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Semi-vortices and cluster-vorticity: new concepts in the Berezinskiĭ-Kosterlitz-Thouless phase transition

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The Berezinskiĭ-Kosterlitz-Thouless (BKT) essential phase transition in the 2d XY model is revisited. Its mechanism is usually described by the (un)binding of vortex–anti-vortex (V–AV) pairs, which does, however, not provide a clear-cut quantitative criterion for criticality. Known sharp criteria are the divergence of the correlation length and a discontinuity of the helicity modulus. Here we propose and probe a new criterion: it is based on the concepts of semi-vortices and cluster vorticity, which are formulated in the framework of the multi-cluster algorithm that we use to simulate the 2d XY model.

Keywords: 2d XY model; essential phase transition; vortices; cluster algorithm.

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1. The 2d XY model

We consider the 2d XY model, or 2d O(2) model, on square lattices of size $L \times L$. At each lattice site $x = (i, j)$, $i, j \in \{1, \ldots, L\}$ there is a classical spin variable $\vec{e}_x \in S^1$, *i.e.* $\vec{e}_x \in \mathbb{R}^2$ and $|\vec{e}_x| = 1, \ \forall x$. It can be parameterized as $\vec{e}_x = (\cos\varphi_x, \sin\varphi_x)$, $\varphi_x \in \mathbb{R}$. In lattice units, the Hamilton function, or Hamiltonian, of a spin configuration $[\vec{e}]$ is given by

$$\mathcal{H}[\vec{e}] = -\sum_{\langle xy \rangle} \vec{e}_x \cdot \vec{e}_y \ , \tag{1}$$

where $\langle xy \rangle$ indicates the nearest-neighbor lattice sites; we see that the spins are coupled ferromagnetically[i]. The model has a global O(2) symmetry, which inspires its application in the description of films of superfluid ^{4}He and of superconductors (although there the $\mathrm{U}(1) = \mathrm{O}(2)$ symmetry is local).

We assume periodic boundary conditions in both directions, *i.e.* the volume has the structure of a torus. As usual, the partition function Z and the thermal expectation value of some observable $A[\vec{e}]$ are given by the functional integrals

$$Z = \int \mathcal{D}\vec{e}\, e^{-\mathcal{H}[\vec{e}]/T} \ , \ \langle A \rangle = \frac{1}{Z} \int \mathcal{D}\vec{e}\, A[\vec{e}] e^{-\mathcal{H}[\vec{e}]/T} \ ,$$

where T is the temperature, cf. footnote i.

Of particular interest are *vortices* in the spin configurations. In order to define them, we consider the relative angle between two nearest-neighbor spins,

$$\Delta\varphi_{x,x+\hat{\mu}} = (\varphi_{x+\hat{\mu}} - \varphi_x) \bmod 2\pi \in (-\pi, \pi) \ , \tag{2}$$

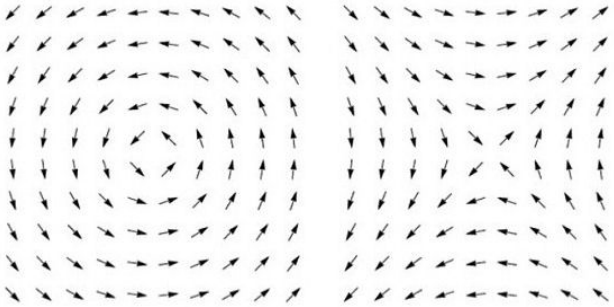

FIGURE 1. Prototypes of a vortex (V, left) and an anti-vortex (AV, right) in the centers of the plots. They show subsets of possible configurations in some region.

where $\hat{\mu}$ is a lattice unit vector in the μ-direction. Note that we are using a non-standard modulo operation, which minimizes the absolute value (the ambiguous case $\Delta\varphi_{x,x+\hat{\mu}} = \pm\pi$ has measure zero). Each plaquette carries a vorticity number

$$v_x = \frac{1}{2\pi} \Big(\Delta\varphi_{x,x+\hat{1}} + \Delta\varphi_{x+\hat{1},x+\hat{1}+\hat{2}} + \Delta\varphi_{x+\hat{1}+\hat{2},x+\hat{2}} + \Delta\varphi_{x+\hat{2},x} \Big) \in \{1, 0, -1\}. \tag{3}$$

$v_x = 1$ means that a vortex (V) is located on this plaquette, for $v_x = -1$ it is an anti-vortex (AV), and for $v_x = 0$ the plaquette is neutral (free of vorticity).

