## Berezinskii-Kosterlitz-Thouless Paired Phase in Coupled XY Models

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We study the effect of a linear tunneling coupling between two-dimensional systems, each separately exhibiting the topological Berezinskii-Kosterlitz-Thouless (BKT) transition. In the uncoupled limit, there are two phases: one where the one-body correlation functions are algebraically decaying and the other with exponential decay. When the linear coupling is turned on, a third BKT-paired phase emerges, in which one-body correlations are exponentially decaying, while two-body correlation functions exhibit power-law decay. We perform numerical simulations in the paradigmatic case of two coupled *XY* models at finite temperature, finding evidences that for any finite value of the interlayer coupling, the BKT-paired phase is present. We provide a picture of the phase diagram using a renormalization group approach.

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An ample variety of physical properties and phenomena emerge when two many-body systems are coupled. There are, of course, different ways of coupling interacting systems, depending on the geometry of the uncoupled systems, on the relevant degrees of freedom and on the way in which the coupling is established. One of them is the socalled weak coupling, when the Hamiltonian term modeling the coupling is a perturbation with respect to the uncoupled Hamiltonians. In this case, if the two systems are separately described by a macroscopic wave functionsuch as superfluids or superconductors—a relative phase between them emerges, as one can see in the Josephson effect between superconductors [1,2], Helium containers [3,4], Bose-Einstein condensates [5,6], and ultracold fermions [7]. In these cases, the microscopic details of the coupling enter only in the Josephson energy ruling the maximum current that can flow through the junction. coupling two superfluids generally gives rise to a dissipationless drag current that is often referred to as the Andreev-Bashkin effect [8]. Previous investigations [9-11] have mainly focused on the three-dimensional (3D) case, where strong enough drag densities have been found to modify the order of the symmetry breaking transition [12].

When the coupling is no longer a perturbation, one can expect that the bulk properties of the uncoupled systems are significantly altered and that new phases may emerge. A typical phenomenon induced by a strong coupling is that the order in the systems is substituted by a phase between them, therefore giving rise to an order parameter expressed in terms of operators of both systems. Several different examples of couplings exist. Among the simplest instances, one can imagine taking two one-dimensional systems and couple them lengthwise, thus creating a ladder geometry. Examples of this kind of coupling include magnetic spin ladders, where two quantum spin chains are put in a ladder geometry; see, e.g., Refs. [13,14]. The bilayer structure, in which two two-dimensional (2D) systems are coupled, is also a paradigmatic configuration, which has been studied in numerous physical systems, ranging from graphene [15] to quantum Hall systems [16] and dipolar models [17]. The bilayer configuration is of particular relevance because it may refer to two quantum or classical systems at finite temperature, or-via the quantum-classical correspondence -to the ladder geometry in which two quantum onedimensional models at zero temperature are coupled.

In this Letter, we address the emergence of a paired phase when two models exhibiting a topological phase transition are coupled. We will refer to the Berezinskii-Kosterlitz-Thouless (BKT) universality class [18] and study the effect of the coupling of two BKT systems. We have two main motivations for our study. First, the BKT transition is not characterized by a local order parameter and by the conventional spontaneous symmetry breaking. Rather, one can locate the critical point in which the system becomes superfluid by looking at the correlation functions, exhibiting a power law (exponential) decay in (outside) the superfluid phase. BKT transitions have been observed in several different 2D physical systems, including superfluid Helium [19], superconducting films and arrays [20,21], as well as bosonic [22,23] and fermionic [24] ultracold systems.

The second motivation is related to the presence and relevance of the coupling between 2D systems in a variety of experimental systems, ranging from layered superconductors [25,26] 2D two-component mixtures [11] and 2D ultracold gases [27]. In the latter case, a single 2D ultracold system is obtained by means of a suitably large transverse confinement: for instance, one can realize a 2D geometry by confining the atoms in a well of an optical lattice along the transverse direction, the transverse confinement frequency increasing with the power laser, with  $\gtrsim 1-10$  kHz [28]. When only two adjacent minima of the vertical lattice are left significantly populated, one would have two 2D ultracold gases with tunable interlayer coupling. In this way, one would study the effect of the bilayer coupling on the 2D physics already observed in single layers [22–24]. Notice that in this case, the coupling is (for bosons) of the form  $b_1^{\dagger}b_2$  (where  $b_{\alpha}$  creates a particle in the  $\alpha$  layer), thereby corresponding to what we refer to as linear coupling.

