) obtained in this way is shown in Fig. 1 for the doping values \( x = 0.091 \) (underdoped), \( x = 0.155 \) (approximately optimally doped), and \( x = 0.222 \) (overdoped). The figure also shows fits to the data at given doping level, where we assume the form \( \ln n_s(T)/m^* \sim a_0 + a_1 \ln(T^*_c - T) + a_2 \ln^2(T^*_c - T) + \ldots \), i.e., a power-law dependence close to \( T^*_c \) with logarithmic corrections. We use the fits to extrapolate to \( T = 0 \). The results show that \( T^*_c \) depends on \( x \) only weakly in the underdoped regime but decreases rapidly in the overdoped. We come back to this below. Furthermore, \( n_s/m^* \) increases much more slowly below \( T^*_c \) in the underdoped regime and extrapolates to a smaller value at \( T = 0 \).

We have also calculated \( n_s \) in units of the total hole density \( n \), shown in Fig. 2, finding that \( n_s/n \) is significantly reduced below unity, in agreement with experiments but in contradiction to BCS theory. The reduction is strongest for the underdoped case. Our results show that spin fluctuations can explain most of the observed reduction of \( n_s \). Also note that \( n_s \) is linear in temperature for \( T \to 0 \) because of the nodes in the gap. The inset in Fig. 2 shows \( \lambda^3(0)/\lambda^3(T) \), where the penetration depth is \( \lambda \propto n_s^{1/2} \), as a function of \( T^*_c - T \). The FLEX approximation yields \( \lambda^3(0)/\lambda^3(T) \propto T^*_c - T \). The same power law has been found experimentally by Kamal et al.\(^9\) It has been attributed to critical fluctuations starting about 10 K below the transition temperature, since it coincides with the critical exponent expected for

![FIG. 1: Static superfluid density as a function of temperature for three values of the doping \( x \) (symbols). The solid curves are fits of power laws with logarithmic corrections as explained in the text. The intersection of \( n_s(T)/m^* \) with the dashed line represents a simplified criterion for the BKT transition temperature \( T_c \).](image-url)
the 3D \textit{XY} model. We here obtain the same power law from the FLEX approximation, which is purely 2D and does not contain critical fluctuations. Instead this rapid increase of \( n_s \propto 1/\lambda^2 \) below \( T^*_c \) is due to the self-consistency, which leads to a more rapid opening of the gap than in BCS theory. We thus conclude that, while critical 3D \textit{XY} fluctuations are expected in a narrow temperature range,\[\text{[18-20]}\] they are not the origin of the observed power law on the scale of 10 K.

Now we turn to the renormalization of \( n_s \) due to phase (vortex) fluctuations. The BKT theory describes the unbinding of thermally created pancake vortex-antivortex pairs.\[\text{[5-7]}\] The relevant parameters are the dimensionless stiffness \( K \) and the core energy \( E_c \) of vortices. The stiffness is related to \( n_s \) by\[\text{[2]}\]

\[
K(T) = \beta \hbar^2 \frac{n_s(T) d}{m^*}, \tag{11}
\]

where \( \beta \) is the inverse temperature and \( d \) is the average spacing between \( \text{CuO}_2 \) layers. Since we use a 2D model to describe double-layer cuprates, we set \( d \) to half the height of the unit cell of the typical representative \( \text{YBa}_2\text{Cu}_3\text{O}_{6+y} \). The stiffness \( K \) is also a measure of the strength of the vortex-antivortex interaction \( V = 2\pi k_B T \ln(r/r_0) \). Here, \( r_0 \) is the minimum pair size, i.e., twice the vortex core radius, which is of the order of the in-plane Ginzburg-Landau coherence length \( \xi_0 \). For the core energy we use an approximate result by Blatter \textit{et al.}\[\text{[1-3]}\]

\[
E_c = \pi k_B T \ln \kappa, \tag{13}
\]

where \( \kappa \) is the Ginzburg parameter. Starting from the smallest vortex-antivortex pairs of size \( r_0 \), the pairs are integrated out and their effect is incorporated by an approximate renormalization of \( K \) and the fugacity \( f = e^{-\beta E_c} \). This leads to the Kosterlitz recursion relations

\[
\frac{dy}{dl} = (2 - \pi K)y, \tag{12}
\]

\[
\frac{dK}{dl} = -4\pi^3 y^2 K^2, \tag{13}
\]