Due to Stokes' Theorem, the periodic boundary conditions imply that the total vorticity of any configuration vanishes, $\sum_x v_x = 0$, hence there is always the same number of V and AV.

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i We do not include a coupling constant, because what matters below is just the ratio $\mathcal{H}/T$, where T is the temperature, which we scale such that it absorbs this coupling. In lattice units (with lattice spacing 1) the dimensions of $\mathcal{H}$ and T are not manifest.

At the critical temperature T_c this model undergoes an essential phase transition, the *Berezinskiĭ-Kosterlitz-Thouless (BKT) transition* [1,2]. For a comprehensive overview, we refer to Ref. [3]. BKT transitions have been experimentally observed in superfluid ^{4}He [4], in various superconductors [5], and recently also in a frustrated magnet [6].

In contrast to finite-order phase transitions, the correlation length ξ does not diverge with a power-law, $\xi \propto (T - T_c)^{-\nu}$, but its behavior at $T \gtrsim T_c$ is exponential,

$$\xi \sim \exp\left(\frac{\text{const.}}{(T - T_c)^{\nu_e}}\right) , \tag{4}$$

where $\nu_e = 0.5$ [7] is an exponential critical exponent.[ii] In Ehrenfest's scheme, this is a phase transition of infinite order, *i.e.* very smooth. It is not related to any spontaneous symmetry breaking (the spontaneous breaking of the O(2) global symmetry is excluded in $d = 2$ by the Mermin-Wagner-Coleman Theorem, so we avoid the expressions "order" and "disorder"). At $T < T_c$ the system remains critical, covering a variety of universality classes.

The critical temperature was numerically measured in numerous works. High precision results were reported in Refs. [8], which are in agreement with $\beta_c \equiv 1/T_c = 1.1199(1)$.

In a sequence of famous papers [1, 2], Berezinskiĭ and later Kosterlitz and Thouless assigned this transition to the vortex dynamics:

- At $T < T_c$ the V and AV appear in pairs close to each other ("bound pairs"): for a given number of V and AV, this structure minimizes the free energy $F = -T \ln Z$, which implies an attractive force between near-by V and AV. Such localized pairs do not significantly affect the long-range correlations, so we are in the *massless phase*.

- At $T > T_c$ these pairs "unbind" as an entropy effect: the attractive force loses its dominance over the high multiplicity of configurations where V and AV are spread over the volume without any specific structure.[iii] We denote them as "free" V and AV, and their significant density does affect long-range correlations, which entails the *massive phase*.

In 2016 Kosterlitz and Thouless were awarded the Nobel Prize (sadly Berezinskiĭ[iv] had passed away in 1980, at the age of only 44) — at that occasion, their work was reviewed in Ref. [10].

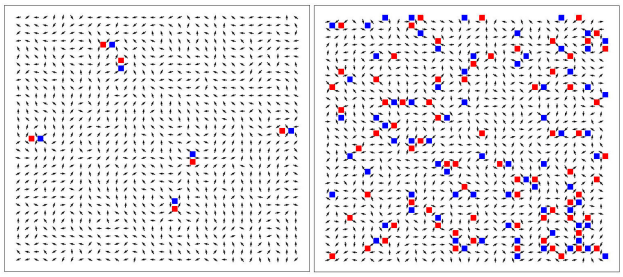

FIGURE 2. Typical configurations at $\beta = 1.12 > \beta_c$ (left) and $\beta = 0.6 < \beta_c$ (right), with V and AV indicated by red (bright) and blue (dark) plaquettes, respectively (and $\beta \equiv 1/T$). We see bound V–AV pairs on the left, and free V and AV on the right.

1.1. Constraint lattice Hamiltonian

Thanks to *universality*, this model — like other models — can be formulated with an (infinite) variety of lattice Hamiltonians. The continuum limit — which corresponds to $\xi \to \infty$, so that the lattice spacing vanishes in units of ξ as an intrinsic scale — is always the same (if suitable conditions are fulfilled, such as locality), hence they all describe the same physics.

