Kosterlitz-Thouless Behavior in Layered Superconductors: The Role of the Vortex Core Energy

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In layered superconductors (SC) with small interlayer Josephson coupling vortex-antivortex phase fluctuations characteristic of quasi two-dimensional (2D) Kosterlitz-Thouless behavior are expected to be observable at some energy scale T_d . While in the 2D case T_d is uniquely identified by the KT temperature $T_{\rm KT}$ where the universal value of the superfluid density is reached, we show that in a generic anisotropic 3D system T_d is controlled by the vortex-core energy, and can be significantly larger than the 2D scale $T_{\rm KT}$. These results are discussed in relation to recent experiments in cuprates, which represent a typical experimental realization of layered anisotropic SC.

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Since the pioneering work of Kosterlitz and Thouless [1] (KT) on the so-called KT transition in the two-dimensional (2D) XY model, much attention has been devoted to the effect of phase fluctuations in quasi-2D superfluid systems. Thin films are natural candidates for the observation of KT physics, as the occurence of the "universal" (i.e., sample independent) jump of the superfluid density, measured in ⁴He superfluid films, or the nonlinear *I-V* characteristic, observed in thin films of conventional SC [2]. Signatures of KT physics can be expected also in layered SC with weak interlayer coupling. A remarkable example of systems belonging to this class are underdoped samples of high-T_c SC [3]. Recently, various experiments ranging from finite-frequency conductivity [4,5], Nerst effect [6] and nonlinear magnetization [7] have been interpreted as signatures of KT phase fluctuations. Nonetheless, any effect reminiscent of the universal jump of the superfluid density at $T_{\rm KT}$, which would be the most direct probe of KT physics, failed to be observed [8-12].

Until now, the 2D-3D crossover in anisotropic layered SC has been discussed mainly within the framework of the anisotropic 3D XY model [13–17]

$$H_{XY} = -\sum_{\langle ij\rangle} J_{ij} \cos(\theta_i - \theta_j).$$
(1)

Here $\theta_{i,j}$ is the superconducting phase on two nearestneighbor sites (i, j) of a coarse-grained lattice, on the same plane $(J_{ij} = J_{ab})$ or in neighboring planes $(J_{ij} = J_c)$. The energy scales J_{ab} , J_c can be related to the measured 3D superfluid density ρ_s at T = 0 as

$$J_{ab} = \frac{\hbar^2 d\rho_s^{ab}}{4m} = \frac{\hbar^2 c^2 d}{\lambda_{ab}^2 16\pi e^2},$$
$$J_c = \frac{\hbar^2 a \rho_s^c}{4m} = \frac{\hbar^2 c^2 a}{\lambda_c^2 16\pi e^2},$$

where λ_{ab} , λ_c represent the in-plane and out-of-plane penetration depth, respectively, *m* is the electron mass, *a*

is the in-plane lattice spacing, and *d* is a transverse length scale (i.e., the interplane distance) used to define the effective 2D areal superfluid density $\rho_s^{2d} = d\rho_s$. In a 2D system vortex fluctuations drive $\rho_s^{2d}(T)$ to zero at $T_{\rm KT}$ given by (we put $\hbar = c = k_B = 1$)

$$\frac{\rho_s^{2d}(T_{\rm KT})}{m} = \frac{8}{\pi} T_{\rm KT},\tag{2}$$

where the temperature dependence of $\rho_s^{2d}(T)$ includes also the effect of other excitations, like long-wavelength phasefluctuations of the model (1) or BCS-like quasiparticles excitations [3,9,18,19]. Within the anisotropic XY model (1) a finite interlayer coupling J_c cuts off the logarithmic divergence of the in-plane vortex potential at scales $\sim a/\sqrt{\eta}$ [13], where $\eta = J_c/J_{ab}$, so that the superfluid phase persists above $T_{\rm KT}$, with T_c at most few percent larger than $T_{\rm KT}$ [14–16]. As far as the superfluid density is concerned, there is some theoretical [14] and numerical [17] evidence that even for moderate anisotropy the universal jump at $T_{\rm KT}$ is replaced by a rapid downturn of $\rho_s(T)$ at a temperature scale $T_d \simeq T_{\rm KT}$.

