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Probing vortex unbinding via dipole fluctuations

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We develop a numerical method for detecting a vortex-unbinding transition in a two-dimensional system by measuring large-scale fluctuations in the total vortex dipole moment $\vec{P}$ of the system. These are characterized by a quantity $\mathcal{F}$ that measures the number of configurations in a simulation for which either P_x or P_y is half the system size. It is shown that $\mathcal{F}$ tends to a nonvanishing constant for large system sizes in the unbound phase, and vanishes in the bound phase. The method is applied to the XY model both in the absence and in the presence of a magnetic field. In the latter case, the system size dependence of $\mathcal{F}$ suggests that there exist three distinct phases, one unbound vortex phase, a logarithmically bound phase, and a linearly bound phase.

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I. INTRODUCTION

Topological defects play a crucial role in two-dimensional classical systems[1] and in $(1+1)$-dimensional quantum systems.[2] The paradigm of these is the XY model, which is known to undergo a vortex-unbinding transition in the Kosterlitz-Thouless (KT) universality class.[3] Highly analogous transitions occur for vortices in superfluids and thin-film superconductors, as well as for dislocations and disclinations in two-dimensional crystals. Worldline dislocations in one-dimensional quantum systems are important for describing tunneling,[4] and the question of whether these are bound or unbound is closely related to whether the system is metallic or insulating.

The KT phenomenology has been highly successful in describing defect unbinding in a variety of situations. For the XY model, fitting to the expected finite-size scaling of the helicity modulus in simulations yields an estimate of $T_{KT}=0.892$.[5] However, the concepts of vortices and defect unbinding are more general than the systems in which a KT transition takes place. In some situations a symmetry-breaking field, for example, a magnetic field tending to align the spins in the XY model, may be present.[6] A recent renormalization-group (RG) study[7] has suggested that vortex unbinding does occur in such systems, although the transition is considerably altered from the KT behavior. It is thus important to develop criteria by which one may determine whether a given system is in a bound or unbound vortex state, which are independent of precise matching to the KT theory. In this paper, we present a method by which this may be accomplished, which focuses on a measure $\mathcal{F}$ of extreme fluctuations in the system vortex dipole moment. Using a Langevin dynamics simulation of the XY model, we show that the method locates T_{KT} with reasonable accuracy. We then include a magnetic field in the Hamiltonian, and show that there are both bound and unbound vortex phases. The bound phase has two distinct behaviors: for smaller fields, $\mathcal{F}$ vanishes as a power of the system size L; for larger fields, $\mathcal{F}$ vanishes exponentially with L. The two behaviors are consistent with the results of the RG analysis,[7] which predicted both a logarithmically bound vortex phase and a linearly confined one, in addition to the unbound (deconfined) vortex phase.

II. CHARACTERIZING VORTEX DIPOLE FLUCTUATIONS

A total vortex dipole moment may be defined for configurations of any system containing vortices with well-defined locations. For concreteness, we will work with the XY model (planar spins of fixed length) on a square lattice. Let $\Delta\theta_{ij}$ denote the angular difference between nearest-neighbor spins ij, which we reduce to the interval $-\pi<\Delta\theta_{ij}\leqslant\pi$ by adding or subtracting 2π if necessary. The vorticity q_i around an elementary plaquette P is then $q_i=(1/2\pi)\Sigma_P\Delta\theta_{ij}$, which takes the values $-1, 0, 1$.[8] For any configuration of the XY system this rule assigns vortex charges to the sites $\vec{R}_i$ of the dual lattice. The corresponding dipole moment could be defined by

$$\vec{P}=\sum q_i\vec{R}_i . \tag{1}$$

However, there is a problem associated with the use of periodic boundary conditions: for a $L\times L$ system one may add (n_i^xL,n_i^yL) to $\vec{R}_i$ (with n_i^x, n_i^y integers) and retain a perfectly sensible definition of $\vec{P}$. For a given configuration, we can use this to reduce $\vec{P}$ so that its components are restricted to the interval $-L/2\leqslant P_{x,y}\leqslant L/2$; or we can extend its definition by adding factors of L so that $\vec{P}$ remains a continuous function as a vortex crosses a periodicity boundary. We will refer to these alternate definitions of the dipole moment as $\vec{P}_{red}$ and $\vec{P}_{ext}$, respectively. Note that $P_{red}^{x,y}$ will jump discontinuously by L whenever a vortex crosses a boundary.