Constraint lattice Hamiltonians for O(N) models have a simple structure, without any derivatives [11]: there is just a constraint δ for all angles between nearest-neighbor spins,

$$\mathcal{H}[\vec{e}] = \begin{cases} 0 & \text{if } |\Delta\varphi_{x,x+\hat{\mu}}| < \delta, \quad \forall x, \mu \\ +\infty & \text{otherwise.} \end{cases} \tag{5}$$

Instead of temperature one varies the constraint angle δ, and the BKT transition occurs in the 2d XY model at $\delta_c = 1.775(1)$ [12]. We confirmed that it is in the BKT universality class by numerically measuring the exponential critical exponent $\nu_e = 0.503(7)$, which is compatible with Kosterlitz' prediction [7]. Further evidence for the BKT universality class is based on the step-scaling function [12, 13].

In Ref. [14] we studied in particular the (un)binding mechanism, by considering various options for a cutoff distance between the nearest V and AV, for being considered a "bound pairs". Indeed, the celebrated mechanism is confirmed again. However, the argument with the free energy does not apply in this formulation, which does not really agree with the established picture: the (un)binding mechanism seems to be a pure entropy effect after all.

1.2. Helicity modulus

A short-coming of the (un)binding mechanism is that it does not provide a clear-cut quantitative criterion for T_c. In par-

ii Here the relation $\sim$ means that this is the term which dominates the divergence, even if there may be a pre-factor with some power of $(T - T_c)$.

iii Schematically we see this by writing the free energy as $F = E_V - TS = (\pi - 2T) \ln L$, where E_V is the (estimated) energy requirement for inserting one V or AV into a "smooth background", and S is the entropy, as reviewed in Ref. [10].

iv His work particularly inspired Polyakov to introduce his famous "dislocations" in gauge theory, with the hope to explain the confinement–deconfinement transition [9].

ticular, the distinction between "bound pairs" and "free" V and AV is not clearly defined.

We have mentioned the divergence of the correlation length for $T \searrow T_c$ as one clear criterion. Another one refers to the *helicity modulus* (or *spin stiffness*): it quantifies how the free energy F reacts to an (infinitesimal) change of the boundary conditions. Say in the $\hat{1}$-direction they are generalized from periodic to twisted,

$$\vec{e}_{x+L\hat{1}} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \vec{e}_x \ . \tag{6}$$

In terms of the *twist angle* α, the helicity modulus Υ — and its dimensionless counterpart $\bar{\Upsilon}$ — are given by

$$\Upsilon := \frac{\partial^2 F}{\partial \alpha^2} \ , \quad \bar{\Upsilon} := \frac{1}{T}\Upsilon \ . \tag{7}$$

For the standard Hamiltonian (1) one obtains[v]

$$\bar{\Upsilon} = \frac{1}{TL^2}\Big\langle \sum_x \vec{e}_x \cdot \vec{e}_{x+\hat{1}} \Big\rangle - \frac{1}{(TL)^2}\Big\langle \Big(\sum_x (e_x^{(1)} e_{x+\hat{1}}^{(2)} - e_x^{(2)} e_{x+\hat{1}}^{(1)}) \Big)^2 \Big\rangle \ , \tag{8}$$

hence this quantity can be numerically measured without ever moving away from $\alpha = 0$ (this is not the case for the constraint Hamiltonian [14]). Theory predicts a discontinuous jump of $\bar{\Upsilon}$ [16], which agrees with the observed jump in the density of superfluid ^{4}He films [4] and in a trapped, ultracold 2d Bose gas [17],

$$\lim_{T \nearrow T_c} \bar{\Upsilon}(T) = \frac{2}{\pi}(1 - 16e^{-4\pi}) \simeq 0.6365 \ ,$$
$$\bar{\Upsilon}(T \geq T_c) = 0, \tag{9}$$

(the small exponential correction to the jump height was discovered in Ref. [18]). This formula refers to infinite volume,

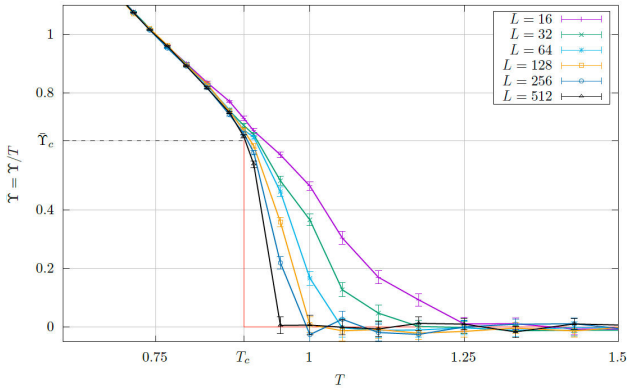

FIGURE 3. Simulation results for the dimensionless helicity modulus $\bar{\Upsilon}$, obtained with the standard Hamiltonian (1), and the theoretically predicted jump in infinite volume.