where \( l = \ln(r/r_0) \) is a logarithmic length scale. For \( T > T_c \), \( K \) goes to zero for \( l \to \infty \), so that the interaction is screened at large distances and the largest vortex-antivortex pairs unbind. The unbound vortices destroy the superconducting order and the Meißner effect and lead to dissipation.\[\text{[4]}\] For \( T < T_c \), \( K \) approaches a finite value \( K_R = \lim_{l \to \infty} K \) and \( y \) vanishes in the limit \( l \to \infty \) so that there are exponentially few large pairs and they still feel the logarithmic interaction. Bound pairs reduce \( K \) and thus \( n_s \), but do not destroy superconductivity. At \( T_c \), \( K_R \) jumps from a universal value of \( 2/\pi \) to zero. The values of \( T_c \) shown below are obtained by numerically integrating Eqs. (12) and (13) with \( n_s \) taken from an interpolation between the points in Fig. 2. It turns out that the renormalization of \( K \) for \( T < T_c \) is very small so that one obtains \( T_c \) from the simple criterion

\[
K(T_c) = \frac{2}{\pi} \text{ or } \frac{n_s(T_c)}{m^*} = \frac{2}{\pi} \frac{4k_B T_c}{\hbar d}, \tag{14}
\]

for the unrenormalized stiffness with an error of less than 1 %. Eq. (14) is satisfied at the intersection of the \( n_s(T)/m^* \) curves with the dashed straight line in Fig. 2.

FIG. 2: Ratio of superfluid density to total hole density for the same doping values \( x \) as in Fig. 1. The inset shows \( \lambda^3(T=0)/\lambda^3(T) = n_s^{3/2}(T)/n_s^{3/2}(T=0) \), where \( \lambda \) is the London penetration depth, as a function of \( (T_c - T) \).

FIG. 3: Temperature scales of the cuprates as functions of doping \( x \). \( T_c \) (solid circles) is the transition temperature obtained from the FLEX approximation with phase fluctuations included by means of BKT theory. At \( T^*_c \) (open circles) Cooper pairs start to form locally; this temperature is given by the transition temperature obtained from the FLEX approximation with spin fluctuations alone. The crosses show the superfluid density (phase stiffness) \( n_s(T=0)/m^* \) for comparison. This curve has been scaled so that it agrees with \( T_c \) in the underdoped regime.
From BKT theory we obtain two important quantities: the transition temperature $T_c$ and the renormalized stiffness $K_R$, which determines the renormalized superfluid density (phase stiffness)

$$\frac{n_s}{m^*} = \frac{4}{\beta \hbar^2 d} K_R.$$  \hspace{1cm} (15)

In Fig. 3 we plot the transition temperature $T_c$ and the temperature $T^*$ where Cooper-pairs form. For decreasing doping $x$, $T^*$ becomes nearly constant and even decreases for the lowest doping level, consistent with the strong decrease of the onset temperature of vortex effects at even lower doping found by Xu et al.\textsuperscript{[13,14]} We have also calculated the superconducting gap $\Delta_0$ extrapolated to $T = 0$ (not shown). $\Delta_0$ is here defined as half the peak-to-peak separation in the density of states. We find approximately $\Delta_0 \approx T_c^*$.\textsuperscript{[66]}

Phase fluctuations lead to a downturn of $T_c$ in the underdoped regime. However, this reduction is not as large as experimentally observed and our value $x \approx 0.14$ for the optimal doping is accordingly smaller than the experimental one of $x \approx 0.16$.\textsuperscript{[67]} We suggest that one origin of this discrepancy is the neglect of the feedback of phase fluctuations on the electronic properties.

Figure 3 also shows the superfluid density $n_s(0)/m^*$ extrapolated to $T = 0$, scaled such that it approaches $T_c$ in the underdoped regime. The density increases approximately linearly with doping except for the most overdoped point, where it turns down again. This behavior agrees well with angle-resolved photoemission (ARPES) results of Feng et al.\textsuperscript{[20,25,26,27]} and with recent $\mu$SR experiments of Bernhard et al.\textsuperscript{[19]} In Ref.\textsuperscript{[16]} a maximum in $n_s$ at a unique doping value of $x_{\text{max}} \approx 0.19$ is found for various cuprates, while we obtain $x_{\text{max}} \approx 0.20$. Our results are consistent with the Uemura scaling\textsuperscript{[16]} $T_c \approx n_s(0)$ in the heavily underdoped regime and with the BCS-like behavior $T_c \approx T^* \approx \Delta_0$ in the overdoped limit. $T_c$ interpolates smoothly between the extreme cases. We find $T_c < T^*$ even for high doping, since $n_s(T)$ and $K(T)$ continuously go to zero at $T^*$ so that Eq. (14) is only satisfied at a temperature $T < T_c^*$, $T_c^*$ becomes much larger than $T_c$. The result for the overdoped case may be changed if amplitude fluctuations of the order parameter and their mixing with phase fluctuations are taken into account. Amplitude fluctuations are governed by $\Delta$, which becomes smaller than the energy scale of phase fluctuations in the overdoped regime.

