

Berezinskii-Kosterlitz-Thouless Phase Transitions with Long-Range Couplings

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The Berezinskii-Kosterlitz-Thouless (BKT) transition is the paradigmatic example of a topological phase transition without symmetry breaking, where a quasicrystalline phase, characterized by a power-law scaling of the correlation functions at low temperature, is disrupted by the proliferation of topological excitations above the critical temperature T_{BKT} . In this Letter, we consider the effect of long-range decaying couplings $\sim r^{-2-\sigma}$ on the BKT transition. After pointing out the relevance of this nontrivial problem, we discuss the phase diagram, which is far richer than the corresponding short-range one. It features—for $7/4 < \sigma < 2$ —a quasicrystalline phase in a finite temperature range $T_c < T < T_{\text{BKT}}$, which occurs between a symmetry broken phase for $T < T_c$ and a disordered phase for $T > T_{\text{BKT}}$. The transition temperature T_c displays unique universal features quite different from those of the traditional, short-range XY model. Given the universal nature of our findings, they may be observed in current experimental realizations in 2D atomic, molecular, and optical quantum systems.

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Two-dimensional interacting systems are well known not to display conventional symmetry-breaking transitions at finite temperature, due to the Hohenberg-Mermin-Wagner theorem [1]. Yet, a phase transition may appear driven by topological defects, according to the celebrated Berezinskii-Kosterlitz-Thouless (BKT) mechanism [2]. In the presence of long-range interactions, the Hohenberg-Mermin-Wagner theorem no longer holds and local order parameters, such as the magnetization [3], may have a nonzero expectation value. The question addressed by this Letter is the fate of the BKT transition when the range of the interactions is increased.

Sak's criterion [4] provides a general argument for understanding whether the long-range, power-law coupling $\sim 1/r^{d+\sigma}$ in the classical $O(N)$ model affects criticality. It can be formulated as follows: at low momenta, the short-range (SR) and long-range (LR) critical scaling of momentum space propagators behave as

$$p^{-2+\eta_{\text{SR}}} \quad \text{vs} \quad p^{-\sigma}, \quad (1)$$

respectively, where η_{SR} is the anomalous dimension of the SR limit. Therefore, one can define a critical value of the

range of the interactions, $\sigma_* = 2 - \eta_{\text{SR}}$, such that, for $\sigma > \sigma_*$, the critical behavior is not affected by the presence of LR interactions. The validity of Sak's criterion for the classical $O(N)$ models has been the subject of considerable scrutiny. Indeed, numerical evidences supporting (or rejecting) Sak's result are notoriously hard to obtain [5–7]. Intense theoretical investigations both via Monte Carlo (MC) simulations [5,8,9], renormalization group (RG) theory [10–12], and conformal bootstrap [13] appeared all to confirm the validity of Sak's conjecture for the LR-SR crossover; so it is fair to conclude that the criterion has been a useful tool to understand the critical behavior of LR interacting systems [14–17]. The criterion is believed to apply to all symmetry-breaking transitions in $d \geq 2$. The status of the $d = 2$ classical XY model, however, is rather different, and only few results (later commented) are known. The main reasons are as follows: (i) Sak's criterion cannot be straightforwardly applied, since in the SR limit the critical behavior is not described by a single RG fixed point, but rather by a whole line of fixed points with a temperature-dependent exponent η_{SR} . (ii) Numerically, the

large number of nonvanishing couplings, coming from the LR nature of the interaction, along with the logarithmic scaling typical of 2D systems (the so-called “Texas state argument” [18]) make the study of the 2D XY universality notoriously challenging.

(iii) In the nearest-neighbor 2D XY model, the classical treatment takes advantage of the duality construction [19], through which one can famously relate the model to the Coulomb gas [20,21] or the sine-Gordon model [21,22]. However, this is no longer the case already for next-to-nearest-neighbors couplings.