Despite the rising interest of the theoretical community in low dimensional binary mixtures [29–32], the influence of interspecies coupling on universal behavior remains largely unknown. In this context, a compelling question is (i) "What is the fate of the quasi-long-range order in the presence of a strong coupling between two BKT systems?". One may as well ask (ii) "Does quasi order occur in the mixed correlators of the coupled system? If so, does it appear already at small couplings?" Previous attempts to answer these questions mainly focused on the study of effective models for coupled topological excitations, such as the coupled sine-Gordon models [33] and the coupled Coulomb gases [34], evidencing the emergence of a composite vortex gas phase as well as a second-order phase transition at strong coupling. However, the results of these investigations cannot be directly applied to our case, since the low energy equivalence between coupled twodimensional superfluids and coupled topological defect gases may be by the presence of the bilayer coupling term.

To address the questions above, we consider the paradigmatic case of two coupled XY models at finite temperature, based on the expectation that similar features emerge for other classical and quantum models in the XY universality class when linearly coupled. The paradigmatic nature of the XY model results in longly certified numerical tools, which allow us to reliably investigate the bilayer case.

*The model.*—The bilayer *XY* Hamiltonian can be written as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos\left(\phi_i - \phi_j\right) - J \sum_{\langle ij \rangle} \cos\left(\psi_i - \psi_j\right) + K \sum_i \cos\left(\phi_i - \psi_i\right), \tag{1}$$

where  $S_i = (\cos \phi_i, \sin \phi_i)$  and  $T_i = (\cos \psi_i, \sin \psi_i)$  are the XY spins with n = 2 components defined on the first and the second layer, respectively, each being a 2D system. We will also use the notation  $S_i = e^{i\phi_i}$  and  $T_i = e^{i\psi_i}$ . Notice that we are considering the symmetric case where the intralayer coupling takes the same value J on both layers. The critical line separating the region with power law correlations from the one with exponential correlations in model (1) has been studied in literature [35]. Moreover, several properties of coupled and layered XY models and two-component systems have also been investigated [29,36–40], as well as coupled 3D XY models [41,42]. Here our focus is on the quasiorder for pairs of spins on different layers arising in a 2D bilayer system.

When K = 0, the two layers are decoupled and the behavior of the model is that of the standard 2D XY model [11,18]: a superfluid phase and the normal state are separated by the BKT transition occurring at  $T_{\rm BKT} \approx 0.893J$  [43–47]. The normal state is characterized by the exponential decay of the phase-phase correlator; in the superfluid phase, on the other hand, one finds the peculiar algebraic decay of correlations functions.

In the other limiting case,  $K \to \infty$ , the spins on the upper and lower layers are constrained to be parallel, i.e.,  $\phi_i = \psi_i \forall i$ , so that the effective Hamiltonian reduces, up to additive constants, to

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \cos{(\phi_i - \phi_j)}, \qquad (2)$$

i.e., that of a 2D XY model with coupling constant J' = 2J, therefore with critical temperature  $T'_{BKT} \approx 1.786J$ .

Results for the phase diagram.-We want to study the full phase diagram of the model, away from the two limiting cases just analyzed. From the theory of bilayer systems and two-component mixtures [11,48] one may expect that, apart from the normal and superfluid phases of the BKT transition, a phase involving variables (operators in the quantum case) of both layers can emerge. The question is whether it emerges only for large values of the coupling K or not. To make a comparison with a similar, yet different, analytically solvable case, let us consider the square lattice Ashkin-Teller model [49]. The Hamiltonian has a form similar to Eq. (1),  $H_{AT} = -J \sum_{\langle ij \rangle} s_i s_j J \sum_{\langle ij \rangle} t_i t_j - K \sum_{\langle ij \rangle} s_i s_j t_i t_j$ , with  $s_i$ ,  $t_i = \pm 1$ . The model has indeed a phase whose order parameter is  $\langle st \rangle$  [49]. However, apart from the fact that spin variables are discrete in the Askhin-Teller model and continuous in the bilayer XY model, there are two remarkable differences: first, the coupling is quartic for the former; second, the bilayer XY



FIG. 1.  $\beta J - \beta K$  phase diagram, showing the paired phase *C* appearing for finite values of  $\beta K$ . Left panel: Monte Carlo results (L = 64) obtained from the fit of correlation functions c(k) and z(k) as described in the text. The lower line has been obtained using the PCC technique, as in the next panel, while the upper line guides the eye. Middle panel: Monte Carlo results (L = 64) obtained through the PCC technique, allowing the Kasteleyn-Fortuin clusters to extend on a single layer only (upper red line) or on both layers (lower red line). Right panel: RG phase diagram; see main text.

model exhibits quasiorder and no spontaneous symmetry breaking at finite temperature.