However, recent measurements of $\rho_s(T)$ in strongly underdoped YBa₂Cu₃O_{6+x} (YBCO) samples [11,12] (with large $\eta \sim 10^{-4}$ anisotropy [12,20]), showed that no downturn of $\rho_s(T)$ is observed at the KT temperature defined by Eq. (2), but eventually at a scale $T_d \approx T_c$ [11]. Analogously, recent measurements of the phase-fluctuations diamagnetism in underdoped Bi₂Sr₂CaCu₂O_{8+ δ} (Bi2212) [7] revealed that the phase correlation length ξ above T_c can be fitted with the typical KT law, provided that the effective KT temperature is few kelvin smaller than T_c . In both cases, by looking at the system from below or above T_c , it appears that the typical temperature scale where vortex fluctuations become relevant is always near T_c , regardless of the value (2) of the $T_{\rm KT}$ of the pure 2D case.

In this Letter we analyze the role played by the interlayer coupling and the vortex-core energy at the crossover from 2D KT to 3D superconducting behavior in layered SC. In particular, we focus on the behavior of the superfluid density below T_c and of the correlation length above T_c . We carry out a renormalization group (RG) analysis using the mapping between the thermal metal-SC KT transition in two dimensions and the quantum metal-insulator transition in the 1D sine-Gordon model [21]. Indeed, a similar model has been studied in Ref. [22] to investigate the superfluid-insulator transition in optical lattices of 1D boson chains, where the tunneling interchains amplitude plays the same role of the Josephson coupling in layered SC. We show that in the presence of a finite interlayer coupling the superfluid density looses its universal character. The jump in $\rho_s(T)$ at $T_{\rm KT}$ observed in the 2D case is replaced by a downturn curvature at a temperature T_d which depends on the vortex-core energy μ . While in XY models, where μ is fixed by the in-plane coupling J_{ab} [see Eq. (6)], $T_d \simeq T_{\rm KT}$, in the general case the ratio $T_d/T_{
m KT}$ increases as μ/J_{ab} increases. Analogously, by approaching the transition from above, the increasing of the phase-fluctuation correlation length is controlled by the scale T_d instead of the $T_{\rm KT}$ of the pure 2D system. Based on these results, we argue that the various experimental data in cuprates concerning KT behavior can be reconciled if μ is larger than the typical XY value.

Let us first recall briefly the basic features of the KT transition using the analogy with the quantum 1D sine-Gordon model [2,21], defined as

$$H_{sg} = \frac{v_s}{2\pi} \int_0^L dx \bigg[K(\partial_x \theta)^2 + \frac{1}{K} (\partial_x \phi)^2 + \frac{2g_u}{a^2} \cos(2\phi) \bigg].$$
(3)

Following standard definitions [21], θ and $\partial_x \phi$ represent two canonically conjugated variables for a 1D chain of length *L*, with $[\theta(x'), \partial_x \phi(x)] = i\pi \delta(x' - x)$, *K* is the Luttinger-liquid (LL) parameter, v_s the velocity of 1D fermions, and g_u is the strength of the sine-Gordon potential. For $g_u = 0$ the action of the model (3) can be simplified by integrating ϕ and rescaling $\tau \rightarrow v_s \tau$, so that

$$S_0 = \frac{K}{2\pi} \int dx d\tau [(\partial_x \theta)^2 + (\partial_\tau \theta)^2], \qquad (4)$$

equivalent to the gradient expansion of the model (1), with τ as the second spatial dimension. Note that in the Hamiltonian notation (3) the coefficient of the dual field is 1/K, while the rotational in-plane symmetry of the model (1) is recovered in the action (4). Besides the long-wavelength phase fluctuations present in Eq. (4), vortex configurations are possible, which require $\oint \nabla \theta = \pm 2\pi$ over a closed loop. Since ϕ is the dual field of the phase θ , a 2π kink in the field θ is generated by the operator $e^{i2\phi}$ [21], i.e., by the sine-Gordon potential in the Hamiltonian (3). The correspondence between the quantum 1D and the classical 2D system is then completed by using

$$K \equiv \frac{\pi J_{ab}}{T}, \qquad g_u \equiv y = 2\pi e^{-\beta\mu}, \tag{5}$$