The bound vortex phase has the property that the dipole moment remains finite, since the pairs do not separate; in the unbound phase, the diffusion of vortices implies a diffusion of the dipole moment, so that its magnitude can become arbitrarily large. In a finite system, this presumably translates into the statement that the diffusion constant of $\vec{P}_{ext}$ becomes very small below the unbinding temperature.

A feature of vortex-unbinding transitions is that the transition occurs via rare but extreme fluctuations.[9] One way to characterize such fluctuations is to look for system configurations with extreme values of $\vec{P}_{red}$. Loosely speaking, if we wish to characterize a configuration in terms of an effective single vortex-antivortex pair, when P_x or P_y is $L/2$, the pair is at its maximum separation. If such extreme configurations persist as $L\rightarrow\infty$, the system is then in an unbound phase. By contrast, we expect the number of such configurations to vanish in the large-size limit when the system is in a bound phase.

This expectation may be more carefully justified by considering effective theories of vortices in their bound and unbound phases. An unbound vortex system behaves as a two-dimensional metal in which the discreteness of the underlying vortex charges may be neglected. An effective Hamiltonian takes the form[10]

$$H_{unb}^{eff}=\frac{K}{2}\int d^2x d^2x' \rho(\vec{x})G(|\vec{x}-\vec{x}'|)\rho(\vec{x}')+\frac{\mu}{2}\int d^2x \rho^2(\vec{x}), \tag{2}$$

where $\rho(\vec{x})$ is the vortex density, $G(r)\sim -(2\pi)^{-1}\ln(r/a)+\text{const}$, with a being a microscopic length of order the lattice constant of the system, and μ is an effective chemical potential, essentially the core energy of the vortices. For this continuum system, we can adopt a definition of the (x component of the) dipole moment that incorporates the periodic boundary condition,

$$\begin{aligned} P_{eff}^{x}&=\frac{L}{2\pi}\int d^2x \rho(\vec{x})\sin\left[\frac{2\pi x}{L}\right] \\ &=\frac{L}{2\pi}\mathrm{Im}\{\rho(k_x=2\pi/L,\ k_y=0)\}. \end{aligned} \tag{3}$$

The fraction $\mathcal{F}$ of configurations with $P_{eff}^x=L/2$ is thus given by the probability of finding $\mathrm{Im}[\rho(k_x=2\pi/L,k_y=0)]=\pi$. This is easily evaluated by reexpressing H_{unb}^{eff} in terms of a wave-vector sum instead of a real-space integral. Noting that the Fourier transform of $G(r)$ for small wave vectors is $G(k)\sim 1/k^2$, one obtains

$$\mathcal{F}\propto \exp\left\{-\frac{1}{L^2T}\left[\frac{1}{2}K\left(\frac{L}{2\pi}\right)^2+\mu\right]\right\}\approx e^{-K/8\pi^2 T} \tag{4}$$

for the probability of obtaining an extreme dipole fluctuation in the large-size limit. Notice that the $\mathcal{F}$ does not vanish as $L\rightarrow\infty$, supporting our argument above that large dipole fluctuations survive in the unbound vortex state.

To analyze the bound vortex state, we focus on the two-dimensional Coulomb particle Hamiltonian

$$H_{CG}=\frac{K}{2}\int d^2x d^2x' m(\vec{x})G(|\vec{x}-\vec{x}'|)m(\vec{x}'), \tag{5}$$

where $m(\vec{x})$ is an integer degree of freedom, and the partition function involves a sum over all complexions of m satisfying $\int d^2x m(\vec{x})=0$. The probability of an extreme fluctuation in the system dipole moment may be expressed as

$$\begin{aligned} \mathcal{F}&\propto\sum_{\{m\}} e^{-H_{CG}[m]/T}\delta(\mathrm{Im}\, m(\vec{k}_d)-\pi) \\ &=\int_{-\infty}^{\infty} d\lambda e^{-i\lambda\pi}\sum_{\{m\}} e^{-H_{CG}[m]/T}e^{i\lambda \mathrm{Im}\, m(\vec{k}_d)}, \end{aligned} \tag{6}$$

