

Change of quasiparticle dispersion in crossing T_c in the underdoped cuprates

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(Received 12 February 2004; revised manuscript received 7 June 2004; published 29 September 2004)

One of the most remarkable properties of the high-temperature superconductors is a pseudogap regime appearing in the underdoped cuprates above the superconducting transition temperature T_c . The pseudogap continuously develops out of the superconducting gap. In this paper, we demonstrate by means of a detailed comparison between theory and experiment that the characteristic change of quasiparticle dispersion in crossing T_c in the underdoped cuprates can be understood as being due to phase fluctuations of the superconducting order parameter. In particular, we show that within a phase fluctuation model the characteristic back-turning BCS bands disappear above T_c whereas the gap remains open. Furthermore, the pseudogap rather has a U shape instead of the characteristic V shape of a $d_{x^2-y^2}$ -wave pairing symmetry and starts closing from the nodal $\vec{k}=(\pi/2, \pi/2)$ directions, whereas it rather fills in at the antinodal $\vec{k}=(\pi, 0)$ regions, yielding further support to the phase fluctuation scenario.

DOI: 10.1103/PhysRevB.70.094522

PACS number(s): 71.10.Fd, 71.27.+a, 74.25.Jb, 74.72.-h

I. INTRODUCTION

More than 15 years after the discovery of the high- T_c superconductors, the mechanisms leading to their unusual properties are still under debate. Especially the pseudogap phase, which appears in various experiments below a characteristic temperature T^* in the underdoped region of the phase diagram as a reduction of spectral weight,^{1,2} might be a key to a better understanding of the high- T_c superconducting (SC) cuprates. In 1995 Emery and Kivelson³ proposed that the proximity to the Mott insulating phase implies a strongly reduced phase stiffness $J \sim \rho_s(0)/m^*$ compared to the usual BCS case. This causes the phase ordering temperature $T_\varphi \sim J$ to be much lower than the mean-field pairing temperature T_c^{MF} . Taking this idea one step further³ implies that at least part of the pseudogap behavior might be due to a kind of “preformed” Cooper pairs which form at a temperature $T^* \equiv T_c^{MF}$ well above the actual SC transition temperature $T_c \equiv T_\varphi$, where phase coherence among these pairs finally sets in. This phase fluctuation scenario also explains quite naturally the strongly enhanced Nernst signal above T_c in the underdoped cuprates.⁴

In previous work, we have already shown that indeed 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 simulation of an XY model, yields results which compare very well with scanning tunneling measurements over a wide temperature range.^{1,2} Furthermore, this phenomenological phase fluctuation model was also able to explain the possible “violation” of the in-plane optical integral in underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi2212).⁵

However, for the phase fluctuation description to be correct over a wide temperature range, one needs a mechanism that produces “cheap” vortices, so that the only energy scale is the stiffness J and the dominating fluctuation channel is that of the phase of the SC order parameter. Mechanisms that can lead to a small vortex core energy range from the more

conventional picture of a granular superconductor, where the vortices arrange themselves to reside in the insulating regions between the SC grains, up to the existence of a competing order that exists inside the vortex cores. As soon as the superconducting order parameter is suppressed inside the vortex core, the system develops the competing order instead of going into a normal conducting paramagnetic state and thus has a much smaller vortex energy compared to a conventional BCS superconductor. Recently, it was shown⁶ that vortices with a staggered-flux core can provide a way to understand the low vortex energy over a wide temperature range above T_c . In all cases, the small phase stiffness and the low vortex core energy have the same origin, which is the proximity to the Mott-insulating state.

In this paper, we present theoretical results on the quasiparticle dispersion, which—when compared with experimental data—give a clear fingerprint towards a possible phase fluctuation scenario for the origin of the pseudogap. Earlier angle-resolved photoemission spectroscopy (ARPES) results have shown deviations from the simple BCS $d_{x^2-y^2}$ -wave form of the SC gap in underdoped Bi2212,^{7,8} which might be due to a change in the pairing interaction in the proximity of the AF insulating phase. By analyzing the temperature dependence of the quasiparticle (QP) dispersion, we want to show that the change of the QP dispersion in crossing T_c from the SC to the pseudogap region can be understood quite naturally by the assumption that the pseudogap is caused by phase fluctuations of the SC gap. Moreover, the phase fluctuation scenario also explains the deviations from the simple $d_{x^2-y^2}$ -wave form of SC and pseudogap⁹ in the underdoped cuprates. Using the ARPES with tunable excitation photon energy we disentangle bilayer splitting related effects and determine the true dispersion and the leading edge gap (LEG) function corresponding to the bonding band in the pseudogap regime of Pb-Bi2212.

