Vortex description of the first-order phase transition in the two-dimensional Abelian-Higgs model

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We use both analytical arguments and detailed numerical evidence to show that the first-order transition in the type-I two-dimensional Abelian-Higgs model is commensurate with the statistical behavior of its vortex fluctuations, which behave as an ensemble of attractive particles. The clustering instabilities of such ensembles are shown to be connected to the process of phase nucleation. Calculations of the vortex equation of state show that the temperature for the onset of clustering is in qualitative agreement with the critical temperature. The vortex description provides a general gauge invariant mesoscopic mechanism for the first-order transition and applies for arbitrary type-I couplings.

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The role of topological excitations in the dynamics and thermodynamics of gauge field theories is a subject of wide interest and great promise, ranging in scope from the understanding of vortex phases in superconductors, necessary for practical applications, to the clarification of the mechanisms of charge confinement in non-Abelian gauge theories, such as quantum chromodynamics.

Topological excitations are important as finite-energy vehicles of disorder. Thus, phase transitions between a state of long range (e.g., magnetic) order and disorder can sometimes be understood by the proliferation of topological excitations, each bringing about disorder comparable to its size [1]. This is true in the XY model in two spatial dimensions, which displays a Kosterlitz-Thouless (KT) transition to a disordered state due to vortex pair unbinding [2]. Furthermore, there is evidence that the second-order transition in the three-dimensional (3D) XY universality class is associated with vortex string proliferation [1,3].

In this paper we show how a *first-order* phase transition in a simple gauge theory is intimately connected to the dynamics of its topological excitations and provide detailed numerical evidence in support of this view. Our results suggest a dual vortex gas picture of the transition, in analogy to the KT case. In the type-I Abelian gauge theory, however, vortices have attractive interactions, leading to characteristic metastability and collapse.

For its simplicity and close relationship to the XY model, we study the Abelian-Higgs (or Landau-Ginzburg) model in two dimensions. The phase structure of this model in three dimensions was examined in [4,5]. The Lagrangian density $\mathcal{L}$ is

$$\mathcal{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{1}{2}|D_\mu\phi|^2-\frac{\lambda}{8}(|\phi|^2-v^2)^2, \qquad (1)$$

where ϕ is a complex scalar field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ is the field strength for the gauge potential A_μ, and $D_\mu=\partial_\mu+ieA_\mu$. Here, we focus on the first-order regime (type-I) where e^2 is larger than the scalar coupling λ.

While the Abelian-Higgs system describes the long-wavelength behavior of an ideal superconductor [4,5], the 2D nature of our model precludes direct application to the description of real superconducting films. This is because even for thin films, the excursion of the vector potential into three dimensions fundamentally alters the nature of the interactions away from type-I behavior [6]. As a result, vortices interact via long-range potentials and the material exhibits a continuous transition. Nonetheless, we believe that the connections we draw below, between metastability and the attractive vortex interaction, are of general theoretical interest and may generalize qualitatively to more realistic situations.

The standard argument [7] for a first-order transition in gauge+scalar field theories relies on large e, for which the gauge field is very massive and can be integrated out. This is only justifiable as $\kappa\equiv\sqrt{\lambda}/e\to 0$, as it requires a separation of scales between "heavy" gauge degrees of freedom, which do not participate in the transition dynamics, and "light" scalar field fluctuations. The result is a "free energy" $F[\phi]$, that is, both nonconvex and, generally, gauge dependent. Nevertheless, $F[\phi]$ yields the correct qualitative picture for certain aspects of the transition [4].

A description of the critical system in terms of gauge invariant degrees of freedom, for arbitrary $\kappa<1$, is therefore desirable and may shed light on the mechanism of the transition. While vortices exist only as fluctuations at high temperature they become the only stable magnetic excitations of Eq. (1) at low temperatures. Moreover, arbitrarily low energy excitations can be produced by the superposition of vortices and antivortices. These arguments suggest that vortices are relevant degrees of freedom at criticality. In type-I, vortices attract each other independent of the sign of their quantized flux (topological charge) [8]. Thus, Abrikosov vortex lattices (such as those found in type-II superconductors) are not formed in applied magnetic fields. Instead type-I systems enter an *intermediate state*, forming a nonextensive multiwinding vortex, with the normal phase restored at its core. We argue that the attractive vortex interactions in type-I systems allow for a vortex description of the first-order phase transition.