and for the standard Hamiltonian (1) the convergence towards this value for increasing L is very slow: even at $L = 2048$, $T = T_c$, it is still 6.6% too high [8]. The constraint Hamiltonian behaves much better: at $L = 64$, $\delta = \delta_c$, it already agrees with the theory to a precision below 1% [14], which was the first convincing numerical confirmation of the prediction (9). In Fig. 3 we show new simulation results with the standard Hamiltonian, which are consistent with Ref. [8], though we are limited to $L \leq 512$.

2. Proposal for a new criticality criterion

Let us now proceed to our suggestion for a new criterion to identify the critical temperature T_c. It is based on the Wolff cluster algorithm [19], which is not only most efficient to simulate this model, but it also allows us to introduce physical quantities, like semi-vortices [20]. The idea is related to the stochastic formulation of merons (semi-instantons) in the 2d O(3) model [21].

Let us begin by sketching the multi-cluster algorithm. A configuration $[\vec{e}]$ is efficiently updated by the following steps:

- 1. Choose a random vector $\vec{r} \in S^1$ with uniform probability. The line orthogonal to $\vec{r}$ through the origin is denoted as the Wolff line. "Flipping" a spin variable $\vec{e}_x$ means that it is reflected in the Wolff line.
- 2. Check all links between nearest-neighbor lattice sites, say x and $x + \hat{\mu}$ (possibly across the periodic boundaries). We consider putting a "bond" which "attaches" the spin variables $\vec{e}_x$ and $\vec{e}_{x+\hat{\mu}}$. If we flip one of these two spins, the contribution of this spin pair to the Hamiltonian $\mathcal{H}$ changes by some amount that we call $\Delta\mathcal{H}$.

  If $\Delta\mathcal{H} \leq 0$, we do not put a bond. In particular, this means that we never put a bond if $\vec{e}_x$ and $\vec{e}_{x+\hat{\mu}}$ point to opposite sides of the Wolff line.

  If $\Delta\mathcal{H} > 0$, we put a bond with probability $1 - e^{-\Delta\mathcal{H}/T}$.
- 3. All spins which are (directly or indirectly) connected by bonds form one *cluster*. We identify all the clusters; thus the entire configuration is divided into a set of clusters.
- 4. Each cluster is flipped with probability $1/2$: in this case, all the spins of a cluster are flipped collectively.
- Return to 1.

This algorithm fulfills the required conditions of detailed balance and ergodicity [19]. It turns out that the cluster size distribution scales with the correlation length to some fractal dimension D, *i.e.* the histogram stabilizes as a function of (cluster size)$/\xi^D$, thus exhibiting a universal behavior [20].

Let us assume the steps 1 to 3, *i.e.* we have a "map" of clusters. The V and AV can only be located at the boundaries between the clusters; for a plaquette inside a cluster all spins

[v] There is some confusion about the correct term, but it has been reproduced carefully in Refs. [15].

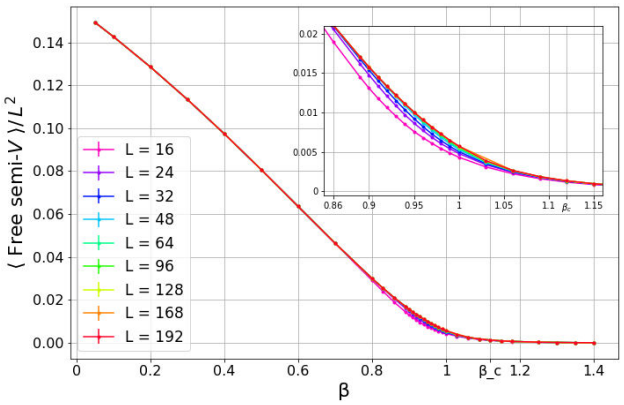

FIGURE 4. The temperature-dependent density of free semi-V, as defined in this section, in volumes $L \times L$, with $\beta = 1/T$.

point to the same side of the Wolff line, hence these plaquettes are neutral. It turns out that a V or AV on a plaquette can only involve spins belonging to exactly two clusters [15, 20].