Since below T_c the QP excitations are perfectly BCS like unless in the extremely underdoped region,¹⁰ it is tempting to

start from the BCS ground state and see how it is destroyed by including phase fluctuations.^{11–14}

II. MODEL AND CALCULATIONS

In the following we use a phenomenological phase fluctuation model which has already been shown to successfully account for the pseudogap observed in tunneling experiments² and which was also able to explain the possible “violation” of the in-plane optical integral in underdoped Bi2212.⁵ We consider the Hamiltonian

$$H = H_0 + H_1, \quad (1)$$

where H_0 is the usual tight-binding Hamiltonian of noninteracting electrons on a two-dimensional (2D) square lattice:

$$H_0 = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - \mu \sum_{i, \sigma} n_{i\sigma}. \quad (2)$$

Here, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron of spin σ on the i th site of the 2D square lattice and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator. t denotes an effective nearest-neighbor hopping term and μ is the chemical potential. The angles $\langle \dots \rangle$ indicate sums over nearest-neighbor sites of the 2D square lattice.

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

$$H_1 = -g \sum_{\vec{i}\vec{\delta}} (\Delta_{i\vec{\delta}} \Delta_{i\vec{\delta}}^\dagger + \Delta_{i\vec{\delta}}^\dagger \Delta_{i\vec{\delta}}), \quad (3)$$

with $\vec{\delta}$ connecting 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 unimportant for the further calculation. It can be either of pure electronic origin, like spin fluctuations, or phonon mediated. The only important thing is that there exists an effective pairing interaction that produces a finite local $d_{x^2-y^2}$ -wave gap 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 number

$$\langle \Delta_{i\vec{\delta}}^\dagger \rangle = \frac{1}{\sqrt{2}} \langle c_{i\uparrow}^\dagger c_{i+\vec{\delta}\uparrow}^\dagger - c_{i\downarrow}^\dagger c_{i+\vec{\delta}\downarrow}^\dagger \rangle = \Delta e^{i\Phi_{i\vec{\delta}}}, \quad (4)$$

with a *constant* magnitude Δ and a *fluctuating* bond-phase field $\Phi_{i\vec{\delta}}$. In order to get a description, where the *center-of-mass* phases of the Cooper pairs are the only relevant degrees of freedom,¹⁵ we write the $d_{x^2-y^2}$ -wave bond-phase field in the following way:

$$\Phi_{i\vec{\delta}} = \begin{cases} (\varphi_i^- + \varphi_{i+\vec{\delta}}^-)/2 & \text{for } \vec{\delta} \text{ in the } x \text{ direction,} \\ (\varphi_i^- + \varphi_{i+\vec{\delta}}^-)/2 + \pi & \text{for } \vec{\delta} \text{ in the } y \text{ direction,} \end{cases} \quad (5)$$

where φ_i^- is the *center of mass* phase of a Cooper pair localized at lattice site \vec{i} .

In order 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

$$F[\varphi_i] = -J \sum_{\langle ij \rangle} \cos(\varphi_i - \varphi_j), \quad (6)$$