Vortices are radial static classical solutions, obeying

$$\frac{d^2\sigma}{dr^2}+\frac{1}{r}\frac{d\sigma}{dr}-\left[e^2n^2\frac{a^2}{r^2}+\frac{\lambda}{2}(\sigma^2-v^2)\right]\sigma=0, \qquad (2)$$

$$\frac{d^2a}{dr^2}-\frac{1}{r}\frac{da}{dr}-e^2\sigma^2 a=0, \tag{3}$$

in temporal gauge $A_0=0$, where $\phi=\sigma(r)e^{in\theta}$. θ is the polar angle, n is an integer, $\vec{A}(r)=A_\theta\vec{e}_\theta$; $A_\theta=n/er-a(r)/r$, with boundary conditions $\sigma(r=0)=a(r\to\infty)=0$, $\sigma(r\to\infty)=v$, $a(r=0)=n/e$. For r larger than the core size, the vortex behaves like a point source for massive scalar and magnetic fields. Then the vortex profiles can be written as [9]

$$\sigma(r)=v-f(r), \quad f(r)=a_S v q K_0(m_S r), \tag{4}$$

$$A_\theta(r)-\frac{n}{er}=-a_G v m K_1(m_G r), \tag{5}$$

where $m_S=\sqrt{\lambda}v$, $m_G=ev$, a_S,a_G are dimensionless constants, and K_i are the modified Bessel functions of order i. The profiles (4) and (5) correspond to Yukawa (massive) charges q, m in two dimensions, in contrast to the familiar Coulomb logarithmic vortex solutions of the 2D XY model.

In the XY model the importance of topological charges to the phase transition is demonstrated by rewriting the partition function in terms of vortex degrees of freedom [10]. Unfortunately because the Abelian-Higgs system is non-Gaussian, it is impossible to perform an exact dual transformation to a partition function written exclusively in terms of a one- and two-body vortex terms. It is nevertheless possible to perform this rewriting approximately.

We begin with a superposition ansatz for an *arbitrary* number N of vortices, by constructing scalar and gauge vortex fields centered at N different loci x_i, $i\in\{1,N\}$,

$$\phi(X,x_1,\ldots,x_N)=\frac{\phi(X-x_1)\cdots\phi(X-x_N)}{v^{N-1}}, \tag{6}$$

$$\vec{A}(X,x_1,\ldots,x_N)=\vec{A}_1(X-x_1)+\cdots+\vec{A}_N(X-x_N). \tag{7}$$

This ansatz is exact when the vortices are all coincident or all widely separated. Substituting Eqs. (6) and (7) into the static part of the Hamiltonian gives

$$H=\sum_i \epsilon_i+\sum_{\langle i,j\rangle}[m_i(x)V_G(|x-y|)m_j(y)+q_i(x)V_S(|x-y|)q_j(y)]+\cdots, \tag{8}$$

where the terms not shown correspond to three- and four-body effects, which are negligible in a low-density vortex ensemble. The charges $m_i(x)=\pm n\delta(x)$ are integers of either sign, corresponding to quanta of magnetic flux, whereas $q_i=|m_i|$ is always positive [9,11]. For well-separated vortices at distance r the potentials are $V_G(r)=a_G v_{\rm eq}^2 K_0(m_G r)$ and $V_S(r)=-a_S v_{\rm eq}^2 K_0(m_S r)$ [9]. $v_{\rm eq}$ is a measure of $\sigma(T)$ and a_S,a_G are weakly varying with the couplings and have been computed numerically by Speight [11]: for $\kappa<1$, $a_S>a_G$. Then the two-body potential for a pair of like-charge vortices is

$$V(r)\simeq -q_i q_j v_{\rm eq}^2[a_S^2K_0(m_S r)-a_G^2K_0(m_G r)], \tag{9}$$

demonstrating that in type-I, when $\kappa<1$, the scalar (attractive) part of the potential dominates the interaction.

