Classical Phase Fluctuations in High Temperature Superconductors

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Phase fluctuations of the superconducting order parameter play a larger role in the cuprates than in conventional BCS superconductors because of the low superfluid density ρ_s of a doped insulator. In this paper, we analyze an XY model of classical phase fluctuations in the high temperature superconductors using a low temperature expansion and Monte Carlo simulations. In agreement with experiment, the value of ρ_s at temperature $T = 0$ is a quite robust predictor of T_c, and the evolution of ρ_s with T, including its T-linear behavior at low temperature, is insensitive to microscopic details.

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Two classes of thermal excitations are responsible for disordering the ground state of a superconductor: amplitude and phase fluctuations of the complex order parameter. A consensus has not yet been reached on the relative importance of the two in the high temperature superconductors, since both are anomalous. The low superfluid density (phase stiffness) of the doped insulator implies that phase fluctuations play an unusually large role [1]. Yet the nodes in the d-wave gap function support more quasiparticle (amplitude) excitations at low temperature than in a *clean* s-wave superconductor.

This paper reports an analytical and numerical study of the thermal evolution of the in-plane helicity modulus, $\gamma_\parallel(T)$, of a quasi-two-dimensional classical XY model of phase fluctuations in a high temperature superconductor [2]. In doing this, we are ignoring the widely discussed effects of thermally excited nodal quasiparticles, i.e., spin $1/2$ excitations. As discussed below and in Ref. [4], we believe this neglect is justified because the nodal quasiparticles are not sensitive to the onset of superconductivity [5]. As such, the spectral weight removed from the superfluid density per thermally excited spin is small [6]. We also neglect the quantum dynamics of the phase since, with sufficient screening, the phase fluctuations are predominantly classical down to quite low temperature [7].

The calculations focus on the scaled curve, $\gamma_\parallel(T)/\gamma_\parallel(0)$ vs T/T_c, and the value of the dimensionless ratios $A_1 = T_c/\gamma_\parallel(0)$ and $A_2 = T_c\gamma'_\parallel(0)/\gamma_\parallel(0)$. [Here $\gamma'_\parallel(T) \equiv d\gamma_\parallel(T)/dT$.] These nonuniversal quantities turn out to be rather insensitive to microscopic details of the model, such as the strength of the interplane coupling and the exact short-distance nature of the interactions, as shown in Fig. 1 and in the tables. Figure 1 also shows that the model results agree well with experiment [8], when the helicity modulus of the model is related to the in-plane superfluid density ρ_s as determined by

$$\frac{\gamma_\parallel(T)}{a_\perp} = \frac{\hbar^2\rho_s(T)}{4m^*} = \frac{(\hbar c)^2}{16\pi e^2\lambda_{ab}^2(T)}, \qquad (1)$$

where $a_\perp$ is the spacing between planes and λ_{ab} is the London penetration depth within the CuO_2 planes.

There is strong empirical evidence that classical phase fluctuations determine much of the important physics in the superconducting state of the high T_c superconductors, and also some properties of the normal state, especially in underdoped materials [1]. Most notably, T_c increases roughly linearly with the zero-temperature superfluid density [9] [$A_1 = T_c/\gamma_\parallel(0) \sim 1$], whereas the characteristic energy scale for pairing, $\Delta_o/2$, is both quantitatively large compared to k_BT_c and decreases as the doping increases. Furthermore, angle-resolved photoemission spectroscopy and other measurements of the superconducting gap reveal that pair formation occurs at a crossover temperature well above T_c [10–12]. It is important to note that