To determine the full phase diagram of the bilayer *XY* model, we perform Monte Carlo (MC) simulations of the Hamiltonian of Eq. (1) on a  $2 \times L \times L$  lattice, *L* being the linear dimension of each layer. We vary  $\beta J$  and  $\beta K$ , where as usual  $\beta = (k_B T)^{-1}$ . Monte Carlo updates use the Swendsen-Wang algorithm [45,50] after embedded cluster decomposition [51]. We sample the following correlation functions

$$c_{\uparrow}(k) = \sum_{|i-j|=k} \exp(i\phi_i - i\phi_j), \qquad (3)$$

$$c_{\downarrow}(k) = \sum_{|i-j|=k} \exp(i\psi_i - i\psi_j), \qquad (4)$$

$$z(k) = \sum_{|i-j|=k} \exp(i\phi_i + i\psi_i - i\phi_j - i\psi_j), \qquad (5)$$

where the summations extend over all *i*, *j* pairs separated by *k* lattice sites along the *x* or *y* direction. Because of the symmetry of the system upon exchange between the upper and lower layers,  $c_{\uparrow}(k)$  and  $c_{\downarrow}(k)$  coincide across the whole phase diagram, let us call them c(k). All correlation functions are well fitted by the function  $Q(r) = (r/r_{alg})^{\alpha} \exp(-r/r_{exp})$ , where  $r_{alg}$  is the characteristic length associated to the algebraic decay and  $r_{exp}$  is the characteristic length associated to the exponential decay.

To tell apart the exponential and algebraic behavior, we compare  $r_{exp}$  with L, the linear system size used in the MC simulation, using the following qualitative criterion: if  $r_{exp}$  is smaller than L/10, then we mark the decay as exponential, otherwise it is marked as algebraic, since the exponential characteristic length  $r_{exp}$  is neglectable when compared to the dimensions of the system being studied.

This allows us to obtain the phase diagram shown in Fig. 1(a), identifying the three phases. We denote by A the usual superfluid BKT phase, characterized by the algebraic decay of c(k) [52]. The correlation function z(k) is also found to be algebraically decaying in the A phase. The normal phase, denoted by B, is characterized, as usual, by the exponential decay of c(k). We checked that in the B phase z(k) is exponentially decaying, as well. Finally, we observe a third C phase, that is instead characterized by the exponential decay of c(k) and the algebraic decay of z(k). Notice that, within the precision we can achieve, for small values of K one always has a range of values of J for which there is the C phase. In other words, the C phase extends up to vanishing values of K.

We dub the C phase BKT-paired phase, since each layer has the one-body correlation function c(k) decaying exponentially, while the two-body correlation function z(k) has an algebraic behavior. Since z(k) is the correlation function between  $S_iT_i$  and  $S_jT_j$  for *i* and *j* far apart from each other, this is related to a quasi-long-range order for the pair variables  $S_iT_i$  in the different sites of the bilayer system. The phase transition between A and C appears to be a conventional BKT line and in agreement with Ref. [35]. It is worth noting that despite some similarities between the phase diagram presented in Fig. 1 and the one discussed in Ref. [33], we find no trace of any actual symmetry breaking while our paired BKT phase appears also at infinitely small coupling strength. Moreover, to the best of our knowledge, the presence of power law four point correlations was not investigated in previous studies.

To further numerically investigate these two transition lines, we resort to probability-changing cluster (PCC) algorithm, introduced in Ref. [45] for the single-layer BKT transition. Following the approach therein, at first the *XY* variables are mapped onto two Ising models, using Wolff's embedded cluster formalism [51]. Subsequently, the temperature of the system is tuned in progressively smaller increments, looking for the 1/2 percolation threshold of the Kasteleyn-Fortuin clusters defined from each Ising model [45], signaling the BKT transition. It can in fact be shown [53,54] that the spin-spin correlation function  $\langle S_i S_j \rangle$  equals  $p_{ii}$ , the probability that the site *i* and *j* belong to the Kasteleyn-Fortuin same cluster, effectively linking the presence of a percolating cluster spanning the whole system to the onset of quasi-long-range order. In the present case, one can identify two different critical lines through the 1/2 percolation threshold criterion, depending on whether the clusters by which percolation is identified are allowed to extend on a single layer or on both layers, respectively. The results we obtain, shown in Fig. 1(b), are compatible with the identification of the A, B, and C phases obtained by the study of correlation functions. We now supplement this analysis by a RG calculation.