where the phase stiffness J determines the Berezinskii-Kosterlitz-Thouless transition temperature T_{BKT} to a quasi-phase-ordered state which we take as T_c . The XY free energy is defined on a coarse-grained lattice with the *scale* of the lattice spacing given by the pair coherence length¹⁵ $\xi_0 \sim v_F/\pi\Delta$. Now, the underdoped cuprates are in an intermediate coupling regime between large BCS mean-field pairs and tightly bound BEC pairs,^{16,17} with the pair-size coherence length ξ_0 given by 3–4 times the basic Cu-Cu lattice spacing. For a typical 36×36 fermionic lattice, which is numerical feasible, we would only have a 9×9 phase lattice on top of it. This would not allow for any proper temperature scaling of the phase correlation length $\xi(T)$ and obscure the Kosterlitz-Thouless transition. Therefore we have chosen to set $\Delta_{sc} = 1.0 t$. This yields $\xi_0 \lesssim 1$ and allows the Monte Carlo (MC) phase simulation to be carried out on the same $L \times L$ lattice that is used for the diagonalization of the fermionic Hamiltonian.⁵ In addition, the choice of $\Delta_{sc} = 1.0 t$ automatically introduces the important short distance cutoff. Finally we set $T_c \approx \frac{1}{4} T^*$, where we had the scanning tunneling microscopy (STM) experiments of Ref. 1 in mind.

III. EXPERIMENTAL DETAILS

The ARPES experiments were carried out using angle-multiplexing electron energy analyzers. Spectra were recorded either with $h\nu = 21.218$ eV photons from a He source or using radiation from the U125/1-PGM beamline at the BESSY synchrotron radiation facility. The total energy resolution was set to 17 meV [full width at half maximum (FWHM)] at $h\nu = 38$ eV. The angular resolution was kept below 0.2° both along and perpendicular to the analyzer entrance slit. Data shown in Fig. 4 were taken with $0.2^\circ \times 0.3^\circ$ angular resolution. The data were collected on two similar underdoped, modulation-free single crystals of Pb-Bi 2212 ($T_c = 77$ K).

IV. DISCUSSION OF RESULTS

A. Dispersion

Figure 1 shows the quasiparticle dispersion calculated from our phenomenological phase fluctuation model for 10% doping ($\langle n \rangle = 0.9$). The spectral weight is plotted along the $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi)$ direction through the Brillouin zone (BZ). The free dispersion would cross the Fermi surface close to the $(\pi,0)$ point. One can clearly see that the characteristic (back-turning) Bogoliubov quasiparticle band disappears in the pseudogap state above T_c . Instead, one obtains a sharp quasiparticle dispersion which runs straight towards the Fermi energy and then fades out at a distance of the order of the SC gap Δ_{sc} . This is in complete agreement with the

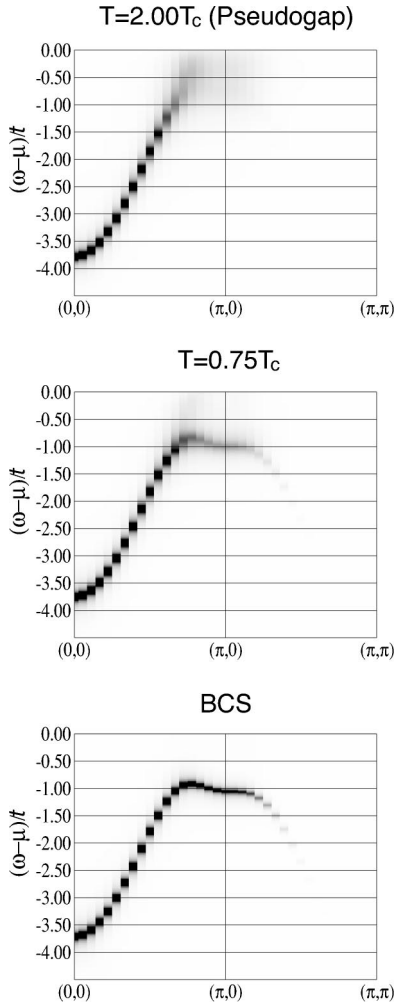


FIG. 1. Spectral weight $A(\vec{k}, \omega)$ in the pseudogap state ($T=2.0 T_c$, top) and in the superconducting state slightly below T_c ($T=0.75 T_c$) calculated from the phase fluctuation model. For comparison we also show the spectral weight for the phase coherent BCS limit (bottom).

experimentally observed dispersion in underdoped Bi2212 which is shown in Fig. 2.