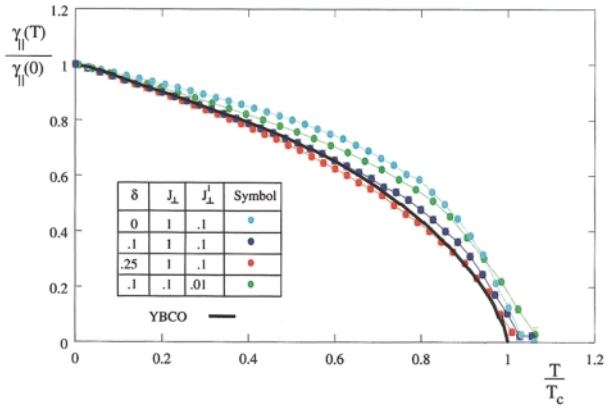

FIG. 1 (color). Superfluid density vs temperature, scaled by the zero-temperature superfluid density and by T_c, respectively. Experimental data on YBCO is depicted by the black line, and is taken from Hardy *et al.* [8] (The data are essentially the same for a range of doping concentration.) Our Monte Carlo results for system size $16 \times 16 \times 16$ are the filled symbols. Calculations are for two planes per unit cell, with coupling $J_\parallel = 1$ within each plane, and $J_\perp$ and $J'_\perp$ between alternate planes, as defined in Eq. (3). Monte Carlo points above T_c are nonzero due to finite size effects. Except where explicitly shown, error bars are smaller than symbol size.

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$A_2 = T_c\gamma_\parallel'(0)/\gamma_\parallel(0)$ is roughly constant for various materials and doping concentrations. This implies that the fluctuations predominantly responsible for the T-linear dependence of the superfluid density at low T are also responsible for the ultimate destruction of the superconducting state at T_c.

The following arguments have been made against this interpretation of the data: (1) The *nonuniversal* ratio $A_1 = T_c/\gamma_\parallel(0)$ should [13] theoretically lie in the range 4–8, rather than in the 0.5–1 range observed experimentally. (2) For weakly coupled layers, a phase only model would [14] yield a $\rho_s(T)$ curve that looks like a rounded Berezinskii-Kosterlitz-Thouless (BKT) discontinuity, unlike what is seen in experiments. (3) Quantum effects suppress classical phase fluctuations [15] for temperatures below the plasma frequency. (4) If pairing occurs in a substantial range of temperatures above T_c, the effects of fluctuation superconductivity should be observed, contrary to experiment [13].

Our present results show that the classical XY model *is* quantitatively consistent with experiments. As can be seen from the tables, A_1 lies in the range 0.6–1.8 for the wide range of parameters we have explored, consistent with experiment. Figure 1 shows that $\gamma_\parallel(T)$ of the XY model closely matches the experimentally measured $\rho_s(T)$ curves. The third suggestion has been previously shown to be incorrect [7], due to screening by the substantial background normal fluid. Specifically, in a two-fluid model of a superconductor, the classical model is reliable down to a classical to quantum crossover temperature which can be well below T_c: $T_{\rm class} \propto T_c/\sigma_N$, where σ_N is an average of the optical conductivity of the normal component in units of the quantum of conductance. The fourth point overlooks the fact that fluctuation superconductivity is only significant close to T_c where the correlation length is long. In conventional superconductors the observed fluctuations involve amplitude and phase and are Gaussian, while for the high T_c superconductors, true critical fluctuations in the XY universality class are detected in a remarkably broad range of temperatures [16].

A classical XY model on a tetragonal lattice will be used to study the effects of phase fluctuations in a quasi-two-dimensional superconductor at wavelengths that are long enough for amplitude fluctuations to be unimportant. The in-plane unit cell area $a_\parallel^2$ does not enter into the evaluation of T_c or the temperature dependence of $\gamma_\parallel(T)$. Here $a_\parallel$ is a short-distance cutoff which will be discussed at the end of the paper. In general, the interaction energy, V, depends on the phase difference, $\theta_{ij} \equiv \theta_i - \theta_j$, between nearest-neighbor sites $\langle i, j\rangle$. Because of gauge invariance and time reversal symmetry, V can be expanded in a cosine series,

$$V(\theta_{ij}) = \sum_n A_n \cos(n\theta_{ij}) . \tag{2}$$

The first harmonic, $\cos(\theta)$, corresponds to the transfer of one pair of electrons between neighboring cells; each successive harmonic transfers a higher number of pairs. We keep only the first two terms in the cosine series for couplings within a plane, and the first cosine term for the weaker Josephson coupling between planes.