The statistical mechanics of particles with a finite-range, soft-core attractive potential was studied in several simple settings [12], aimed at elucidating thermodynamic gravitational instabilities. Unfortunately the 2D Yukawa gas of Eq. (9) was not among these.

Nevertheless, systems in this class share important qualitative properties: they always display a first-order transition between an (almost) ideal gas state at high T and a clustered phase at low T [12]. The latter is *not* an extensive thermodynamic phase. It consists of a single bound cluster containing most of the particles. Qualitatively this clustering transition occurs at $T_{\rm cl}$, such that the kinetic energy equals the interaction energy per particle. This gives a rough estimate of the vortex gas clustering temperature [12], $T_{\rm cl}\sim\epsilon/2=0.019$, where ϵ measures the strength of the interaction. We estimate ϵ from Ref. [13], by averaging the strength of vortex-vortex and vortex-antivortex pair interactions, $\epsilon=(\epsilon_{vv}+\epsilon_{v\bar{v}})/2$, where $\epsilon_{vv}\simeq 0.62v_{\rm eq}^2$ and $\epsilon_{v\bar{v}}=3.80v_{\rm eq}^2$. Vortex interactions are softened by a small order parameter, $v_{\rm eq}=\sigma(T_c^+)\simeq 0.13$.

The equation of state for the almost ideal (low-density) gas of vortices at high T can be computed by standard cluster expansion methods in the particle density, which we take as the (canonical) vortex density ρ. For simplicity we model the attractive potential as a square well with a strength ϵ and an interaction length l. Then

$$P\simeq\rho T(1-\rho B_2), \quad B_2=\frac{\pi l^2}{2}\left(\exp\frac{\epsilon}{T}-1\right), \tag{10}$$

where we neglected terms proportional to $\rho^n, n\geqslant 3$. The correction to the ideal gas behavior is negative as expected for an attractive potential. For high T, B_2 vanishes. Interactions are most important at low T and the pressure P vanishes at $T_{\rm cl}$:

$$T_{\rm cl}\simeq\frac{\epsilon}{\ln(1+2/\rho\pi l^2)}. \tag{11}$$

Attributing the change in σ to vortices, in analogy to the KT transition, we estimate $\rho\pi l^2\simeq 0.37=\sigma(T_c^-)-\sigma(T_c^+)$, and take ϵ as above to obtain $T_{\rm cl}\simeq 0.020$. Both estimates of $T_{\rm cl}$ are compatible with the measured T_c, see Figs. 1 and 2.

In spite of the qualitative agreement with T_c measured numerically we must note that these estimates of $T_{\rm cl}$ are very qualitative. For our choice of parameters the exact two-vortex potential is not known. Moreover, the virial expansion is notoriously unreliable near a clustering transition. To establish $T_{\rm cl}$ quantitatively will require a direct numerical molecular dynamics study of the vortex ensemble using the exact intervortex potential or the Yukawa gas interaction of Eq. (9).

The strength of the vortex ensemble picture lies in its several qualitative predictions, namely, that (1) the vortex density ρ will behave as a disorder parameter, vanishing *discontinuously* in the superconducting phase [14], (2) the vor-

