Precursor effects of the superconducting state caused by \( d \)-wave phase-fluctuations above \( T_c \)

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One of the hallmarks of high-temperature superconductors is a pseudogap regime appearing in the underdoped cuprates below a characteristic temperature \( T^* \), that is higher than the superconducting (SC) transition temperature \( T_c \). The size of this pseudogap temperature regime scales with the superconducting gap. In addition, high-frequency conductivity experiments in underdoped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) (Bi2212)\(^1\) have indicated a SC scaling behavior of the optical conductivity. Furthermore, a strongly enhanced Nernst signal was measured above \( T_c \) in underdoped samples of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (LSCO), which is usually associated with the presence of vortices in the superconducting state and, therefore, implies that \( T_c \) corresponds to a loss of phase rigidity rather than a vanishing of the pairing amplitude\(^2\). Recently, a field-enhanced diamagnetism was found in the pseudogap state of Bi2212, which scales exactly like the Nernst signal\(^3\) and further supports the vortex description for the loss of phase coherence at \( T_c \).

All these experiments point towards a picture, where the pseudogap arises from phase fluctuations of the superconducting gap\(^4\). In previous work\(^4\), we provided a detailed numerical solution of a minimal model which, however, contains key ideas of the phase-fluctuation scenario: In this scenario, below a “mean-field” temperature \( T_{MF} \equiv T^* \), a \( d_{x^2-y^2} \)-wave gap amplitude is assumed to develop. However, the SC transition is suppressed to a considerably lower temperature \( T_c \) by phase fluctuations\(^5\). In the intermediate temperature regime between \( T^* \) and \( T_c \), the phase fluctuations of the gap give rise to the pseudogap phenomena. In this previous work, it was shown that a two-dimensional BCS-like Hamiltonian with a \( d_{x^2-y^2} \)-wave gap and phase fluctuations, which were treated by a Monte-Carlo (MC) simulation of an \( XY \) model, yields results which compare very well with scanning tunneling measurements over a wide temperature range\(^6\). Furthermore, this phenomenological phase fluctuation model was also able to explain the “violation” of the in-plane optical integral in underdoped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) (Bi2212)\(^7\) and the characteristic change of the quasiparticle dispersion observed in crossing \( T_c \) in underdoped Bi2212 samples\(^8\).

Here, we consider in detail two other experiments, which critically probe the phase-fluctuation scenario. The first one is the optical response. Our calculations were, in particular, motivated by optical studies of the Berkeley group\(^9\). In this seminal work high-frequency optical response, i.e. the complex frequency dependent conductivity, was used to capture the short-time scale dynamics of the phase correlations. Indeed, the pseudogap conjecture had early on led to an intensive search for normal state “remnants” of the SC state, such as the infinite d. c. conductivity. However, it was not before this Corson et al. work that it was realized that the short phase-correlation times require a high-frequency optical probe to make the conductivity enhancement over normal-state values observable.

We give a detailed analysis of the temperature and frequency dependence of the optical conductivity \( \sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega) \) within our phenomenological phase fluctuation model, which, for completeness, is reintroduced in section II. In section III we compare the calculated paraconductivity due to \( d \)-wave phase fluctuations above \( T_c \) with the high-frequency conductivity experiments of Ref.\(^9\). Salient features of these experiments are reproduced in \( \sigma(\omega) \) above \( T_c \); at sufficiently high frequencies, the phase-fluctuating state becomes indistinguishable from the SC state. In this latter case \( \sigma_2(\omega) \), i.e. the imaginary part, shows the usual BCS-like behavior falling off as \( 1/\omega \), with a prefactor being proportional to the phase-stiffness energy. This generates in our calculations a scaling behavior of \( \sigma_2(\omega, T) \), in agreement with exper-
iment, in that all $\omega \sigma_2(\omega, T)$ curves collapse onto a single curve at the Kosterlitz-Thouless (KT)-temperature $T_c = T_{KT}$.

Since, in the phase fluctuation scenario, the pseudogap is due to phase fluctuations of the SC order parameter, one might ask, how much of the characteristic magnetic properties of a superconductor are still observable in the pseudogap state of the underdoped cuprates.

These magnetic precursor effects of the ideal superconducting state are twofold. Firstly, one would expect a form of fluctuating diamagnetism which partially screens an applied magnetic field already above $T_c$. Secondly, one would also expect that the paramagnetic spin (or Pauli) susceptibility is reduced in a characteristic way below $T^*$ due to the formation of incoherent singlet-pairs, accompanied by the reduction of spectral weight at the Fermi surface.