$$H = -J_\parallel \sum_{\langle ij\rangle_\parallel} \{\cos(\theta_{ij}) + \delta\cos(2\theta_{ij})\} - \sum_{\langle kl\rangle_\perp} \{J_\perp^{kl}\cos(\theta_{kl})\} , \tag{3}$$

where the first sum is over nearest-neighbor sites within each plane, and the second sum is over nearest-neighboring planes. The coupling, $J_\parallel$, will be assumed to be isotropic within each plane and the same for every plane, but the coupling between planes, $J_\perp^{kl}$, is different for crystallographically distinct pairs of neighboring planes. It will be assumed that $J_\parallel$, $J_\perp$, and δ are positive, since there is no reason to expect any frustration in the problem [17], and that $\delta \le 0.25$, since for $\delta > 0.25$ there is a secondary minimum in the potential for $\theta_{ij} = \pi$, which is probably unphysical. The sensitivity of various computed quantities to variations in δ in this range is a measure of the importance of "microscopic details."

It follows from simple and general considerations that most features of the thermal evolution of the superfluid density of $YBa_2Cu_3O_{7-\delta}$ (YBCO) shown in Fig. 1 are reproduced by such a model. The critical phenomena are in the same universality class as the classical 3D XY model, which is consistent with the observed behavior [16] in $YBa_2Cu_3O_{7-\delta}$ within about 10% of T_c. Furthermore, the helicity modulus is linear in the temperature, as observed in $YBa_2Cu_3O_{7-\delta}$. As first pointed out by Roddick and Stroud, the T-linear behavior is characteristic of classical phase fluctuations [18,19]. Indeed, using linear spin-wave theory, it is straightforward to obtain the first terms in the low temperature series for γ,

$$\frac{\gamma_\parallel}{a_\perp}(T) = J_\parallel(1 + 4\delta) - \frac{\alpha(1 + 16\delta)}{4(1 + 4\delta)} T + \mathcal{O}(T^2) , \tag{4}$$

where α is a numerical integral which varies from $\alpha = 1$ in the 2D limit ($J_\perp \to 0$) to $\alpha = 2/3$ for $J_\perp \to \gamma_\parallel(0) = J_\parallel(1 + 4\delta)$ for one plane per unit cell. Note that the T-linear term is independent of $J_\parallel$ and so is much less dependent on microscopic parameters (such as doping) than is $\gamma_\parallel(0)$.

A more quantitative comparison between the classical model and experimental data can be undertaken by studying various dimensionless ratios, particularly $A_1 = T_c/\gamma_\parallel(0)$ and $A_2 = T_c\gamma_\parallel'(0)/\gamma_\parallel(0)$. Here, T_c is computed numerically by means of the Binder parameter [20] for systems of size up to $24 \times 24 \times 24$. Errors in T_c are limited by the resolution with which the Binder crossing point is computed in each case. The quantities $\gamma_\parallel(0)$ and $\gamma_\parallel'(0)$ are obtained from Eq. (4).

TABLE I. Single layer: The dimensionless ratios $A_1 = T_c/\gamma_\parallel(0)$ and $A_2 = T_c\gamma'_\parallel(0)/\gamma_\parallel(0)$ which characterize the superfluid density vs temperature for systems with one layer per unit cell. $J_\perp$ and T_c are quoted in units of $J_\parallel$.