(iv) It is known that, in the SR limit, the physics of the 2D classical XY model can be related to the one of the 1D quantum XXZ model via its transfer matrix [23]. This approach is based on the mapping to hard-core bosons, and therefore to the XXZ model, and cannot be straightforwardly applied to the case of XY LR interactions, as one should show the RG irrelevance of terms violating the hard-core condition. Moreover, let us remark that a 2D boson gas at finite temperature with (isotropic) $1/r^3$ density-density interaction does exhibit a BKT transition [24]; but this interaction corresponds to a quantum 1D XXZ in which only in the $z-z$ interaction is long range.

(v) Finally, we observe that the treatment of the SR XY model in 2D is very much simplified by the introduction of the Villain model [25,26], which can be mapped exactly onto the Coulomb gas and shares the same universality class of the SR XY model. The physical reason of their connection in the SR regime is that the (gapped) amplitude fluctuations of the corresponding $O(2)$ action are irrelevant [27]. Thus, once the periodic nature of the phase is taken care of, all the relevant information is present in the theory. However, in the LR regime, the interplay between amplitude and phase fluctuations cannot be neglected and it is not known whether they still share the same universality class.

Despite these difficulties, the study of the LR XY model is of great interest. Indeed, since its introduction, the BKT mechanism [28–31] has been found to quantitatively describe the universal scaling appearing in several 2D systems with $U(1)$ symmetry, ranging from thin ^4He films [32] to quasi-2D layered superconductors [33–37], exciton-polariton systems [38], cold atoms in 2D traps [39,40], and 2D electron gases at the interface between insulating oxides in artificial heterostructures [41–43]. Apart from these experimental realizations, topological defects are expected to be relevant in several natural phenomena outside the condensed matter realm, such as DNA tangling or stripe formation [44–46]. To understand how σ_* is modified is then a crucial question in all the cases in which a LR tail of the interaction can be added or tuned, especially because the spin-wave interaction term, already present in the SR case, may destroy, partially or totally, the topological nature of the phase transition. Moreover, the physics of LR interacting systems has recently experienced a new wave of interest, due to the current experimental realizations

on atomic, molecular, and optical (AMO) systems. In particular, trapped ions [47,48], Rydberg gases [49], and optical cavities [50,51] allowed the observation of plenty of exotic equilibrium and dynamical phenomena induced by LR interactions, including entanglement and correlations propagation [52,53], dynamical phase transitions [54,55], time crystals [54,56,57], and defect scaling [58,59]. These experimental results stimulated an impressive theoretical activity to characterize the equilibrium and dynamical critical scaling induced by LR interactions in a wide variety of different systems [17,60–65]. Despite this outpouring theoretical activity and the long-standing relation between topological scaling and LR interactions, the possible corrections induced by power-law decaying couplings to the topological BKT scaling remain an open question, testable in experiments.

Model and preliminaries.—We consider a system of planar rotators on a 2D lattice of spacing a , described by the Hamiltonian

$$\beta H = \frac{1}{2} \sum_{\mathbf{i}, \mathbf{j}} J_{|\mathbf{i}-\mathbf{j}|} [1 - \cos(\theta_{\mathbf{j}} - \theta_{\mathbf{i}})], \quad (2)$$

where $\mathbf{i}, \mathbf{j} \in \mathbb{Z}^2$ and $J_{|\mathbf{i}-\mathbf{j}|}$ has a power-law tail: $J_{|\mathbf{i}-\mathbf{j}|} \sim [g/(|\mathbf{i}-\mathbf{j}|^{2+\sigma})]$ for $|\mathbf{i}-\mathbf{j}| \gg 1$. The exponent σ is assumed positive in order to ensure additivity of the thermodynamic quantities [66]. For the following arguments, the specific form of the couplings is not important, as long as there are no frustration effects nor competing interactions.

Let us now summarize what we do know for sure about the LR XY model (2): (a) For $\sigma < 2$, at low enough temperatures, the system magnetizes, as rigorously proven in [3]. MC simulations at $\sigma = 1$ indicate an order-disorder transition and no BKT phase at finite temperature [67]. Moreover, for $\sigma \leq 1$ the critical exponents of the ferropar-amagnetic transition are expected to be mean field [11]. (b) In agreement with (a), the spin-wave theory in which the cosine is expanded to the quadratic order, *without* imposing the periodicity, as in the original Berezinskii calculation [28], does also magnetize for $\sigma < 2$, since the contribution of the spin fluctuations is of the form $\int d^2q/q^\sigma$ and thus infrared finite. (c) An upper bound for σ_* has to be $\sigma_* = 2$, i.e., for sure there is BKT for $\sigma > 2$, as one can deduce even from Sak’s argument, since η is positive. This result is supported by the self-consistent harmonic calculation recently presented in [68], which anyway is unable to make even qualitative predictions for $\sigma < 2$.