*RG approach.*—Mermin-Wagner theorem [55] forbids spontaneous breaking of continuous symmetries in two dimensions and, thus, only quasi-order, characterized by power law correlations, can arise in our model. Such effect can be described by RG theory via the explicit introduction of topological defects [18,56]. Even the functional RG approach [57,58], which overcomes the traditional perturbative methods [59–61], does not completely describe the BKT transition [62]. Nevertheless, a novel technique has been recently devised in order to allow nonperturbative treatment of quasi-order [63].

We shall now employ a simplified version of this approach to the bilayer case, showing how it is possible to provide an estimate for the MC phase diagram. First of all, we are going to derive the mean field solution of our problem; then we are going to use it to compute the effective spin stiffness in the low temperature phase, which will serve as the initial condition of the traditional BKT flow equations [64,65]. Finally, solving the BKT flow equations with the MF initial condition, we will be able to locate the vortex unbinding transition.

Within our framework, it is convenient to employ a Hubbard-Stratonovich transformation [20,66,67], in order to introduce the continuous field representation of the bilayer model under study. Following this procedure, the bilayer XY model can be mapped into two coupled complex  $|\varphi|^4$  theories, whose action reads,

$$S[\phi] = \frac{1}{2} \sum_{\sigma,q} \frac{\varphi_{\sigma}(q)\varphi_{\sigma}(q)}{K^{\sigma}(q)} + \sum_{l} \int U(|\varphi_{l}|) d^{2}x, \quad (6)$$

where  $U(|\varphi|) = \log(I_0(|\varphi|))$  is the local potential of the model, written in terms of the zeroth order Bessel function  $I_0$ , and  $K^{\sigma}(q) = 2J\varepsilon_0(q) + 2\mu + \sigma 2K$  the momentum space couplings, apart for a multiplicative  $\beta$  factor. The index  $l \in \{1, 2\}$  labels two different complex fields, which represent the spin variables in the two different layers, while  $\sigma \in +, -$  labels the symmetric and antisymmetric

combinations of these fields  $\varphi_{\pm}(q) = [\varphi_1(q) \pm \varphi_2(q)]/\sqrt{2}$ . The coefficient  $\mu$  has to be introduced in order to have a positively defined exchange matrix, as needed in the Hubbard-Stratonovich transformation [66].

In the following, we are going to only consider the continuum limit of the action in Eq. (6), discarding lattice effects. This leads to a spurious  $\mu$  dependence in our treatment [63,66,68], which is solved by fixing  $\mu = K$  in agreement with the optimal choice discussed in [63]. Imposing the vanishing of each of the two effective modes  $\varphi_{\pm}$  masses  $\mu_{\pm} = [1/K^{\pm}(0) - 1/2]$ , one obtains, respectively, the lower and the upper phase boundaries in Fig. 1(c).

Above each boundary one of the effective modes acquires a finite expectation value which can be obtained solving the saddle point equation

$$0 = \frac{\partial S[\varphi]}{\partial \varphi_{\pm}}\Big|_{\varphi = \text{const}},\tag{7}$$

where  $S[\varphi]$  is defined in Eq. (6). The field density is defined according to  $\rho_{\text{MF},\sigma} = |\varphi_{\text{MF},\sigma}|^2$ , where  $\varphi_{\text{MF},\sigma}$  is the constant solution of the saddle point expression in Eq. (7).

As anticipated, the low energy behavior of the model cannot be described simply considering the static MF solution, which provides an unphysical symmetry breaking scenario. In order to account for vortex fluctuations, we consider the continuum limit expression of the action in Eq. (6),

$$S_c[\varphi] = \sum_{\sigma} \int d^2x \frac{|\nabla \varphi_{\sigma}(x)|^2}{2m_{\sigma}} + \text{local terms}, \quad (8)$$

where  $m_{\pm}^{-1} = [J/K^{\pm}(0)^2]$ . Introducing the Madelung representation  $\varphi_{\sigma} = \sqrt{\rho_{\sigma}} e^{i\theta_{\sigma}(x)}$  and assuming that the field density remains frozen at the MF expectation  $\rho_{\sigma} = \rho_{\text{MF},\sigma}$ , we obtain the phase only action [63]

$$S[\theta] = \sum_{\sigma} \int d^2 x \frac{\rho_{\sigma}}{2m_{\sigma}} \partial_{\mu} \theta_{\sigma} \partial_{\mu} \theta_{\sigma}, \qquad (9)$$

which features two independent BKT transitions, one for each phase variable [69].