In experiment, the fluctuation-induced diamagnetism is only important close to $T_c$. Since, at higher temperatures, the paramagnetic spin response is typically one-order-of-magnitude larger than the diamagnetic response, we concentrate here on the spin susceptibility $\chi_s$. This latter quantity dominates the T-dependence of the paramagnetic susceptibility in the experiments.

In section IV, it is shown that the Pauli spin susceptibility extracted from our phase-fluctuation model can qualitatively account for the observed paramagnetic properties over a wide range of temperatures in the pseudogap regime. Section V, finally, presents a summary of our results.

II. PHASE-FLUCTUATION MODEL

We consider the Hamiltonian\textsuperscript{14}

$$H = H_0 + H_1,$$ \hspace{1cm} (1)

where $H_0$ is the usual tight-binding operator of non-interacting electrons on a two-dimensional (2D) square lattice, i.e.,

$$H_0 = -t \sum_{(ij),\sigma} \{ \hat{c}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}_{j\sigma} \hat{c}_{i\sigma} \} - \mu \sum_{i,\sigma} n_{i\sigma}. \hspace{1cm} (2)$$

Here, $c_{i\sigma} \ (\hat{c}_{i\sigma})$ creates (annihilates) an electron of spin $\sigma$ on the $i$\textsuperscript{th} site of the (2D) square lattice and $n_{i\sigma} = c_{i\sigma} \hat{c}_{i\sigma}$ is the number operator. $t$ denotes an effective nearest-neighbor hopping-term and $\mu$ is the chemical potential. The $(ij)$ sum is over nearest-neighbor sites of the 2D square lattice. For simplicity of our minimal model, we set longer-ranged hoppings $t'$ equal to zero. All calculations were done for 10\% doping, which corresponds to a typical underdoped cuprate situation.

The second part of the Hamiltonian $H_1$ contains a BCS-like $d$-wave interaction, which is given by

$$H_1 = -g \sum_{\vec{i}\vec{\delta}} (\Delta^\dagger_{\vec{i}\vec{\delta}} \Delta^\dagger_{\vec{i}\vec{\delta}'} + \Delta^\dagger_{\vec{i}\vec{\delta}'} \Delta^\dagger_{\vec{i}\vec{\delta}}), \hspace{1cm} (3)$$

with $\vec{\delta}$ connecting site $i$ to its nearest-neighbor sites. The coupling constant $g$ stands for the strength of the effective next-neighbor $d_{x^2-y^2}$-wave pairing-interaction. The origin of this pairing interaction is not essential for the further calculation. It can be either of purely electronic origin, like spin fluctuations, or phonon mediated. The only important point is, that there exists an effective pairing interaction, that produces a finite $d_{x^2-y^2}$-wave gap amplitude as one goes below a certain temperature $T^*$. In contrast to conventional BCS theory, we consider the pairing-field amplitude not as a constant real number, but rather as a complex quantity

$$\Delta^\ast_{\vec{i}\vec{\delta}} = \frac{1}{\sqrt{2}} (c^\dagger_{\vec{i}\uparrow} c^\dagger_{\vec{i}\downarrow} - c^\dagger_{\vec{i}\downarrow} c^\dagger_{\vec{i}\uparrow}) = \Delta e^{i\theta_{\vec{i}\vec{\delta}}}, \hspace{1cm} (4)$$

with a constant magnitude $\Delta$ and a fluctuating bond-phase field $\Phi_{\vec{i}\vec{\delta}}$. In order to get a description, where the center of mass phases of the Cooper pairs are the only relevant degrees of freedom, the $d_{x^2-y^2}$-wave bond-phase field is written in the following way

$$\Phi_{\vec{i}\vec{\delta}} = \begin{cases} (\varphi^\uparrow + \varphi^\downarrow)/2 & \text{for } \vec{\delta} \text{ in } x\text{-direction} \smallskip \end{cases}$$

$$\begin{cases} (\varphi^\uparrow + \varphi^\downarrow)/2 + \pi & \text{for } \vec{\delta} \text{ in } y\text{-direction}, \end{cases} \hspace{1cm} (5)$$

where $\varphi_i$ is the center of mass phase of a Cooper pair localized at lattice site $\vec{i}$.