Effective model.—We decompose the coupling as $J_{|\mathbf{i}-\mathbf{j}|} = J_{|\mathbf{i}-\mathbf{j}|}^S + g|\mathbf{i}-\mathbf{j}|^{-(2+\sigma)}$, where J^S is a SR term taking into account the small-distance behavior of the coupling. At low temperatures, the spin direction varies smoothly from site to site and, as a consequence, we can expand the SR term for small phase differences as $\cos[\theta(\mathbf{x} + \mathbf{r}) - \theta(\mathbf{x})] \sim 1 - |\nabla\theta|^2/2$. The same, however, it is not automatically true for the LR term, since far-away pairs, whose phase

difference is not necessarily small, give a significant contribution to the Hamiltonian.

These considerations allow us to write a continuous version of the Hamiltonian in Eq. (2) in terms of the field $\theta(\mathbf{x})$, namely, the Euclidean action

$$S[\theta] = \frac{J}{2} \int d^2x |\nabla\theta|^2 + S_{\text{LR}}, \quad (3)$$

where the LR part can be written as

$$S_{\text{LR}} = -\frac{g}{2\gamma_{2,\sigma}} \int d^2x (\cos\theta \nabla^\sigma \cos\theta + \sin\theta \nabla^\sigma \sin\theta), \quad (4)$$

with $\gamma_{2,\sigma} = 2^\sigma \Gamma((1+\sigma)/2) \pi^{-1} |\Gamma(-\sigma/2)|^{-1}$, by using the definition of (bulk) fractional derivative (see Supplemental Material [69]). The first and the second term in Eq. (3) account for the short- and long-range contributions, respectively, with $J \sim 1/T$ and $g \sim 1/T$ being the temperature-dependent couplings [70].

If $g = 0$, by following the usual duality procedure [26], one can take into account the periodic nature of the field θ in Eq. (3) by isolating the topological configurations and introducing the vortex fugacity $y = \exp(-\varepsilon_c)$, ε_c being the corresponding core energy. This, in turn, leads to the Kosterlitz-Thouless RG equations [26,29,30,72] (see [73,74] for textbook presentations), which feature a line of stable Gaussian fixed points for $y = 0$ and $J > 2/\pi$, describing the power-law scaling observed in the low-temperature BKT phase. For g small enough, we expect to have then a continuum theory described by the three parameters J , g , and y .

In order to explore the effects of LR interactions, we deform the traditional BKT fixed-points theory with the nonlocal operator in the second term of Eq. (3). Since only those fixed points that are stable under topological perturbation correspond to an infrared limit of the SR BKT theory, we can restrict ourselves to the region in which the topological excitations are irrelevant ($(J > 2/\pi)$). The relevance of the LR perturbation depends on the scaling dimension Δ_g of the coupling g , which is defined according to the asymptotic behavior $g_\ell \approx \exp(\Delta_g \ell)$ for $\ell \gg 1$, where as usual in the BKT literature, we put $\ell = \ln(r/a)$. On the other hand, due to the Gaussian nature of the measure,

$$\langle \cos[\theta(\mathbf{x}) - \theta(\mathbf{x}')] \rangle = e^{-\frac{1}{2}(\theta(\mathbf{x}) - \theta(\mathbf{x}'))^2} = |\mathbf{x} - \mathbf{x}'|^{-\eta_{\text{SR}}(J)}, \quad (5)$$

where $\eta_{\text{SR}}(J) = 1/2\pi J$ is the exponent of the SR two-point function [26,29,30]. Following Eq. (5), the scaling dimension of the LR term reads

$$\Delta_g = 2 - \sigma - \eta_{\text{sr}}(J), \quad (6)$$

so that the LR perturbation becomes relevant only if $\sigma < 2 - \eta_{\text{SR}}(J)$, similar to the traditional spontaneous symmetry-breaking (SSB) case [11], but with a temperature-dependent anomalous dimension. This confirms that for $\sigma > 2$ the LR perturbation is always irrelevant, as expected.