The situation is complicated by the Josephson coupling between CuO$_2$ layers. This coupling leads to the appearance of Josephson vortex lines connecting the pancake vortices between the layers.\textsuperscript{[12]} They induce a linear component in the vortex-antivortex interaction. This contribution becomes relevant at separations larger than $\Lambda = d/\epsilon$, where $\epsilon < 1$ is the anisotropy parameter.\textsuperscript{[22]} $\Lambda$ acts as a cutoff for the Kosterlitz recursion relations and eventually leads to an increase of $T_c$ relative to the BKT result $T_c^{\text{BKT}}$ and to the breakdown of 2D theory close to the transition temperature.\textsuperscript{[22,23,24]} The experiments of Corson et al.\textsuperscript{[13,14]} also show that the BKT temperature $T_c^{\text{BKT}}$ extracted from the data is significantly smaller than the experimental $T_c$. Thus $T_c$ as calculated here is a lower bound of the true transition temperature.

The feedback of phase fluctuations on the electrons is not included in our approach. We expect the phase fluctuations in this regime to lead to pair breaking.\textsuperscript{[18]} However, simulations of the XY model suggest that this feedback is rather weak.\textsuperscript{[18]} Neglecting the feedback, the electronic spectral function shows the unrenormalized superconducting gap for $T_\text{c} < T < T_c^*$. Since there is no superconducting order in this regime, we identify this gap with the (strong) pseudogap, which thus is automatically $d_{x^2-y^2}$-wave-like and of the same magnitude as the superconducting gap for $T < T_c$. Thus in this picture the pseudogap is due to local Cooper pair formation in the absence of long-range phase coherence. Pair breaking due to phase fluctuations should partly fill in this gap.

Figure 4 shows $T_c$, $T_c^*$, and $T^*$ on a different temperature scale. $T^*$ is the highest temperature where a weak pseudogap is obtained from FLEX, i.e., where the density of states at the Fermi energy starts to be suppressed. The inset shows this suppression for $x = 0.155$. The temperature $T^*$ becomes much larger than $T_c$ in the underdoped regime, in agreement with experiments.\textsuperscript{[13,14]}

To conclude this section, we discuss the effect of a normal-state pseudogap due to a mechanism other than incoherent Cooper pairing. Let us assume a suppression of the density of states close to the Fermi surface in the normal state, e.g., due to the formation of a charge-density wave.\textsuperscript{[21]} This decreases the number of holes available for pairing and should thus reduce $T_c$. To check this, we have performed FLEX calculations with a pseud-
FIG. 5: Transition temperatures in the presence of a normal-state pseudogap. The open squares show the transition temperature $T_c^*$ obtained from the FLEX approximation with a $d$-wave pseudogap in the normal-state dispersion. The amplitude of the pseudogap is taken from experiments. The open circles show the corresponding values without a pseudogap, see Fig. 1. The solid squares denote $T_c$ in the presence of the pseudogap and with phase fluctuations included, assuming the two effects to be independent. The solid circles show the corresponding results without pseudogap. The inset of Fig. 5, even if $T_{c}^{*}$ is not well-defined for $\Delta = 0$. Indeed, using a Ward identity on equal footing with spin fluctuations would be a formidable task.

III. DYNAMICAL CASE

In this section, we calculate the dynamical phase stiffness, which is the quantity obtained by Corson et al. We first note that the superfluid density can also be obtained from the imaginary part of the conductivity,

$$\frac{n_s}{m^*} = \frac{1}{e^2} \lim_{\omega \to 0} \omega \sigma_2^S(\omega),$$

as can be shown with the help of Kramers-Kronig relations. We have recalculated $n_s/m^*$ in this way and find identical results compared to Eq. (8).