$J_\perp$	0	0	0	0.01	0.01	0.01	0.1	0.1	0.1
δ	0	0.1	0.25	0	0.1	0.25	0	0.1	0.25
A_1	0.89	0.72	0.6	1.1	0.828	0.625	1.324	0.986	0.73
A_2	0.22	0.335	0.38	0.27	0.381	0.388	0.3066	0.432	0.437
T_c	0.89	1.01	1.2	1.1	1.16	1.25	1.324	1.38	1.46

Experimentally $A_2 \sim \frac{1}{2}$, and A_1 is in the range 0.6–1.3 for underdoped and optimally doped materials. Tables I and II show the ratios A_1 and A_2 for various choices of parameters in the classical XY model. Note that $A_2 \sim \frac{1}{2}$ for δ not too small, whereas A_2 is about a factor of 2 smaller for $\delta = 0$. The shape of the $\rho_s(T)$ vs T curves, as quantified by A_2, is remarkably robust, especially if we compare the cases of $\delta = 0.1$ to $\delta = 0.25$. The ratio A_1 is a little more sensitive to the value of δ, but it is comfortably in the experimental range for δ between 0.1 and 0.25, and only slightly larger for $\delta = 0$. The relative insensitivity of A_1 to δ and to the details of the interplane couplings, $J_\perp$, demonstrates that when classical phase fluctuations govern the physics, $\rho_s(0)$ is a quantitatively good predictor of T_c.

Hardy *et al.* have demonstrated [8] that when $\rho_s(T)/\rho_s(0)$ is plotted vs T/T_c, for various dopant concentrations in $YBa_2Cu_3O_{7-\delta}$, the data collapse approximately onto one curve. Since $T_c \propto \rho_s(0)$, this amounts to scaling out T_c for both axes. Thus the unique shape of the normalized ρ_s vs T curve may be attributed to the existence of a single energy scale, the transition temperature. We have also used Monte Carlo calculations to evaluate the superfluid density for $0 < T < T_c$. The results are scaled as in Hardy *et al.* [8] and compared with their data in Fig. 1. As anticipated, for δ not too near zero, the model is insensitive to the value of δ, and in remarkable agreement with experiment, considering that no parameters have been tuned.

A much-discussed feature of the systematics of T_c in the high temperature superconductors [21] is the observed increase of T_c within each family of materials with the number of planes per unit cell, n. Within the classical phase model, the fact that phase fluctuations lead to a particularly large suppression of T_c below its mean-field value (see Table III) leads to an increased sensitivity to even weak couplings in the third direction. This produces a strong increase of T_c with n, although possibly not quite as strong as observed experimentally. However, it should be noted that other things may change with n; for example, in a three-plane material, the central plane may have a different hole concentration than the others.

Mean-field theory is a standard method of estimating the effects of weak higher-dimensional couplings on the critical temperature of quasi-one-dimensional or quasi-two-dimensional systems. For instance, for one plane per unit cell ($n = 1$) this approach leads to an implicit equation for the three-dimensional T_c

$$\chi_{2d}(T_{\mathrm{MF}})2J_\perp = 1\,, \tag{5}$$

where $\chi_{2d}(T)$ is the susceptibility of an isolated plane. For the case $\delta = 0$, we have computed the interplane mean-field transition temperature, which is also presented in Table III, using the Monte Carlo results of Gupta and Baillie [22] for $\chi_{2d}(T)$. This mean-field theory always gives an upper bound to T_c.

Phase fluctuations should also have detectable effects on other equilibrium properties, such as the specific heat, the diamagnetic susceptibility, and $\gamma_\perp$. In contrast to $\gamma_\parallel$, these quantities depend on $a_\parallel$. The classical XY model at temperatures $T \ll T_c$ has a specific heat per unit area in a CuO_2 plane equal to $C = k_B/2a_\parallel^2$. The specific heat [23] at $T = 2$ K of good crystals of optimally doped YBCO is roughly $5 \times 10^{-4}k_B$ per planar copper; if we assumed that all of this specific heat were due to phase fluctuations, it would imply $a_\parallel = 32$ lattice constants.