Let us now consider the case $\sigma < 2$. There, the LR perturbation becomes relevant at small temperatures, since $\eta_{\text{SR}} \simeq 0$ for $T \simeq 0$. Since η_{SR} in Eq. (6) is the one of the SR unperturbed theory, we can apply the results of the traditional BKT theory [75] as long as the LR perturbation is not relevant. In particular, we know that topologically excitations are irrelevant for $\eta_{\text{SR}} < 1/4$, so that, in the range $7/4 < \sigma < 2$, a subset of the BKT fixed points remains stable and we have quasi-long-range order (QLRO) for a certain temperature window. This result is rather nontrivial, since in SSB transitions the traditional Sak's result [4] predicts the irrelevance of LR couplings at all temperatures for $\sigma > 2 - \eta_{\text{SR}}$.

RG flow.—These results may be confirmed by deriving the flow equations for the LR term at the leading order in g for $y = 0$, obtaining [69]

$$\begin{aligned} \frac{dg_\ell}{d\ell} &= [2 - \sigma - \eta_{\text{SR}}(J_\ell)]g_\ell, \\ \frac{dJ_\ell}{d\ell} &= c_\sigma \eta_{\text{SR}}(J_\ell)g_\ell, \end{aligned} \quad (7)$$

where $c_\sigma = (\pi/2)a^{2-\sigma} \int_1^\infty du u^{1-\sigma} \mathcal{J}_0(2\pi u)$ and $\mathcal{J}_0(x)$ is the zeroth-order Bessel function of the first kind. As shown in the Supplemental Material [69], the above result is reliable as long as $a^{2-\sigma}g_\ell \ll J_\ell$ or, equivalently, as long as $dJ/d\ell \ll J_\ell$. The RG flow is depicted in Fig. 1 As expected, we see that the flow equations (7) support a line of SR fixed points $g = 0$, which becomes unstable for $\eta_{\text{SR}}(J) < 2 - \sigma$. As long as our hypothesis of small g holds, we can explicitly identify the form of the flow trajectories of Eqs. (7),

$$g_\ell(J) = \frac{\pi(2-\sigma)}{c_\sigma} [(J_\ell - J_\sigma)^2 + k], \quad (8)$$

where k is a real number and $J_\sigma = [2\pi(2-\sigma)]^{-1}$. The sign of k divides the trajectories that met the fixed point $g = 0$ and those that do not, the first ones ending at (starting from) the fixed-point line for $J \leq J_\sigma$ ($J > J_\sigma$). The separatrix corresponds to the semiparabola with $k = 0$, $J \leq J_\sigma$. For $k > 0$, $g \rightarrow \infty$, showing the existence of a new low-temperature phase, where LR interactions are relevant. The critical temperature T_c , below which this new phase appears, is such that $\eta_{\text{SR}}(J_c) > 2 - \sigma$.

Since, as in the traditional BKT calculation [29], Eqs. (7) were derived for small g and y , its use for $T < T_c$ is, in principle, not justified, since LR interactions are relevant and g_ℓ grows indefinitely. However, let us notice that the

scaling of g_ℓ with T for $T \rightarrow T_c^-$ can be reliably predicted from Eqs. (7), since in this limit the flow spends a divergent amount of RG time ℓ in the vicinity of the line of fixed points $g = 0$. This scaling is derived in the Supplemental Material [69]. Moreover, we can guess the infrared form of the action in the low-temperature phase by observing that the rigorous result of Ref. [3] implies that for $T < T_c$ the system displays finite magnetization and, then, phase fluctuations are limited even at large distances. Therefore, the expansion of the trigonometric function in Eq. (3) is justified, leading to an action of the form