where we have adopted the same definition of P_{eff}^x as in Eq. (3), with $\rho(\vec{x})$ replaced by $m(\vec{x})$, and $\vec{k}_d\equiv(2\pi/L,0)$. In the bound state the integer nature of $m(\vec{x})$ may not be ignored; however, we can make progress by adopting the dual description of the partition function.[6] This involves employing the Poisson resummation formula to rewrite Eq. (6) as

$$\begin{aligned} \mathcal{F}\propto&\int_{-\infty}^{\infty} d\lambda e^{-i\lambda\pi}\int \mathcal{D}\phi\sum_{\{n\}} e^{-H_{CG}[\phi]/T}e^{i\lambda\ \mathrm{Im}\ \phi(\vec{k}_d)} \\ &\times\exp\left[-2\pi i\sum_{\vec{x}} \phi(\vec{x})n(\vec{x})\right]. \end{aligned} \tag{7}$$

The integration over the continuous field ϕ may be carried through, with the result

$$\begin{aligned} \mathcal{F}\propto\int_{-\infty}^{\infty} d\lambda e^{-i\lambda\pi}\sum_{\{n\}} \exp\Bigg[&-\frac{T}{2K}\sum_{\vec{k}} |2\pi n(\vec{k}) \\ &-\lambda\ \mathrm{Im}\, n(\vec{k}_d)\,\delta_{\vec{k},\vec{k}_d}|^2/G(k)\Bigg]. \end{aligned} \tag{8}$$

A bound vortex fixed point is generated by replacing K with a renormalized value, and by exchanging the sum over integers n in Eq. 8 with a functional integral over continuous fields.[11] The resulting model represents the rough phase of a solid-on-solid model. Once the integer sum has been replaced by an integral, the $\lambda\,\mathrm{Im}\, n(\vec{k}_d)$ term in the integrand may be shifted away and the functional integral in fact has no dependence on λ. It then immediately follows that $\mathcal{F}=0$ for the bound vortex phase.

These considerations lead us to expect that one should observe large vortex dipole fluctuations in the unbound phase, but not in the bound one. We now demonstrate this is indeed the case using a Langevin dynamics simulation.

III. SIMULATION

Our simulations focus on the XY model for which we assign dynamics to the spins and coupling to a heat bath to generate a distribution of configurations. The equations of motion for our system are taken to be

$$\Gamma\frac{d^2\theta(\vec{x})}{dt^2}=\frac{\delta H_{XY}}{\delta\theta(\vec{x})}+\zeta(\vec{x})-\eta\frac{d\theta(\vec{x})}{dt}. \tag{9}$$

Γ is an effective moment of inertia for the XY spins, which for simplicity we set to 1 in the simulations, ζ is a random torque that models coupling to a heat bath, and η is the viscosity. To satisfy the fluctuation-dissipation theorem, the random torques are drawn from a distribution satisfying $\langle\zeta(\vec{r},t)\zeta(\vec{r}',t')\rangle=2\eta T\delta_{\vec{r},\vec{r}'}\delta(t-t')$ with T being the temperature of the system. Finally, our XY Hamiltonian is

$$H_{XY}=-K\sum_{\langle\vec{x},\vec{x}'\rangle}\cos[\theta(\vec{x})-\theta(\vec{x}')]-h\sum_{\vec{x}}\cos\theta(\vec{x}), \tag{10}$$

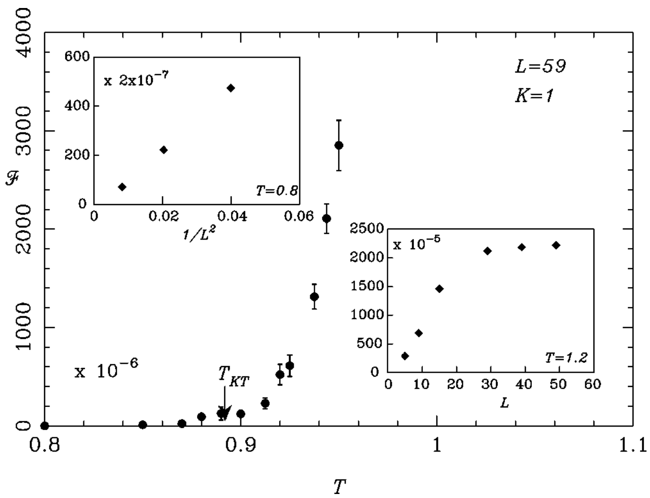

FIG. 1. $\mathcal{F}$ vs temperature for XY system with $h=0$, $L=59$. $\mathcal{F}$ drops sharply in the vicinity of the known Kosterlitz-Thouless temperature. Left inset: $\mathcal{F}$ vs $1/L^2$ for $T=0.8$, demonstrating $\mathcal{F}$ vanishes in the bound vortex state. Right inset: $\mathcal{F}$ vs L for $T=1.2$, demonstrating $\mathcal{F}$ approaches a nonzero constant in the unbound vortex state.