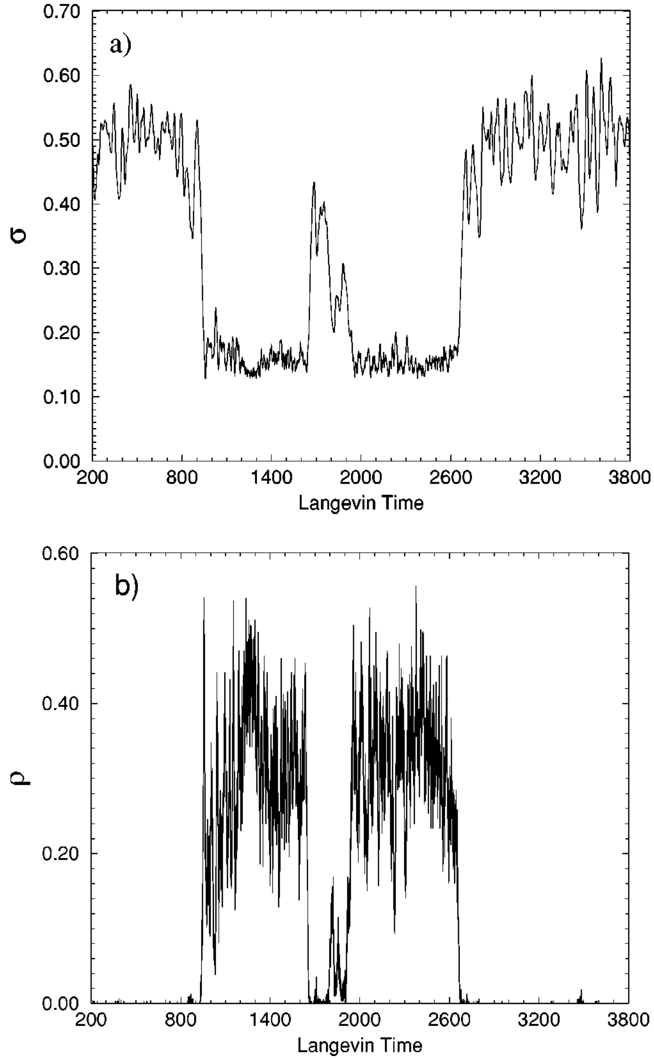

FIG. 1. (a) A characteristic time evolution of the average scalar modulus σ at $T=0.01844$, close to phase coexistence. σ jumps abruptly between the normal and superconducting phases. (b) The total vortex density ρ for the same trajectory as in (a). ρ is a disorder parameter vanishing in the superconducting phase.