$$S_g = -\frac{\bar{g}}{2} \int d^2x \theta \nabla^\sigma \theta, \quad (9)$$

where $\bar{g} = g\gamma_{2,\sigma}^{-1}$. Being the above action quadratic, the properties of this exotic low-temperature phase can be worked out: in particular, the scaling of the magnetization for $T \rightarrow T_c^-$ is found to be [69]

$$\ln m \sim -e^{B(T_c - T)^{-1/2}}, \quad (10)$$

where B is a nonuniversal constant. Since all the derivatives of m with respect to T vanish at $T = T_c$ (essential singularity), and since m is linked to the derivative of the free energy with respect to the external field, we have that the phase transition between the ordered and disordered phase is actually of infinite order. Moreover, the connected correlation functions have a power-law decay for $T < T_c$ given by $\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{0}) \rangle_c \sim r^{-2-\sigma}$, where $\mathbf{S}(\mathbf{r}) = (\cos \theta_r, \sin \theta_r)$.

We have so far assumed $y = 0$; let us now consider the effect of topological excitations. At leading order in both g and y , the two perturbations remain independent and, since the vortices contribute to the J_ℓ flow only beyond leading order in y , Eqs. (7) are unchanged. Moreover, one has $dy_\ell/d\ell = (2 - \pi J_\ell)y_\ell$ valid up to second-order terms in y_ℓ and g_ℓ . Then, in agreement with what we stated above, as long as $7/4 < \sigma < 2$, the temperature range T between T_c and T_{BKT} of the line of fixed points $g = y = 0$ remains stable under both topological and LR perturbations (see Fig. 1). In the low-temperature phase, instead, it is natural to suppose y to be irrelevant, because a non-negligible LR coupling increases the cost of highly nonlocal topological excitations. This idea is made more rigorous in the Supplemental Material [69], where the interaction energy between vortices in the low-temperature phase is computed, and it is shown that they cannot proliferate.

Summarizing, for $\sigma \in (7/4, 2)$ we find three phases: (i) an ordered phase for $T < T_c$ with finite magnetization and temperature-independent power-law correlation functions, (ii) an intermediate BKT phase for $T_c < T < T_{\text{BKT}}$, where the magnetization vanishes and the exponent of the two-point correlation function depends on T , and (iii) a disordered phase for $T > T_{\text{BKT}}$. Because of the LR character of the interactions, also the high-temperature phase

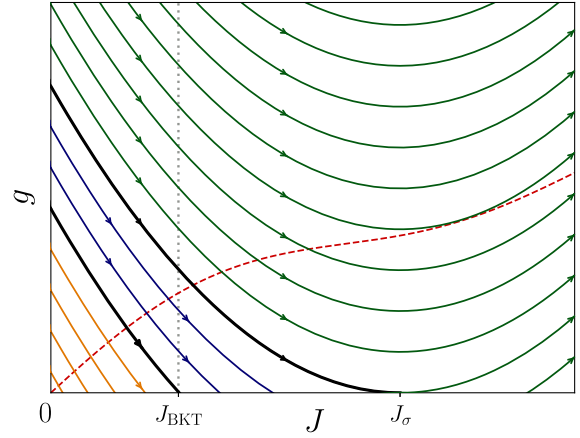


FIG. 1. Sketch of the RG flow lines for $7/4 < \sigma < 2$ in the $y = 0$ plane. The dashed red line is a possible realization of the physical parameters line, from which the flow starts, as the temperature is varied. On the right (left) of the gray dotted line, the vortex fugacity y is irrelevant (relevant) ($\dot{y}_\ell/y_\ell \geq 0$). The two separatrices (bold black lines) divide the flow in three regions: a high-temperature region (orange, the flow ends up in the disordered phase), an intermediate one (blue, the flow reaches a $g = 0$ fixed point), and the low-temperature region (green, the LR perturbation brings the system away from the critical line).

displays power-law decaying two-point functions $\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{0}) \rangle \sim r^{-2-\sigma}$ [76–78]. As $\sigma \rightarrow 7/4^+$, the critical temperature T_c reaches T_{BKT} from below. Therefore, for $\sigma < 7/4$, all the fixed points in the BKT line become unstable either with respect to topological or LR perturbations and the intermediate phase vanishes, leaving only a SSB phase transition. However, our approach cannot reliably be used to fully characterize this transition: as T approaches T_c from below, the RG flow slows down close to the $g = 0, J = J_\sigma$ fixed point. Since, for $\sigma < 7/4$ and $J_\sigma < J_{\text{BKT}}$, y grows indefinitely, away from the $y \ll 1$ regime. Our results are summarized in Fig. 2.