where y is the vortex fugacity. In the 2D XY model (1) (with $J_c = 0$) one has a single energy scale given by J_{ab} , so that the vortex-core energy μ is given by [1,2]

$$\mu_{XY} = \pi J_{ab} \ln(2\sqrt{2}e^{\gamma}) \simeq 1.6\pi J_{ab}, \tag{6}$$

where γ is the Euler's constant. However, μ depends in general on the details of the microscopic superconducting model under consideration, so it will be taken as a *free* parameter in the following, while the value (6) will be used just for the sake of comparison with the XY model (1). It is worth noting that the limitations of the XY model as an effective phase-only model have been pointed out in Ref. [18], as far as the role of the phase-interaction terms beyond Gaussian level are concerned. The effect of the interlayer coupling J_c of Eq. (1) can be incorporated in the sine-Gordon model (3) as an interchain hopping term, so that the full Hamiltonian becomes

$$H = \sum_{m} H_{sg}[\phi_{m}, \theta_{m}] - \frac{v_{s}g_{J_{c}}}{\pi a^{2}} \sum_{m'=m\pm 1}^{m} \int_{0}^{L} dx \cos[\theta_{m} - \theta_{m'}],$$
(7)

where *m* is the chain (layer) index and $g_{J_c} \equiv \pi J_c/T$. We derived the perturbative RG equations for the couplings of the model (7) by means of the operator product expansion, in close analogy with the analysis of Ref. [22]. Under RG flow an additional coupling g_{\perp} between the phase in neighboring chains is generated

$$\frac{g_{\perp}}{2\pi} \sum_{\langle m,m'\rangle} \int dx \bigg[-K(\partial_x \theta_m)(\partial_x \theta_{m'}) + \frac{1}{K} (\partial_x \phi_m)(\partial_x \phi_{m'}) \bigg].$$
(8)

The superfluid coupling K_s is defined, as usual [17], as the second-order derivative of the free energy with respect an infinitesimal twist δ of the phase, $\partial_x \theta_m \rightarrow \partial_x \theta_m - \delta$. The interlayer term (8) contributes as $K \rightarrow K(1 - ng_{\perp})$ to the current-current coefficient, where n = 2 is the number of nearest-neighbors chains (layers). Thus, the in-plane stiffness J_s is defined as:

$$K_s = K - nKg_{\perp}, \qquad J_s = \frac{\rho_s^{2d}}{4m} = \frac{K_sT}{\pi}.$$
 (9)

The full set of RG equations for the couplings K, K_s , g_u , g_{J_c} reads

$$\frac{dK}{d\ell} = 2g_{J_c}^2 - K^2 g_u^2, \tag{10}$$

$$\frac{dg_u}{d\ell} = (2 - K)g_u,\tag{11}$$

$$\frac{dK_s}{d\ell} = -g_u^2 K_s^2,\tag{12}$$

$$\frac{dg_{J_c}}{d\ell} = \left(2 - \frac{1}{4K} - \frac{K_s}{4K^2}\right)g_{J_c},$$
(13)

with $\ell = \log(a/a_0)$, where a_0 , a are the original and RG rescaled lattice spacing, respectively. Observe that for $g_{J_{\alpha}} = 0$ the first two equations reduce to the standard ones of the KT transition [1], with a fixed point at K =2, $g_u = 0$, and K_s coincides with K. Thus, one sees that at K > 2 the g_u coupling is irrelevant, the quantum 1D system is a LL and the vortex-antivortex pairs are bound in the classical 2D system. At K < 2 the g_u term is relevant, the ϕ field is locked in a minimum of the $\cos(2\phi)$ potential and the 1D system is an insulator. In the classical case this corresponds to the proliferation of vortexes (large vortex fugacity) in the metallic phase. The physical superfluid stiffness is given [2] by the asymptotic value of the running coupling $K_s(\ell) = K(\ell)$. Thus, J_s is finite below T_{KT} , since $K(\ell)$ flows to a finite value [in particular $K(\infty) = 2$ at $T_{\rm KT}$, in accordance to Eq. (2)], and it goes to zero above the transition, since $K(\ell)$ scales to zero. The KT temperature is defined by the highest temperature where $K(\infty) = 2$, and it is given (at small g_u) by $K(T) - 2 = 2g_u(T)$, which yields $T_{\rm KT} \simeq \pi J_{ab}/2.$