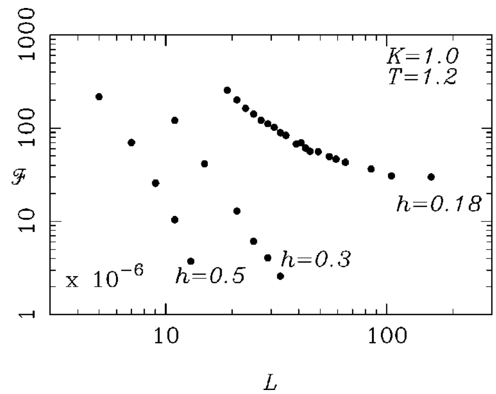

FIG. 2. $\mathcal{F}$ vs system size for XY system for $h=0.18$, 0.30, 0.50 for fixed temperature $T=1.2$ (error bars are smaller than symbols). $\mathcal{F}$ approaches a constant for large system sizes for smallest field, vanishes as a power law for intermediate field (straight line on log-log plot); and vanishes exponentially for the largest field (downward curvature on log-log plot). The three different behaviors indicate an unbound vortex phase, a logarithmically bound phase, and a linearly confined phase.

where we take the angles $\theta(\vec{x})$ to reside on an $L\times L$ square lattice. To perform the simulation, we have discretized the time derivative in Eq. (9) and used a standard random number generator[12] to generate a realization of $\zeta(\vec{r},t)$ at each time step. A typical run consists of 10^6 Langevin sweeps for equilibration, followed by 9×10^6 measurement steps. In accumulating the data, we repeated runs for each set of parameters with ~10 different seeds, allowing us to estimate our statistical errors. Simulations were performed for system sizes as large as $L=199$, although most of the simulations were in the range $19\leqslant L\leqslant59$.

Our measurement consists of counting the number of times a component of the system dipole moment $\vec{P}_{ext}$ passes through $(n+\frac{1}{2})L$ for n any integer. We then plot the number of such events divided by the total simulation time, yielding a measure of the fraction of configurations $\mathcal{F}$ for which the system has attained its maximal value. One advantage of the Langevin dynamics approach is that the vortex dipole moment $\vec{P}_{ext}$ changes by several steps with each Langevin sweep, but these steps are always much smaller than L except for very small values of L. This allows us to detect when $\vec{P}_{ext}$ has passed through $(n+\frac{1}{2})L$ even if in the immediate time step before and the step after $\vec{P}_{ext}$ was not measured to be precisely at this value. A larger number of events can then be accumulated than one might in a Monte Carlo simulation employing a cluster algorithm, since the configurations generated in the latter are not related in any simple way, forcing one to count only configurations for which $\vec{P}_{ext}$ is precisely $(n+\frac{1}{2})L$. Note that we count passages in both directions; this tells us how often $\vec{P}_{red}$ visits its extremal value.

As a check on the method, we first present results of simulations in the absence of the symmetry-breaking field, for which vortices unbind in a Kosterlitz-Thouless transition. Figure 1 illustrates these for $L=59$, $h=0$, and $K=1$. One can see $\mathcal{F}$ decreases sharply as the temperature approaches $T\approx0.9$ from above, so that $\mathcal{F}$ appears to be vanishing quite close to the accepted value of $T_{KT}^{XY}=0.892$. The differing behavior of $\mathcal{F}$ above and below the transition can be further confirmed by examining its size dependence: for T below the transition temperature, $\mathcal{F}$ decreases with system size, apparently approaching zero as $L\to\infty$, whereas for higher values of T, $\mathcal{F}$ *increases*, approaching a constant value from below. These differing size dependences strongly support the idea that $\mathcal{F}$ distinguishes the bound and unbound phases.