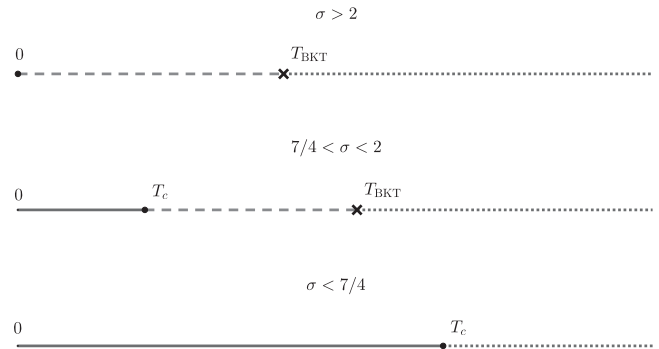


FIG. 2. Sketch of the possible phases of the model: ordered with magnetization (solid black), BKT QLRO (dashed light gray), disordered (dashed dark gray). If $\sigma > 2$, we find the usual SR phenomenology with a BKT phase transition. For $\sigma < 2$, an ordered phase appears at low temperatures, the BKT QLRO phase disappearing for $\sigma < 7/4$.

Conclusions.—We have shown that the introduction of LR power-decaying couplings in the 2D XY model Hamiltonian produces a rich phase diagram, different from the SR case [29] and from the one of $O(N)$ LR systems [4]. Remarkably, for $7/4 < \sigma < 2$, the system displays both BKT QLRO in the temperature interval $T_c < T < T_{\text{BKT}}$ and actual long-range order for $T < T_c$.

The introduction of complex interaction patterns in systems with $U(1)$ symmetry is known to generate exotic critical features, as in the anisotropic 3D XY model [79], coupled XY planes [80], 2D systems with anisotropic dipolar interactions [81,82], or four-body interactions [83], and high-dimensional systems with Lifshitz criticality [84,85]. This Letter constitutes a further milestone along this path, as it identifies a peculiar critical behavior, namely, a nonanalytic exponential vanishing of the order parameter, that eludes the current classification of universal scaling behaviors [86].

Our predictions may be tested in several low-dimensional AMO systems. It would be interesting to perform extensive numerical simulations in order to observe the scaling of the critical quantities, and especially the magnetization, close to the low-temperature end point of the BKT line in the regime $7/4 < \sigma < 2$. These simulations will be useful to classify this unprecedented transition and to investigate possible corrections near the $\sigma = 7/4$ end point due to higher-order effects caused by spin-wave excitations [87]. Further investigation is also needed to compare our results with the LR diluted model studied in [88,89]. In this model, at $\sigma = 1.875$, the numerical simulations presented in [89] do not find any intermediate BKT region, but the general question of whether the 2D LR diluted XY model and the 2D LR nondiluted one have the same phase diagram remains open.

Our results have also implications for LR quantum XXZ chains [71,90,91]. One would need to perform the exact mapping of the classical 2D LR XY model to an effective 1D quantum model, following the calculation presented in [23] and valid for the classical 2D SR XY model. If the nonlocal, LR terms violating the hard-core boson condition can be shown to be irrelevant, then one could put in correspondence our phase diagram with that of the LR quantum XXZ chains having LR couplings both for $x - y$ and $z - z$ terms [71]. This seems to be confirmed by the similar structure of the RG flow equations of [71] with our Eqs. (7) taken at low temperatures. If this is the case, then the two lines, black and white, of Fig. 1 in [71] would merge in a point, with the XY phase disappearing, corresponding to our $\sigma = 7/4$ point. Finally, we mention that it would be interesting to study in detail the phase diagram of the 2D LR Villain model for $\sigma < 2$.

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