As an initial value $g_{J_c} \neq 0$ is considered, the interchain (interlayer) coupling increases under RG [14–16], leading to larger values of the LL parameter $K(\ell)$ and stabilizing the metallic 1D phase. However, when the initial g_u coupling is sufficiently large the second term in the right-hand side of Eq. (10) dominates and $K(\ell)$ goes to zero, leading to the insulating 1D phase. In the classical 2D analogous case, the effects of g_{J_c} are easily readable through the behavior of K_s , which is controlled by the g_u coupling alone. Whenever $K(\ell)$ scales to large values the g_{μ} coupling is irrelevant and K_s flows to a constant; see Fig. 1. This effect guarantees the persistence of the superfluid phase in a range of temperature above $T_{\rm KT}$. Indeed, the initial decrease of $K_s(\ell)$ is cut off at a finite length scale by the interlayer coupling, which brings again $K(\ell)$ to large values and $g_{\mu}(\ell)$ to zero, giving a finite asymptotic value of $K_s(\ell)$. As the temperature increases further and the g_u term dominates, both K and K_s scale to zero, the scaling dimen-



FIG. 1 (color online). RG flow of the couplings $K(\ell)$ and $K_s(\ell)$ at various temperatures for $\mu = \mu_{XY}$ and $\eta = 10^{-4}$. Inset: critical temperature T_c as a function of η for a bare stiffness $J_0(T) = J_{ab}(1 - T/4J_{ab})$ (see text).

sion of g_{J_c} becomes negative and one observes a "layer decoupling" above T_c [15,16].

The critical temperature T_c is defined by the vanishing of the $K_s(\ell \to \infty)$. Alternatively, to account for the perturbative character of the RG equations, one can compute J_s by stopping the RG flow at the scale ℓ^* where g_{J_c} is of order one [23]. The two definitions are equivalent, and lead to the estimate of the critical temperature T_c reported in the inset of Fig. 1. For the sake of completeness, we also added a temperature dependence of the bare couplings, using $J_0(T) = J_{ab}(1 - T/4J_{ab})$, as due to long-wavelength phase fluctuations in the XY model (1) [17,18], and we keep the ratios $\eta = J_c/J_{ab}$ and μ/J_{ab} fixed. For $\mu = \mu_{XY}$ the calculated values of T_c/J_{ab} show a remarkable quantitative agreement with Monte Carlo simulations on the anisotropic XY model [17]. The fact that larger values of μ lead to a larger critical temperature has a direct counterpart on the temperature dependence of the superfluid stiffness $J_s(T)$, as we show in Fig. 2. As one can see, when $J_c = 0$ we recover the standard jump of J_s at $T_{\rm KT}$, which is easily identified as the temperature where the curve $J_s(T)$ intersects the line $2T/\pi$, according to Eqs. (2) and (9) above. As μ increases the g_u coupling decreases, and the renormalization of $J_s(T)$ with respect to $J_0(T)$ below $T_{\rm KT}$ becomes negligible. As soon as a finite interlayer coupling is switched on, the jump of $J_s(T)$ at $T_{\rm KT}$ disappears and it is replaced by a rapid bending of $J_s(T)$ at some temperature T_d . However, while for $\mu \leq \mu_{XY} T_d$ coincides essentially with $T_{\rm KT}$, for a larger vortex-core energy T_d rapidly increases and approaches the temperature T_c estimated above.

These results offer a possible interpretation of the experiments in underdoped YBCO [12], where $\eta \sim 10^{-4}$ [20], but the measured $J_s(T)$ goes smoothly across the $T_{\rm KT}$ estimated from Eq. (2). We calculated $J_s(T)$ as done



FIG. 2 (color online). Temperature dependence of $J_s(T)$ in two dimensions (lines) and in the layered 3D case (symbols). Here $J_0(T) = J_{ab}(1 - T/4J_{ab})$. The $T_{\rm KT}$ is identified by the intersection between $J_s(T)$ and the straight line $2T/\pi$. The results for $\mu \leq \mu_{XY}$ show a rapid downturn of $J_s(T)$ at $T_d \approx T_{\rm KT}$. As μ increases T_d increases as well, so that at $T_{\rm KT}$ no effect is observed in $J_s(T)$ reminiscent of the jump present in two dimensions.