We now turn to the case $h>0$, for which we show some typical results in Fig. 2. Previous discussion[7] suggests three possible dependences of $\mathcal{F}$ on system size. At high temperatures and low fields, the vortices will remain unbound; then $\mathcal{F}$ will remain finite in the limit of large system size. This would seem to describe the case of the $h=0.18$ curve in Fig. 2. (Interestingly, the asymptotic value of $\mathcal{F}$ is approached from above, indicating that the symmetry-breaking field has had some effect). At intermediate values of h, we might find a bound vortex phase with logarithmically interacting vortices: then $\mathcal{F}$ would decrease with system size as a power law in $1/L$. The $h=0.3$ curve in Fig. 2 seems to correspond to this case. Finally, at large values of h, there could be a phase in which the vortices interact with a linear binding potential, and then $\mathcal{F}$ will decrease exponentially with L. The $h=0.5$ curve in Fig. 2 is consistent with this behavior.

Our results indicate that in the presence of a magnetic field, there exists an unbound vortex state and two different bound vortex states in the XY model. This behavior is precisely what was predicted in the RG analysis of Ref. 7. At low temperatures, vortex-antivortex pairs are connected by a string of overturned spins, leading to linear confinement. As temperature is increased, fluctuations can lead to a roughening of the strings binding the vortices, driving the effective string tension to zero. The vortex-antivortex pairs nevertheless retain a logarithmic attraction and remain bound as the system passes through the transition. At still higher temperatures, a second transition occurs in which the vortices do ultimately unbind. A remarkable feature of these transitions is that, according to the RG analysis,[7] they are not associated with singularities in the free energy.[13] Measurements of the specific heat and magnetization in our simulations are consistent with this expectation. Thus, one is forced to probe the vortices directly in order to detect their unbinding, as we have done by probing the system vortex dipole moment. It is interesting to note that in the absence of singularities in the free energy, it is unclear whether or not vortex unbinding should be thought of as a true thermodynamic phase transition. To our knowledge, this is the first example of a defect-unbinding transition that does not have the full character of a phase transition.[14]

In summary, we have developed a method of detecting vortex unbinding in two-dimensional systems by tracking extreme fluctuations in the vortex dipole moment of the system. For a system of linear size L, the fraction of configurations, $\mathcal{F}$, having a dipole moment component P_x or P_y equal to its largest value, consistent with periodic boundary conditions $(L/2)$, approaches a constant for large sizes when vortices are unbound, and vanishes when the vortices are bound. We have demonstrated this for the Kosterlitz-Thouless transition in the XY model, for which $\mathcal{F}$ can locate the transition temperature with reasonable accuracy. In the presence of a magnetic field tending to orient the spins, we have found that there is an unbound vortex state and two possible bound vortex states, one consistent with logarithmic binding of the vortices, the other with linear confinement. The method presented here is easily generalizable, and should be applicable to systems with other topological, pointlike defects.

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[1] D.R. Nelson, *Defects and Geometry in Condensed Matter Physics* (Cambridge University Press, New York, 2002).

[2] A.O. Gogolin, A.A. Nersesyan, and A.M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, New York, 1998).

[3] J.M. Kosterlitz and D. Thouless, J. Phys. C **6**, 1181 (1973); J.M. Kosterlitz, *ibid.* **7**, 1046 (1974).

[4] E. Kolomeisky and J.P. Straley, Rev. Mod. Phys. **68**, 175 (1996).

[5] P. Olsson, Phys. Rev. B **52**, 4526 (1995).

[6] J.V. José, L.P. Kadanoff, S. Kirkpatrick, and D.R. Nelson, Phys. Rev. B **16**, 1217 (1977).

[7] H.A. Fertig, Phys. Rev. Lett. **89**, 035703 (2002).

[8] The sum of $\Delta\theta_{ij}$ does not necessarily vanish. This is a consequence of having constrained these to the finite interval.

[9] N.D. Antunes, L.M.A. Bettencourt, and M. Kunz, cond-mat/0201149 (unpublished).

[10] G. Foltin, cond-mat/0101060 (unpublished).

[11] P.M. Chaikin and T.C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, New York, 1995).

[12] W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery, *Numerical Recipes, 2nd ed.* (Cambridge University Press, New York, 1996). We used the program ran1.f described here.

[13] However, singularities *can* appear in correlation functions and transport coefficients, and the transitions are associated with diverging length scales (Ref. 7). The possibility of such unusual transitions has been pointed out in Ref. 14

[14] D. Ruell, *Statistical Mechanics: Rigorous Results* (Addison Wesley, Reading, 1989).