To account for the proximity to the Mott insulating state and thus the low superfluid density, we perform a quenched average over all possible phase configurations with the statistical weight given by the classical $XY$ free energy

$$F[\varphi_{\vec{i}}] = -J \sum_{(ij)} \cos (\varphi_{\vec{i}} - \varphi_{\vec{j}}). \hspace{1cm} (6)$$

Here, the phase stiffness $J$ determines the Kosterlitz-Thouless transition temperature $T_{KT}$ to a quasi phase-ordered state, a temperature, which we take as $T_{KT} \approx T_c/2$. Finally, we set $T_c = T^*$, where we have the STM experiments of Ref. 8 in mind, which corresponds to a large pseudogap regime.

In Ref. 14 the justification for using a minimal model and, in particular, the use of a classical $XY$ interaction in Eq. 5, has been carefully discussed. Our belief, that this model contains key ideas of the cuprate phase-fluctuation scenario, has been substantiated there by a detailed numerical solution and the fact that characteristic and crucial features of STM studies could be reproduced over a wide temperature range.

Recent work on a BCS-Hamiltonian with classical phase fluctuations can also be found in Ref. 13.

III. PARACondUTIVITY

In a conventional BCS superconductor, superconducting (SC) fluctuations with short-range phase coherence typically survive no more than 1K above $T_c$. Within a
phase fluctuation scenario for the underdoped cuprates, one would expect that pairing remains over a wide temperature range above $T_c$, together with phase correlations which are of finite range in space and time. Hence, although the system is in the normal state, signatures of the ideal SC state should still be observable considerably above $T_c$, if the experiments probe short enough time scales. A likely candidate to observe these effects are high-frequency conductivity experiments.

Indeed, microwave conductivity experiments on underdoped Bi2212 were able to track the phase-correlation time in the normal state up to 25K above $T_c$. These experiments show, that the SC transition is “smeared out” over a considerable temperature range, when viewed at high-enough frequencies (short-enough time scales). The imaginary part of the conductivity finally disappears more than 25K above $T_c \approx 74$K and shows a superconducting scaling behavior already above $T_c$. The real part of the conductivity displays a characteristic peak near $T_c$ at finite frequencies, on top of a “background conductivity” of normal conducting electrons. This peak was interpreted by the authors of Ref. 11 as signature of the partially phase coherent electrons.

All experiments were carried out with frequencies of a few hundred GHz, which corresponds to $\omega \lesssim 0.01t$. In order to compare these experiments with our phase fluctuation model, some compromise has to be made, since finite-size effects become important below $\omega_{\text{low}} \approx 0.03t$. Therefore, we have chosen a set of frequencies $\omega = \{0.1t, 0.2t, 0.3t, 0.4t\}$, which are, on the one hand, much larger than $\omega_{\text{low}}$, and on the other hand much smaller than the relevant energy scale, i.e. the SC gap size in our model ($\Delta_{\text{sc}} = 1.0t$). Thus, in the following, one always should keep in mind that the frequency closest to experiment is $\omega = 0.1t$.

The optical conductivity from our phase-fluctuation model, i.e. $\Sigma_{xx}^c(\tilde{k}, \omega) = e^2 \langle k_x \rangle - D_c(\tilde{k}, \omega + i\eta)/i(\omega + i\eta)$, was obtained by averaging the Matsubara current-current correlation function

$$D_c(\tilde{l}, \tilde{l}', \tau') = -i \text{Tr}\{\hat{\rho}_c T_\tau \hat{J}_c^\dagger(\tilde{l}, \tau) \hat{J}_c(\tilde{l}', \tau')\},$$

and the operator for the local kinetic energy in x-direction

$$k_x(\tilde{l}) = -it \sum_\sigma (c^\dagger_{\tilde{l}, \sigma} c_{\tilde{l}, \sigma} + c^\dagger_{\tilde{l}, \sigma} c_{\tilde{l}, \sigma})$$

over all possible phase configurations using Eq. (6). Here, $\hat{\rho}_c$ is the usual statistical operator, and

$$\hat{J}_c(\tilde{l}) = it \sum_\sigma (c^\dagger_{\tilde{l}, \sigma} c_{\tilde{l}, \sigma} - c^\dagger_{\tilde{l}, \sigma} c_{\tilde{l}, \sigma})$$

denotes the paramagnetic current density operator in x-direction.

Fig. 1 plots our results for the imaginary part of the optical conductivity, i.e. $\sigma_2(\omega, T)$, as a function of temperature for different frequencies $\omega < \Delta_{\text{sc}}$ ($\Delta_{\text{sc}} = 1.0t$). The dotted vertical line indicates $T_c \equiv T_{KT}$. Note, that the change of $\sigma_2(\omega, T)$ at the superconducting transition $T_c \equiv T_{KT}$ becomes less pronounced at higher frequencies and is smeared out over a finite range of temperatures $T > T_c \equiv T_{KT}$.