The angle-resolved data presented in Fig. 2 provide an insight into how the pseudogap is actually created near k_f . In the superconducting state a characteristic BSC-like back-dispersion is easily seen. This clarity is achieved by the careful choice of the excitation photon energy. Exactly near $h\nu = 38$ eV the emission probability for the bonding band is much higher than for the antibonding band^{18,19} and bilayer-related complications are thus avoided. Above T_c in the pseudogap state the characteristic BCS behavior is replaced by the straight dispersion and strong depletion of the spectral weight towards E_f , which, as will be shown below, still leaves the energy gap in the spectrum.

Furthermore, Fig. 1 shows that the sharp quasiparticle features close to the $(\pi, 0)$ point are getting lost above T_c within the phase fluctuation model. The sharp coherent $(\pi, 0)$ peaks disappear and broad incoherent weight *fills in* the gap. Exactly this behavior was observed before in photoemission studies of the pseudogap^{9,20-23} and is also responsible for the

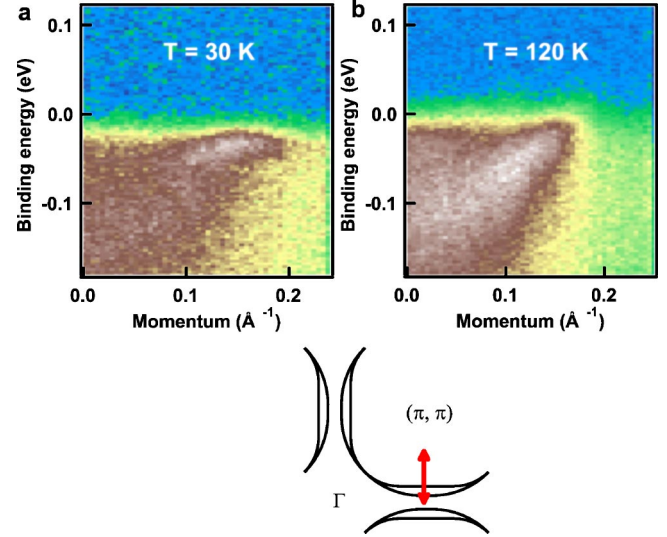


FIG. 2. (Color online) (a) Superconducting state. Energy distribution of the photoemission intensity along the direction shown as a red arrow on the sketch below. The BCS-like dispersion is clearly observed for the bonding band. (b) Pseudogap state. No more bending back of the dispersion is observed. Instead, spectral weight fades upon approaching the Fermi level.

characteristic temperature dependence of the scanning tunneling gap in the underdoped cuprates,^{1,2} where the pseudogap fills in instead of closing. Interestingly, not only SC fluctuations,²⁴ but also staggered flux fluctuations²⁵ can lead to this temperature dependence of the $(\pi, 0)$ -photoemission peak.

The disappearance of the characteristic BCS bands above T_c within the phase fluctuation picture can be understood by the fact that the BCS wave function is a coherent superposition of wave functions with a different number of electron pairs²⁶

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |\phi_0\rangle = \sum_N \lambda_N |\Psi_N\rangle, \quad (7)$$

where $|\Psi_N\rangle$ is an N -particle wave function. The quantum-mechanical uncertainty in the particle number is given by

$$(\Delta N)^2 = 4 \sum_k u_k^2 v_k^2. \quad (8)$$

Now $v_k^2 = 1 - u_k^2$ is the momentum distribution function for $T=0$ and the weight of a quasiparticle peak at momentum k is given by $v_k^2 (u_k^2)$ for $E < E_f$ ($E > E_f$).

In the normal metallic state with $\Delta=0$, one gets a sharp cutoff in $v_k^2 (u_k^2)$ at the Fermi wave vector $k=k_f$ so that $(\Delta N)^2 \equiv 0$. In the BCS superconducting state, however, $v_k^2 (u_k^2)$ are finite also beyond the Fermi wave vector k_f , which means that also for $k > k_f$ ($k < k_f$) one gets spectral weight at $E < E_f$ ($E > E_f$). This produces the characteristic BCS band structure, with bands approaching E_f from below (above) and then turning back to higher binding (quasiparticle) energies.