In the classical XY model $a_\parallel \sim r_v$, where r_v is the radius of a vortex core. Recent muon spin rotation (μSR)

TABLE II. Double layer: The dimensionless ratios $A_1 = T_c/\gamma_\parallel(0)$ and $A_2 = T_c\gamma'_\parallel(0)/\gamma_\parallel(0)$, which characterize the superfluid density vs temperature curve, for systems with two layers per unit cell; the two values of $J_\perp$ are between planes within a unit cell and between unit cells.

$J_\perp$:$J'_\perp$	1:0	1:0	1:0	1:0.01	1:0.01	1:0.01	1:0.1	1:0.1	1:0.1
δ	0	0.1	0.25	0	0.1	0.25	0	0.1	0.25
A_1	1.38	1.03	0.78	1.52	1.12	0.83	1.6975	1.252	0.916
A_2	0.279	0.402	0.426	0.306	0.437	0.452	0.3318	0.4772	0.4906
$J_\perp$:$J'_\perp$	0.1:0	0.1:0	0.1:0	0.1:0.01	0.1:0.01	0.1:0.01	0.1:0.1	0.1:0.1	0.1:0.1
δ	0	0.1	0.25	0	0.1	0.25	0	0.1	0.25
A_1	1.13	0.836	0.645	1.2	0.907	0.675	1.324	0.986	0.73
A_2	0.271	0.376	0.394	0.29	0.407	0.411	0.3066	0.432	0.437

TABLE III. Variations as a function of the number of planes per unit cell: The coupling between planes within the unit cell is $J_\perp = 0.1$, and between planes of different unit cells is $J'_\perp = 0.01$, and $\delta = 0$. Similar data exist for $\delta > 0$. T_{MF} is the interplane mean-field estimate of T_c obtained as described in the text.

n	1	2	3	4	∞
$\frac{d\rho(0)}{dT}$	0.2472	0.2384	0.2365	0.2348	0.2315
T_c	1.09	1.20	1.24	1.26	1.324
T_{MF}	1.111	1.287	1.334	1.361	1.394

measurements [24] have found that r_v grows substantially at low fields, and tends to a zero field value which is on the order of 100 Å (26 lattice constants) and which is only weakly temperature dependent nearly up to T_c. Thus, if we estimate $a_\parallel$ using the μSR data, it is consistent to attribute a large fraction of the low temperature specific heat to classical phase fluctuations. The contribution of critical fluctuations to the specific heat near T_c may also be dominated by classical phase fluctuations, but a quantitative comparison of the theoretically expected (nonuniversal) critical amplitudes with experiment is not straightforward.

Finally, we address the remarkable measurements of the frequency dependent superfluid density in BSCCO of Corson *et al.* [25]. Without making any explicit assumptions concerning the dynamics, we can interpret these results in terms of a finite size scaling hypothesis, in which we associate a length scale, $L(\omega)$, with the finite measurement frequency, and

$$\gamma(T, L) \sim L^x T \tilde{\gamma}[L/\xi(T)], \tag{6}$$

where $\xi(T)$ is the correlation length of the infinite system at temperature T. Since BSCCO is highly anisotropic, we follow Corson *et al.* [25] in assuming that the finite frequency response is essentially two dimensional, in which case $x = 0$, and $\xi(T)$ is infinite for all $T < T_{\mathrm{BKT}}$, the BKT transition temperature. This implies that γ is approximately frequency independent for $T < T_{\mathrm{BKT}}$ and vanishes exponentially as a function of L/ξ at temperatures enough above T_{KT} that $L > \xi(T)$. Indeed, $\gamma(T, L)$ was computed numerically for the two-dimensional XY model by Schultka and Manousakis [3] and we have repeated these calculations for anisotropic three-dimensional models; the results confirm that our model nicely accounts for the observations of Corson *et al.* [25].

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