This inspires the assignment of a vorticity contribution of some plaquette to a given cluster $\mathcal{C}$, we call it $v_{x,\mathcal{C}}$. Flipping the cluster $\mathcal{C}$ (while keeping all other clusters fixed) changes the configuration $[\vec{e}\,]$ to another configuration $[\vec{e}\,']$, and it may change the vorticity of the plaquettes at its boundary. We define

$$v_{x,\mathcal{C}} = \tfrac{1}{2}\,(v_x[\vec{e}\,] - v_x[\vec{e}\,']) \in \{-\tfrac{1}{2}, 0, \tfrac{1}{2}\}\,, \qquad (10)$$

which introduces the concept of *semi-vortices* (semi-V, $v_{x,\mathcal{C}} = 1/2$) and *semi-anti-vortices* (semi-AV, $v_{x,\mathcal{C}} = -1/2$) [20]. Note that $v_{x,\mathcal{C}}$ does not depend on the flipping orientation of the other clusters, which is important for the concept to be sensible. Thus a V is split into two semi-V associated with two clusters (and the same for an AV). The vorticity of a plaquette is retrieved as $v_x = \sum_{\mathcal{C}} v_{x,\mathcal{C}}$.

For a configuration with $N_{\mathcal{C}}$ clusters, all the cluster flips provide an ensemble of $2^{N_{\mathcal{C}}}$ configurations. In two of them all the spins are on the same side of the Wolff line, these are the *reference configurations*. If we start from a reference configuration and flip just one cluster, some semi-V may appear at its boundary, and the same number of semi-AV — they are alternatingly ordered along the boundary [20].

This provides a sharp criterion to define whether or not a V–AV pair is *bound:* this is the case if its semi-V and semi-AV are associated with only two clusters. Under cluster flips, they can only appear or disappear simultaneously, and their signs can only change simultaneously. Here, the binding does not refer to their distance, but to their fate under cluster flips.

The remaining *free semi-V* are therefore supposed to drive the BKT phase transition. Figure 4 shows that — for decreasing temperature T — a significant density of free semi-V does set in around $T_{\rm c}$, but this density looks like a smooth function of T: for increasing size L it does not approach the behavior like an order parameter (zero at $T \geq T_{\rm c}$, non-zero at $T < T_{\rm c}$).

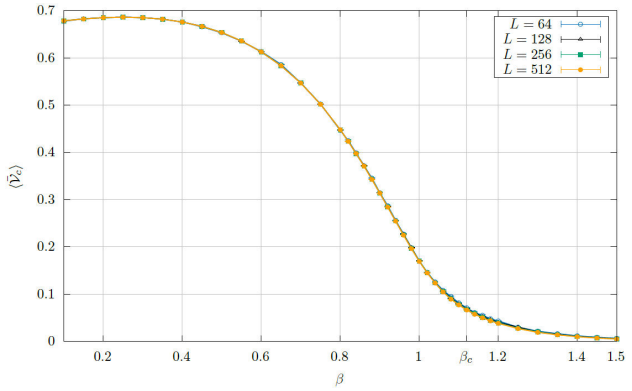

FIGURE 5. Cluster vorticity $\langle \bar{\mathcal{V}}_{\mathcal{C}} \rangle$ as a function of β. It coincides to high accuracy for different lattice sizes L.

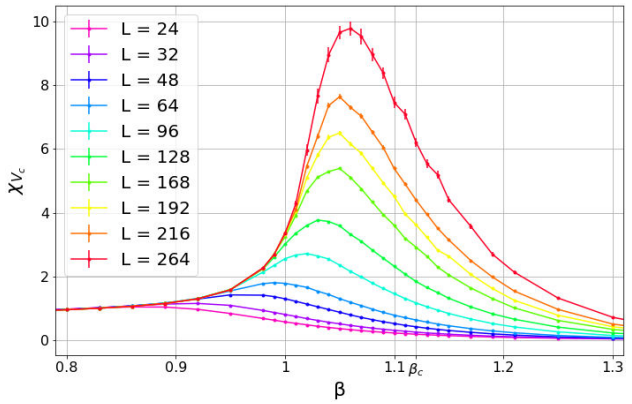

FIGURE 6. Cluster vorticity susceptibility $\chi_{\mathcal{V}}$ as a function of β, for various lattice sizes L.