Now let us see what happens if one introduces an arbitrary phase factor into the BCS wave function²⁶

$$|\Psi_\varphi\rangle = \prod_k (|u_k\rangle + |v_k\rangle e^{i\varphi} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |\phi_0\rangle. \quad (9)$$

Integrating over all possible phases yields²⁶

$$\begin{aligned} |\Psi_N\rangle &= \int_0^{2\pi} d\varphi e^{-iN\varphi/2} \prod_k (|u_k\rangle + |v_k\rangle e^{i\varphi} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |\phi_0\rangle \\ &= \int_0^{2\pi} d\varphi e^{-iN\varphi/2} |\Psi_\varphi\rangle. \end{aligned} \quad (10)$$

This means that one projects into an exact particle-number eigenstate by making the relative phase of the Cooper pairs completely uncertain. Equation (8) is a special case of the general uncertainty relation between phase and particle number:

$$\Delta N \Delta\varphi \gtrsim 1. \quad (11)$$

The above-described behavior corresponds to what is happening in the phase-fluctuation model as a function of temperature. Starting from a phase coherent state at $T=0$ with $\Delta\varphi=0$, the particle number is completely uncertain with ΔN given by Eq. (8). With increasing temperature, one *gradually projects into a state with exact particle number* N . In the temperature range where the phases are completely uncorrelated ($\xi \sim \xi_0$), one then obtains $\Delta N=0$, and the back-turning BCS bands must completely disappear (lose weight for $k > k_f$, as seen in Figs. 1 and 2). At finite temperatures, this situation corresponds to a classical grand canonical average over ensembles with a different number of particles, where each state has a well-defined particle number and is no longer a coherent quantum-mechanical superposition of states with different number of particles. Thus, we obtain a crossover from a BCS-like phase-ordered band structure to a completely new phase-disordered *pseudogapped* band structure.

B. Superconducting gap and pseudogap

Next we want to elucidate the effect of phase fluctuations on the \vec{k} dependence of the quasiparticle pairing gap. Therefore, we have plotted in Fig. 3 the quasiparticle dispersion obtained from MC simulations of the phase fluctuation model along the Fermi surface of the free dispersion $\epsilon(\vec{k})$ at half-filling ($\langle n \rangle = 1.0$). This gives us effectively the gap function $\Delta(\vec{k})$. As can be seen in Fig. 3, below T_c one obtains the characteristic V shape of a gap with $d_{x^2-y^2}$ pairing symmetry. As the temperature is raised, the quasiparticle peaks are getting broader. In the pseudogap state above T_c , the spectral weight is getting rather incoherent close the $\vec{k}=(\pi, 0)$ as was pointed out before. However, close to the nodal point of the gap function one still obtains a sharp quasiparticle dispersion. There, one can clearly see spectral weight shifting to lower binding energies which produces an *extended gapless region* in the pseudogap state close to $\vec{k}=(\pi/2, \pi/2)$ instead of the nodal point in the superconducting state below T_c . This behavior is in complete agreement with photoemission experiments^{9,23} which show that the pseudogap starts closing