The phase stiffness has also been obtained at nonzero frequencies using field-theoretical methods. For small wave vector $q \to 0$,

$$\frac{n_s(\omega)}{m^*} = \frac{1}{e^2} \omega \sigma_2^S(\omega).$$

The imaginary part $\sigma_2^S(\omega)$ of the dynamical conductivity is obtained from the FLEX approximation for the dynamical current-current correlation function using the Kubo formula: For $\omega > 0$ one should not interpret $n_s(\omega)$ as a density. Note also that $n_s^{-1/2}(\omega)$ is no longer proportional to the penetration depth of a magnetic field—for $\omega > 0$ there is also a contribution from the real part of the conductivity, i.e., the normal skin effect.

The resulting phase stiffness $n_s(\omega)/m^*$ is shown in Fig. 1 for $x = 0.122$ (underdoped) at various temperatures. At higher doping the results (not shown) are similar, only the typical frequency scale, which turns out to be the low-temperature superconducting gap $\Delta_0$, is reduced. We find a finite phase stiffness at $\omega > 0$ even for $T \geq T_c^*$. At first glance this is surprising, since the phase is not well-defined for $\Delta = 0$. Indeed, using a Ward identity one can show that the Gaussian part of the phase action vanishes for $T \geq T_c^*$. However, the phase action contains a contribution from the time derivative of the phase besides the stiffness term. While the total action vanishes, each term on its own does not. Thus the stiffness is finite but has no physical significance for $T \geq T_c^*$.

Even slightly below $T_c^*$, $n_s(\omega = 0)/m^*$ obtains a significant finite value, leading to the Meißner effect, and there is a considerable redistribution of weight from energies roughly above twice the low-temperature maximum gap, $2\Delta_0$, to energies below $2\Delta_0$. This redistribution increases with decreasing temperature. Also, a peak develops slightly below $\Delta_0$ followed by a dip around $2\Delta_0$, this

dogap of the form $\Delta_k = \Delta_0 (\cos k_x - \cos k_y)$ included in the normal-state dispersion. The doping-dependent amplitude $\Delta_0$ is chosen in accordance with ARPES experiments by Marshall et al. and by Ding et al. The results are shown by the open squares in Fig. 1. The curve merges with the $T_c$ curve without pseudogap (open circles) at $x = 0.155$, since here the pseudogap is experimentally found to vanish. It is apparent that $T_c^*$ is indeed strongly reduced in the underdoped regime. Thus this density-of-states effect is a possible alternative explanation for the observed downturn of $T_c$.

Next, we consider phase fluctuations in the presence of a normal-state pseudogap. The $T_c$ values naively obtained from BKT theory for this case are shown in Fig. 1 as the solid squares. Phase fluctuations reduce $T_c$ even more, in particular for $x = 0.122$. This is due to the fact that the phase stiffness $n_s/m^*$ increases much more slowly below $T_c$ in the presence of a pseudogap, as shown in the inset of Fig. 1 even if $T_{c}^{*}$ is only slightly reduced. The small stiffness makes phase fluctuations more effective. However, in this picture the reduction of $T_c$ is probably overestimated: Above, we have explained the pseudogap as resulting from incoherent Cooper pairing. This contribution to the pseudogap must not be incorporated into the normal-state dispersion to avoid double counting. This would increase the result for $T_c$. It is clearly important to develop a theory that incorporates phase fluctuations, spin fluctuations, and possibly the charge-density wave on the same microscopic level. However, the inclusion of vortex fluctuations in a FLEX-type theory on equal footing with spin fluctuations would be a formidable task.
structure being most pronounced in the underdoped case. Since $\Delta_0$ is smaller in the overdoped regime, $n_s(\omega)/m^*$ changes more rapidly for small $\omega$ in this case. It is of course not surprising that $2\Delta_0$ is the characteristic frequency of changes in $n_s(\omega)/m^*$ related to the formation of Cooper pairs.

We now turn to the question of how phase fluctuations affect the dynamical phase stiffness $n_s(\omega)/m^*$. This requires a dynamical generalization of BKT theory, which was first developed by Ambegaokar et al. Here, we start from a heuristic argument for the dynamical screening of the vortex interaction. An applied electromagnetic field exerts a force on the vortices mainly by inducing a superflow, which leads to a Lorentz force on the flux carried by the vortices. On the other hand, moving a vortex leads to dissipation in its core and thus to a flux carried by the vortices. On the other hand, moving a vortex leads to a Lorentz force on the vortex interaction:

$$D_v = \frac{2\pi e^2 \xi_{ab} \rho_n k_B T}{\phi_0 d},$$

(19)