Next we define the vorticity of a cluster $\mathcal{C}$ by the number of semi-V generated by its flip out of a reference configuration,

$$\mathcal{V}_{\mathcal{C}} = N_{\text{semi-V}} = N_{\text{semi-AV}}\,. \qquad (11)$$

For a configuration with $N_{\mathcal{C}}$ clusters we obtain the mean cluster vorticity $\bar{\mathcal{V}}_{\mathcal{C}}$, and the mean square $\bar{\mathcal{V}}_{\mathcal{C},2}$,

$$\bar{\mathcal{V}}_{\mathcal{C}} = \frac{1}{N_{\mathcal{C}}} \sum_{k=1}^{N_{\mathcal{C}}} \mathcal{V}_{\mathcal{C}_k}\,, \quad \bar{\mathcal{V}}_{\mathcal{C},2} = \frac{1}{N_{\mathcal{C}}} \sum_{k=1}^{N_{\mathcal{C}}} \mathcal{V}_{\mathcal{C}_k}^2\,. \qquad (12)$$

This takes us to the *cluster vorticity susceptibility*

$$\chi_{\mathcal{V}} = \langle \bar{\mathcal{V}}_{\mathcal{C},2} \rangle - \langle \bar{\mathcal{V}}_{\mathcal{C}} \rangle^2\,. \qquad (13)$$

Figure 5 shows $\langle \bar{\mathcal{V}}_{\mathcal{C}} \rangle$, which hardly depends on the volume, and which increases significantly below $T_{\rm c}$, like the free semi-V density, but again with a smooth behavior.

Hence its peak location $\beta_{\max}$ looks promising as a new criticality criterion. Figure 7 illustrates its thermodynamic extrapolation: we show a 3-parameter fit of the data points to the function $a/L^c + b$ (Fit 1); it leads $b = 1.0959(62)$, with a good fitting quality of $\chi^2/\text{dof} = 1.36$, which misses the consensus of the literature [8], $\beta_{\rm c} = 1.1199(1)$, by $2.14\,\%$, or 3.87σ. We add another fit to the same function, which includes $\beta_{\rm c}$ (Fit 2):

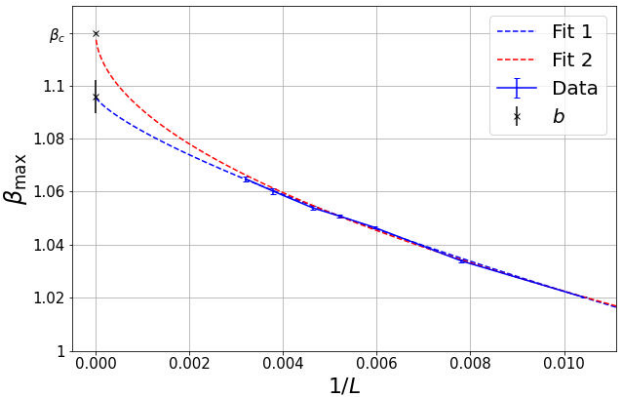

FIGURE 7. Two thermodynamic extrapolations of $\beta_{\max}$, the peak location of $\chi_{\mathcal{V}}$.

it still has a decent quality, with the ratio $\chi^2/\mathrm{dof} = 2.65$, which means that it is still conceivable the $\beta_{\max}$ converges to β_c in the large-L limit. We are in the process of testing this hypothesis with simulations on larger lattices.

3. Final remarks

We have reviewed some aspects of the BKT transition in the 2d XY model, and we arrived at the recently suggested concept of semi-vortices. We search for a new quantity which clearly detects the critical temperature T_c. The cluster vorticity susceptibility $\chi_{\mathcal{V}}$ of Eq. (13) looks promising: it has a peak close to T_c, with a height that rises with the volume L^2.

So far it seems that a natural thermodynamic extrapolation of the peak temperature — based on data up to $L = 264$ — slightly misses T_c. However, we should keep in mind that finite-size effects tend to be very persistent in this model, in particular for the standard Hamiltonian (1). We saw this property in the case of the helicity modulus, and the same holds for the magnetic susceptibility χ_m: at T_c it is predicted to scale as $\chi_m \propto L^{7/4}(\ln L)^{1/8}$ [7], but even size $L = 2048$ is not sufficient to numerically confirm these exponents [8].

Hence, we hope for the large-L peak location of $\chi_{\mathcal{V}}$ to agree with T_c, which would provide a new criterion for the BKT transition.

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