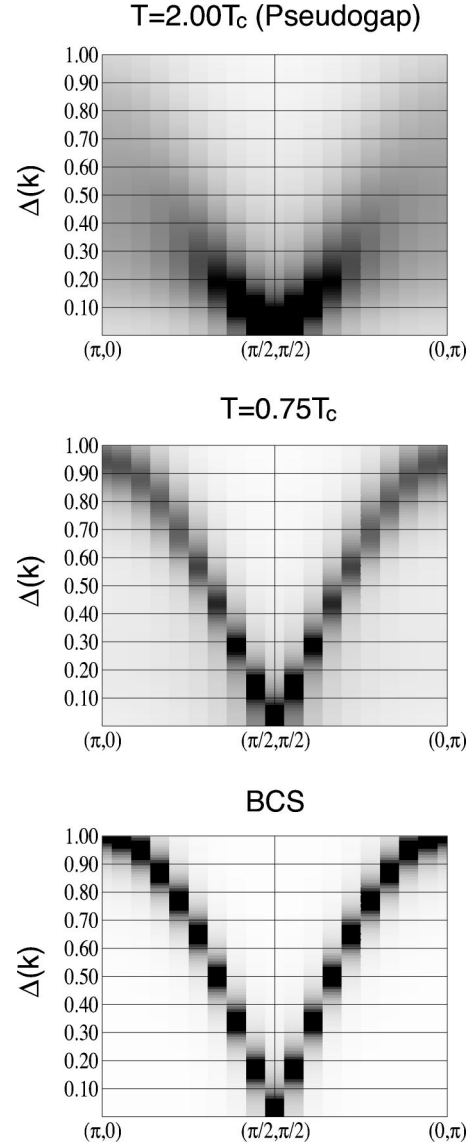


FIG. 3. Gap function $\Delta(\vec{k})$ in the pseudogap state ($T=2.0 T_c$, top) and in the superconducting state slightly below T_c ($T=0.75 T_c$) calculated from the phase fluctuation model. For comparison we also show the BCS gap function (bottom).

from $\vec{k}=(\pi/2, \pi/2)$ where one obtains a finite Fermi arc but rather *fills in* at $\vec{k}=(\pi, 0)$ exactly as in Fig. 3 (top).

Furthermore, the pseudogap $\Delta(\vec{k})$ obtained from phase fluctuations of the local $d_{x^2-y^2}$ pairing amplitude rather has a U-like shape (see Fig. 3, top) than the characteristic V shape of a BCS $d_{x^2-y^2}$ -gap. For comparison, Fig. 4 shows the experimentally observed pseudogap in underdoped Bi2212. One can clearly see that the experimentally determined pseudogap has exactly the U-like form that we have obtained from the phase fluctuation model. This deviation from the pure $d_{x^2-y^2}$ -wave form was also observed in the superconducting state of very underdoped cuprates and interpreted as higher harmonic contributions to the pairing function.^{7,8} However, these experimental results just might indicate the possible relevance of quantum phase fluctuations in this re-

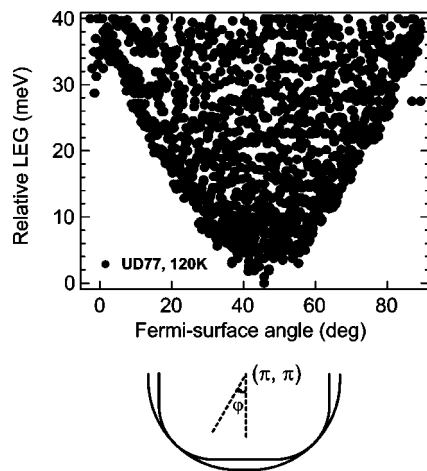


FIG. 4. Values of the leading edge (pseudo) gap (LEG) as a function of the Fermi surface angle within the quadrant of the Brillouin zone (see lower panel) given with respect to the binding energy of the leading edge of a nodal energy distribution curve. The curve joining the low-gap extremity of these data points would represent the \vec{k} dependence of the pseudogap. For details see Ref. 8.

gion of the phase diagram. Our results on the effects of phase fluctuations on the form of the pairing gap could also be of some relevance for electron doped cuprates²⁷ where a possible crossover from a $d_{x^2-y^2}$ (or anisotropic s -wave) to a pure s -wave symmetry of the superconducting gap as a function of electron doping was observed.^{28,29}

V. SUMMARY AND CONCLUSION

In conclusion, we have elaborated the important role that phase fluctuation effects might play in the underdoped cuprates. With a detailed comparison between theory and experiment we were able to show how phase fluctuations influence the quasiparticle spectra. In particular the disappearance of the BCS-Bogoliubov quasiparticle band at T_c and the change from a more V-like superconducting gap to a rather U-like pseudogap above T_c can be explained in a consistent way by assuming that the low-energy pseudogap in the underdoped cuprates is due to phase fluctuations of a local $d_{x^2-y^2}$ -wave pairing gap with fixed magnitude. Furthermore, phase fluctuations can explain why the pseudogap starts closing from the nodal points, whereas it rather fills in along the antinodal directions.

ACKNOWLEDGMENTS

We would like to acknowledge useful discussions and comments by E. Arrigoni, D. J. Scalapino, and S. A. Kivelson. We are grateful to H. Berger for providing us with the high-quality single crystals. This work was supported by the KONWHIR projects OOPCV and CUHE and by the Forschergruppe under Grant No. FOR 538. The calculations were carried out at the high-performance computing centers HLRS (Stuttgart) and LRZ (München).

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