where $c$ is the speed of light, $\xi_{ab} \sim r_0/2$ is the coherence length, $\rho_n$ is the normal-state resistivity, $\phi_0 = hc/2e$ is the superconducting flux quantum, and $d$ is an effective layer thickness. In the renormalization the quantity $D_v/r_0^2$ enters, which according to Eq. (19) is linear in temperature. In the presence of a high density of weak pinning centers the diffusion constant becomes:

$$D_v = D_v^0 \exp(-E_p/k_B T),$$

where $E_p$ is the pinning energy. Matters are complicated by the observation that $E_p$ depends on temperature. Rogers et al. find $E_p(T) \approx E_p^0 (1 - T/T_c^*)$ with $E_p^0/k_B \approx 1200$ K for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Absorbing the constant term in the exponent into the prefactor, the result for the diffusion constant in natural units is

$$\frac{D_v}{r_0^2} \approx C_v \frac{k_B T}{\hbar} \exp\left(-\frac{E_p^0}{k_B T}\right),$$

(20)

where $C_v$ is a dimensionless constant. However, such a large value of $E_p^0$ would lead to a sharp, step-like dependence of $n_s(\omega)/m^*$ on temperature, in contradiction to the smooth behavior shown in Fig. 4 of Ref. 41. In view of these difficulties we treat $D_v/r_0^2$ as a constant parameter and discuss the dependence on $D_v$ below.

To find the effect of phase (vortex) fluctuations on the phase stiffness, the recursion relations [12] and [13] are now integrated numerically up to the cutoff $t = \ln(r/r_0)$, which depends on $D_v/r_0^2$. The resulting renormalized phase stiffness $n_s^\ast(\omega)/m^*$ for constant $D_v/r_0^2 = 10^3 \text{ s}^{-1}$ and $x = 0.122$ is plotted in Fig. 6. Other values of $D_v$ give similar results. Of course, faster vortex diffusion shifts the features at given temperature to higher frequencies. The dashed lines denote the unrenormalized stiffness, i.e., the same data as in Fig. 4 albeit on an expanded frequency scale. The highest frequency used in Ref. 41 (600 GHz) corresponds to $\omega/t \approx 0.01$, also indicated in Fig. 6.

For $T < T_c$ (the upper six curves) the static renormalization has been found to be small, see Sec. II. The renormalization at finite $\omega$ is even weaker so that the renormalized stiffness is in practice identical to the unrenormalized one, which has only a weak frequency dependence for low $\omega$, in agreement with Ref. 41.

When $T$ is increased above $T_c$ (the lower five curves in Fig. 6), a strong renormalization of the stiffness due to phase fluctuations sets in starting at very low frequencies. The Meißner effect is thus destroyed for all $T > T_c$ by
the comparatively slow vortex diffusion. With increasing temperature the onset of renormalization shifts to higher frequencies. At frequencies above this onset, the vortices cannot follow the field and thus do not affect the response, as discussed above. The onset frequencies are always much smaller than $2\Delta_0$. The features at the energy scale $2\Delta_0$ shown in Fig. 8 are due to Cooper-pair formation, are unaffected by phase fluctuations and show no anomaly at $T_c$. They vanish only at $T_\ast^c$.

Finally, in Fig. 8 we plot the renormalized $n^R_\ast(\omega)/m\ast$ for $x = 0.122$ as a function of temperature for various frequencies. This graph should be compared to Figs. 2 and 4 of Ref. 41—note that the quantity $T_\theta$ given there is proportional to $n^R_\ast/m\ast$. We note that Corson et al. assume a thermally activated density of free vortices, $n_f \propto \exp(-E_f/T)$, for $T$ not too close to the BKT transition temperature, and a temperature-independent diffusion constant. Here, we instead integrate the recursion relations explicitly up to the dynamical length scale $\xi$ so that we do not have to make an assumption on $n_f$. One sees that even at $f = 600$ GHz the broadened BKT transition is still much narrower than found by Corson et al. From Eqs. (12) and (13) it is clear that the diffusion constant $D_\ast/r_0^2$ increases with temperature. In the presence of pinning it increases rapidly around $k_B T \sim E_0^\ast$. Since a larger diffusion constant, i.e., more mobile vortices, leads to stronger renormalization, the transition in Fig. 8 would become even sharper if $D_\ast/r_0^2$ were an increasing function of temperature.