Fig. 2: Scaling behavior of the imaginary part of the optical conductivity $\sigma_2(\omega, T)$. In the superconducting state $\sigma_2(\omega, T) \sim 1/\omega$, thus all $\omega \sigma_2(\omega, T)$ curves should collapse onto a single curve. Note, that the higher the frequency, the earlier this collapse starts in the normal state for temperatures $T > T_c \equiv T_{KT}$. The logarithmic scale was chosen for a better comparison with the experimental data of Ref. 11 reproduced in Fig. 3, below.
caused scattering. In a "real" metal, above $T_c$, the finite electronic scattering rate, strongly suppresses the imaginary part $\sigma_2(\omega)$ at low frequencies, so that it can be neglected. This effect can phenomenologically be taken into account by replacing the infinitesimal damping factor $\eta$ in Eq. (7) by a finite marginal-Fermi-liquid (MFL) damping factor $^{19,20}$. Since the inclusion of such a MFL scattering-rate further reduces $\sigma_2(\omega, T)$ above $T \approx 2T_c$, whatever without changing its properties at the SC transition ($T \lesssim 2T_c$) qualitatively, we refrain from burdening our simple model with it.

In Fig. 2, the re-scaled imaginary part of the optical conductivity $\omega \sigma_2(\omega, T)$ is displayed as a function of temperature for the same frequencies $\omega < \Delta_{sc}$, as before. In the superconducting state, all re-scaled curves should collapse onto a single curve, as has been beautifully demonstrated in Ref. $^{11}$ (Fig. 2 of that work, which corresponds to our Fig. 2 is reproduced for comparison in Fig. 3). One can clearly see from our results that this collapse already begins in the normal state above $T_c \equiv T_{KT}$, starting with the highest frequencies, exactly as in Ref. $^{11}$. Also here, the inclusion of an additional MFL scattering-rate reduces the optical conductivity curves above $T \approx 2T_c$, but it does not change the SC high-frequency scaling-behavior below $T \lesssim 1.5T_c$ significantly.$^{20}$

IV. MAGNETIC PROPERTIES

In this section, we study the precursor effects of the SC state caused by d-wave phase fluctuations above $T_c$ appearing in the paramagnetic response. The spin (or Pauli) susceptibility can be obtained from the coupling of the magnetic field $\vec{B}$ to the spin degrees of freedom.

With $\vec{B} \parallel \hat{z}$, one gets:

$$\chi_{\text{spin}}(\vec{q}, \omega) = \frac{N}{V} g^2 \frac{\mu_B^2}{\hbar^2} \frac{1}{\hbar} D_{zz}(\vec{q}, \omega), \quad (11)$$

where $D_{zz}(\vec{q}, \omega)$ is the Fourier transform of the spin-spin correlation function in z-direction, i.e.

$$D_{zz}(x, t, x', t') = -i \langle \hat{\rho}_G[s_z(x, t), s_z(x', t')] \rangle \Theta(t - t'). \quad (12)$$

The static uniform susceptibility is defined by $\chi_{\text{spin}}(\vec{q} \rightarrow 0, \omega = 0)$. For a non-interacting system with a general dispersion $\epsilon(\vec{k})$, the static uniform spin (or Pauli) susceptibility is given by

$$\chi_{\text{spin}}(\vec{q} \rightarrow 0, \omega = 0) = -\frac{1}{V} \frac{1}{g^2 \mu_B^2} \sum_{\vec{k}} \frac{\partial f(\epsilon(\vec{k}) - \mu)}{\partial \epsilon(\vec{k})}, \quad (13)$$

with $f(\epsilon(\vec{k}) - \mu)$ being the Fermi function. For $T \rightarrow 0$, the static uniform susceptibility is proportional to the density of states at the Fermi surface.