FIG. 3 (color online). Correlation length above T_c for different values of η and μ . Each curve stops at T_c , which increases as η increases. We take $J_0(T) = J_{ab}(1 - T/T_{\rm MF})$, with $J_{ab} = 300$ K and $T_{\rm MF} = 100$ K, as appropriate for Bi221 [8]. The dashed line is $\xi \sim e^{\beta\mu(T)/2}$, expected to hold far above T_c . The solid lines are fit with the KT functional form (see text), with $T_d = T_{\rm KT}$, c = 0.25, b = 0.9 for $\mu = \mu_{XY}$, and $T_d = 86.8$ K, c = 0.4, b = 1.21 for $\mu = 3\mu_{XY}$.

in Fig. 2 (taking into account also the measured linear depletion at low T [24]). Using a large vortex-core energy, i.e., $\mu = 6\mu_{XY}$, we found that $J_s(T)$ shows no signature of a rapid downturn at $T_{\rm KT}$, and goes to zero near to the measured T_c . Observe that we did not consider the effects of disorder, which can also smear out the KT transition, as measurements in thin films [4,25] could suggest.

A similar separation between $T_{\rm KT}$ and T_d is observed in the behavior of the correlation length above T_c . Since the quantity experimentally accessible is the vortex density n_V , given at the RG scale $\ell = \ln(a/a_0)$ by $n_V(\ell) =$ $e^{-\beta\mu(\ell)}/a^2 = g_u(\ell)/(2\pi a^2)$, we define the correlation length ξ as $\xi^{-2} \equiv n_V(\ell_s)$, where $a_s = a_0 e^{\ell_s}$ is the length scale where $K_s(\ell_s)$ vanishes above T_c . The behavior of $\xi(T)$ for different values of μ and η is reported in Fig. 3, using parameter values appropriate for Bi2212 compounds. Far above $T_c \ a_s \approx a_0$, so that ξ scales as $a_0/\sqrt{g_u(T)/2\pi}$, as shown by the dashed line. As T approaches T_c ℓ_s increases and ξ shows the exponential increase reminiscent of the KT behavior in two dimensions [1]. However, while in two dimensions, ξ diverges at $T_{\rm KT}$, a finite J_c cuts off at T_c the increasing of ξ , since below $T_c g_u$ becomes irrelevant and K_s flows to a finite value. Nonetheless, the behavior of ξ above T_c is still reminiscent of the KT behavior, $\xi_{\rm KT} \sim a_0 c \times$ $\exp(b/\sqrt{T/T_d-1})$, with c, b of order one, provided that $T_{\rm KT}$ is replaced by a proper scale T_d slightly smaller than T_c . Once again, while for $\mu = \mu_{XY} T_d \sim T_{\text{KT}}$, as the vortex-core energy increases T_d becomes significantly larger than T_{KT} and approaches T_c . This behavior is consistent with recent experiments in Bi2212 compounds [7].

In summary, we analyzed the phase-fluctuations contribution to the 2D KT-3D crossover in strongly anisotropic layered SC. Using a RG approach, we showed that a finite interlayer coupling can shift the temperature scale T_d of vortex unbinding away from the KT temperature $T_{\rm KT}$ of the pure 2D case. Indeed, T_d is essentially controlled by the vortex-core energy, and it coincides with $T_{\rm KT}$ only when $\mu \leq \mu_{XY}$, as within the standard XY model (1). When applied to cuprates, our findings suggest that in these systems μ is definitively larger than expected in the XY model, even though still of order of the in-plane stiffness. The consequences are twofold. First, the lack of any signature of KT behavior in $J_s(T)$ at $T_{\rm KT}$ does not rule out the possibility that phase fluctuation effects play a role in these systems. Second, $\mu > \mu_{XY}$ is not inconsistent with microscopic theories which associated μ to the energy scale of the superfluid stiffness instead of that of the superconducting gap, which would be far too large compared to J_s in underdoped samples [3].

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