Our results show that dynamical BKT theory together with Bardeen-Stephen theory for vortex diffusion and natural assumptions on pinning does not agree quantitatively with the experimental results. We conclude that the finite size effect apparent in the experimental data is not only due to the finite diffusion length. Another possible source is the interlayer Josephson coupling, which leads to the appearance of the Josephson length $\Lambda$ as an additional length scale, as discussed above. This length scale leads to a cutoff of the recursion relations at $l \sim \ln(\Lambda/r_0)$, which becomes small close to $T_\ast^c$ due to the divergence of $r_0 \sim \xi_{ab}$ (neglecting the feedback of phase fluctuations on the quasiparticles). This broadens the transition but cannot easily explain the observed frequency dependence. On the other hand, the experimental observation that the curves for various frequencies start to coincide where the phase stiffness agrees with the universal jump criterion supports an interpretation in terms of vortex fluctuations. We suggest that a better description of the interplay of vortex dynamics and interlayer coupling is required to understand the data.

Note, the origin of the discrepancy may also lie in the FLEX results for $n_\ast(\omega)/m^\ast$, which do not include all effects of temperature-dependent scattering on the conductivity $\sigma$ and in the omission of the feedback of phase fluctuations on the electronic properties. Another effect neglected here is the possible coupling to a charge-density wave perhaps taking the form of dynamical stripes.
IV. SUMMARY AND CONCLUSIONS

In the present paper we have obtained the characteristic energy scales of hole-doped cuprate superconductors from a theory that includes both spin and Cooper-pair phase fluctuations. The former are described by the FLEX approximation, whereas the latter are included by means of the Berezinskii-Kosterlitz-Thouless (BKT) theory, taking the FLEX results as input. Phase fluctuations mainly take the form of vortex fluctuations, since Gaussian phase fluctuations have a large energy gap. Vortices lead to the renormalization of the phase stiffness $n_s(\omega)/m^*$ to $n_s^R(\omega)/m^*$. The stiffness at $T \to 0$ shows a maximum at a doping level of $x \approx 0.2$, in good agreement with experiments. At the transition temperature $T_c$ the renormalized static phase stiffness $n_s^R(\omega = 0)/m^*$ vanishes, leading to the disappearance of the Meißner effect. The ideal conductivity is also destroyed by free vortices. $T_c$ is significantly reduced compared to the transition temperature $T_c^*$ that would result from spin fluctuations alone. The $T_c$ determined from spin and phase fluctuations (vortex) fluctuations is in much better agreement with experiments in the underdoped regime and shows a maximum at optimum doping. Still, our approach does not explain the full reduction of $T_c$. We believe that a further reduction of $T_c$ results from (a) the breaking of Cooper pairs by scattering with phase fluctuations and (b) other instabilities that reduce the density of states in the normal state, for example a charge-density wave. Since the latter effect also suppresses $n_s/m^*$, phase fluctuations can become even more effective and reduce $T_c$ further. It would be desirable to include the pair-breaking effect of phase fluctuations and the possible formation of a charge-density wave on the same microscopic level as the spin fluctuations.

For $T_c < T < T_c^*$, where phase-coherent superconductivity is absent, phase fluctuations lead to a strong renormalization of $n_s/m^*$ at frequencies much smaller than $2\Delta_0$. Our results show the same trends as found in conductivity measurements. However, a three-dimensional description of vortex dynamics might be required to obtain a more quantitative agreement. Local formation of Cooper pairs still takes place in this regime. This leads to a strong pseudogap of the same magnitude $\Delta_0$ and symmetry as the superconducting gap below $T_c$. We also find a frequency dependence of $n_s^R(\omega)/m^*$ at higher frequencies, $\omega \gtrsim \Delta_0$, that is very similar to the superconducting phase. These features vanish only around $T_c^*$. Finally, for $T_c^* < T < T^*$ there is a weak suppression in the density of states at the Fermi energy. Our results reproduce several of the main features common to all hole-doped cuprate superconductors. We conclude that the exchange of spin fluctuations, modified by strong superconducting phase (vortex) fluctuations in the underdoped regime, is the main mechanism of superconductivity in cuprates.

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* Electronic address: timm@physik.fu-berlin.de

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This derivation starts from an attractive pairing interaction, which is decoupled using a Hubbard-Stratonovich transformation. The decoupling field is the complex superconducting gap $\Delta$. A gauge transformation of the fermions then removes the phase from $\Delta$ and couples it directly to the fermions. After the fermions are integrated out, one obtains the effective action of the phase.

One usually writes $\eta = N_0 e^{-\beta E_c}$, where $N_0$ is a factor of order unity. However, the results depend on $N_0$ only very weakly, since the renormalization of $n_s$ below $T_c$ is small.

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