Fig. 4 displays the spin susceptibility $\chi_{\text{spin}}$ as a function of temperature for a constant $d_{x^2-y^2}$-wave gap with phase fluctuations at finite doping ($\langle n \rangle = 0.9$). In Sec. $^2$ we have mentioned already that the fluctuation-induced diamagnetism is only important below $T \sim 1.5T_c$ and that, at higher temperatures, $\chi_{\text{Diam}}$ is at least two orders of magnitude smaller than the paramagnetic current response of the tight-binding electrons. Moreover, the experimentally observed diamagnetic susceptibility close to $T_c$ can be perfectly fitted by an exponential function, which also indicates that the fluctuating diamagnetism is exponentially suppressed at higher temperatures.$^{23}$ Furthermore, one obtains that the paramagnetic spin response is about 5 times larger than the paramagnetic current response of the tight-binding electrons. In addition, the magnetic current response is only weakly tem-
temperature dependent. Hence, we expect that the temperature dependence of the experimentally observed paramagnetic susceptibility is dominated by the spin susceptibility $\chi_{\text{spin}}$ over almost the entire pseudogap region. In Fig. 4 $\chi_{\text{spin}}$ is plotted for our phase-fluctuation model and for a BCS-model with a constant superconducting gap. The phase-fluctuation model exhibits a characteristic temperature dependence of the spin susceptibility, which differs qualitatively from the tight-binding model as well as from the BCS-model. This becomes even more clear for a BCS-temperature-dependent gap, as shown in Fig. 5. From Fig. 5 we can also infer, that a temperature dependent pairing-gap only slightly modifies the temperature dependence of $\chi_{\text{spin}}$ in our phase-fluctuation model. $\chi_{\text{spin}}$ always slightly decreases (nearly linear) below $T^* \equiv T^{MF}_{K,\mu}$ and, then, displays a characteristic downward bending at $T \simeq 2T^{K,\mu}_{K,\mu}$.

These results are very similar to the experimentally observed temperature dependence of the NMR Knight-shift and the magnetic susceptibility in the pseudogap state of various underdoped high-$T_c$ compounds. For comparison, we reproduce in Fig. 6 the $T$-dependence of the Knight-shift experimental data from Ref. 24 in underdoped and overdoped Bi2212. In the pseudogap state, the temperature variation of the NMR Knight-shift scales linearly with the macroscopic magnetic susceptibility $\chi_{\text{spin}}$. In underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) single-crystals, two characteristic temperature scales can be identified in the temperature dependence of the Knight-shift (see Fig. 6). A higher temperature $T_{mK}$, where the Knight-shift starts to decrease from the nearly constant high-temperature value, and a lower temperature $T_{K}^* > T_c$, where it starts to decrease very steeply. These two temperatures are, however, difficult to define exactly. This can be seen from the scaled Knight-shift data of YBCO shown in Ref. 24, and also from our numerical results displayed in Fig. 4 and Fig. 5 since the change as a function of temperature is continuous.

V. SUMMARY AND CONCLUSION

In the high-$T_c$ superconductors, a pseudogap opens at a temperature $T^*$ that is higher than the SC transition temperature $T_c$. There is a rather general consensus that the pseudogap state is crucial for understanding the microscopic pairing mechanism, however key issues are unsettled. One of these is whether it is a precursor state for SC, sharing common features such as pair formation or whether it is even antagonistic to SC.

At present, there is not yet agreement as to which of these possibilities is correct. In part, this is because of the difficulty in determining the experimental consequences of the various theoretical proposals. This is exactly what we seek to improve here.

We have provided a numerical solution of a simplified model which, nevertheless, contains key ideas of the phase-fluctuation pseudogap scenario. Here, the center-of-mass pair-phase fluctuations of a BCS $d$-wave model were determined from a classical 2D $XY$-action by means of a Monte-Carlo simulation. Earlier work concerned with the one-particle excitations have already been found to reproduce salient features of recent STM studies of Bi2212 and Bi2201, and to explain the change of the quasiparticle dispersion in crossing $T_c$ in underdoped cuprates. Here, we concentrate on experiments related to two-particle correlation functions, i.e. the optical and magnetic response functions. They are sensitive, diagnostic tools to search for normal-state remnants of the infinite d. c. conductivity and perfect diamagnetism above...
magnetic susceptibility is dominated by the Pauli spin.

The temperature dependence of the uniform static magnetic susceptibility, which displayed a very characteristic temperature dependence, independent of the details of the gap function used in our model. This temperature dependence is qualitatively very similar to the experimentally observed change of the Knight-shift as a function of temperature in underdoped Bi2212.

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30. It is known, from a variety of experiments (e.g. Fong et al., PRB 61, 14773 [2000]), that there is an increase of AF correlations in the pseudogap if the temperature $T$ is reduced. However, this effect has been detected experimentally in the low-doping regime, especially for dopings where at low $T$ the AF phase appears. We neglect in our discussion the direct influence of antiferromagnetic spin fluctuations. As discussed in Section I, they may, however, be indirectly incorporated in the effective next-neighbor $d_{x^2-y^2}$-pairing interaction used in our BCS-like model (Eqs. (1)-(4)).