The physics of these transitions only depends on the effective phase stiffness  $\rho_{\sigma}/2m_{\sigma}$  which remains finite above the MF phase boundaries, where  $\rho_{\sigma} > 0$ . Therefore, in the trivial MF phase J < 1 both the effective phase stiffnesses vanish, leading to exponentially decaying correlations, while for 1 < J < 1 + 2K (J > 1 + 2K) the effective stiffness of the  $\theta_{+}$  ( $\theta_{-}$ ) phase becomes finite and its renormalization by vortex fluctuations shall be described by the BKT flow equations

$$k\partial_k K_k = -\pi g_k^2 K_k^2, \tag{10}$$

$$k\partial_k g_k = \pi \left(\frac{2}{\pi} - K_k\right) g_k,\tag{11}$$

where the RG scale k denotes the maximum wavelength of the fluctuations integrated by the flow and one has to assume a UV regularization at a microscopic scale  $k = \Lambda$  [64]. At  $k = \Lambda$  one has to use the MF expectations obtained solving the saddle point Eq. (7) to compute the initial conditions  $K_{\Lambda} = J_{\text{eff}}^{\sigma}$ , and  $g_{\Lambda} = 2\pi e^{-\pi^2 K_{\Lambda}/2}$  where  $J_{\text{eff}}^{\sigma} = \rho_{\text{MF},\sigma}/2m_{\sigma}$ . The theoretical prediction for the two BKT transition line was reported in panel (b) of Fig. 1. The upper transition line, which corresponds to the conventional BKT transition. comes from the unbinding of the  $\theta_{-}$  vortices. Such phase boundary appears to be flat at our approximation level since we solve Eq. (7) separately for  $\varphi_{\rm MF,-}$  posing  $\varphi_{\rm MF,+} = 0$ , due to the difficulties encountered in solving the two coupled equations for the expectation values. On the other hand, the K dependence of the lower transition line is only due to the explicit K dependence in the  $m_+$  factor and it is in good agreement with the MC prediction.

Finally, we should compare our results with the corresponding results for two linearly coupled Ising models. Denoting by  $S_i$  and  $T_i$  the spins in the two layers, a phase with order parameter  $\langle ST \rangle \neq 0$  cannot exist (in the paramagnetic phase with  $\langle S \rangle = \langle T \rangle = 0$ ). The same is occurring for the two linear coupled XY models treated in this Letter; i.e., there is no phase with order parameter  $\langle \cos(\phi + \psi) \rangle$ , in agreement with the Mermin-Wagner theorem. What is present is indeed a BKT of the pairs, specific of coupled *two-dimensional* systems with O(2) symmetry, not contradicting the previous result.

Conclusions.-We investigated the occurrence of a BKTpaired phase in coupled XY models, corresponding to an exponential (algebraic) decay for the one-body (two-body) correlation functions. We found that the third phase is present even for very small linear couplings between the layers, within the precision of our simulations. Furthermore, we presented an RG treatment which was found to be in agreement with the aforementioned results. Our investigation calls for a more systematic study of finite sizescaling effects in the J - K phase diagram such as, e.g., precision studies [46,47] at larger lattice sizes of points belonging to the C phase of Fig. 1(a). Experiments with coupled 2D ultracold gases are performed on lattices with a linear size of tens up to a few hundreds of lattices sites, therefore motivating the study of the presence of the BKTpaired phase in realistic setups.

Furthermore, an exciting perspective is represented by a comparison of the present results with the ones obtained for other types of couplings, such as quartic ones, and to consider the case of different J's in the layer. A systematic analysis for small K done at larger sizes would also be important in clarifying whether the critical value for the presence of the BKT transition is zero as the RG approach seems to suggest. Moreover, we think as well that it would

be a deserving subject of future investigations to further analyze the order to quasi-order transition between phases B and C of Fig. 1. Finally, we mention that an interesting perspective is represented by the comparison of our results with analytical findings from suitably derived theories where two sine-Gordon models are coupled in a way fixed by the microscopic coupling.

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