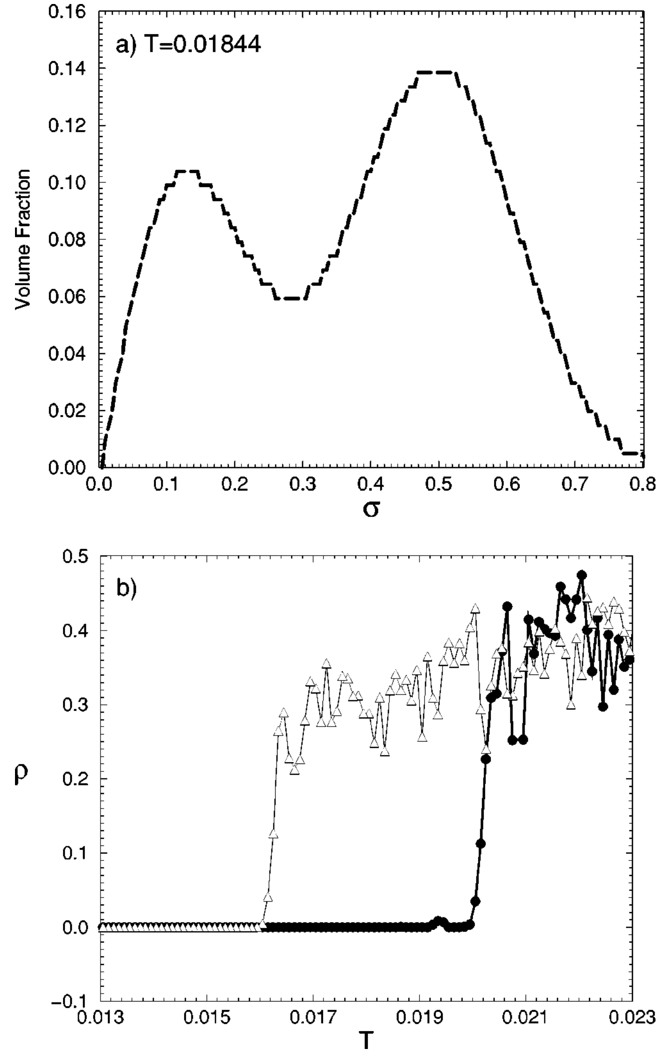

FIG. 2. (a) The probability distribution of the scalar field modulus σ (a gauge invariant) at $T=0.018\,44$, in the critical region, showing coexistence of the normal and superconducting phases. (b) A hysteresis loop for the vortex density ρ obtained by cooling (triangles) and heating (circles) the system through the critical region. Vortices disappear abruptly in the low-temperature phase. The sharp transitions in ρ, and the trajectory dependence as the transition point is crossed at a finite rate are typical signs of the discontinuous nature of the transition.

tex ensemble will show signs of a clustering instability in the metastable phase, and (3) multicharged vortices will be formed locally under sudden nonequilibrium cooling.

To test these predictions we consider the field evolution in contact with a heat bath, given by a system of Langevin field equations. Gauge invariance demands that the evolution preserves Gauss' law. This constraint still allows for several classes of dynamical equations [15], characterized by different gauge invariant stochastic generators. We choose the simple set $\{|\phi|^2,\vec{E}\}$, leading to

$$\partial_t \pi_a = \left[\nabla^2 - e^2|A|^2 - \frac{\lambda}{2}(|\phi|^2-1)\right]\phi_a - 2e\epsilon_{ab}A^i\partial_i\phi_b - 2\phi_i[\eta_s\partial_t|\phi|^2+\Gamma_s], \tag{12}$$

$$\partial_t\phi_i = \pi_i,$$

$$\partial_t E_i = (\vec{\nabla}\times\vec{B})_i + J_i, \quad J_i \equiv -e^2|\phi|^2 A_i - e\epsilon_{ab}\phi_a\partial_i\phi_b,$$

$$\partial_t A_i = E_i + \eta_g\partial_t E_i + \Gamma_g,$$

with $E_i=\partial_t A_i$, $\vec{B}=\vec{\nabla}\times\vec{A}$. The details of this choice are irrelevant to the state of canonical thermal equilibrium reached at long times. The indices a,b refer to the two real components of ϕ, whereas i is a spatial vector index. ϵ_{ij} is the totally antisymmetric rank-2 tensor. The stochastic sources Γ obey fluctuation-dissipation relations

$$\langle\Gamma_{s,g}(x,t)\Gamma_{s,g}(x',t')\rangle = 2\eta_{s,g}T\delta(x-x')\delta(t-t'), \tag{13}$$

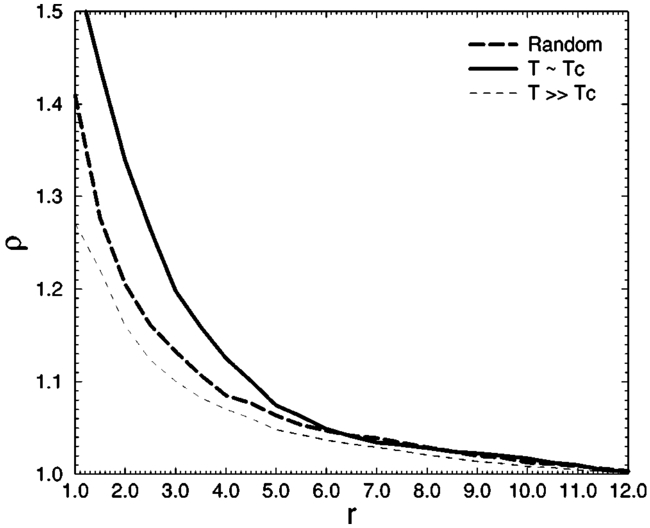

FIG. 3. The density of like-sign vortices $\rho(r)$ in a disk of radius r around a vortex, normalized by the average vortex density. Lines correspond to the metastable region (solid), the near-ideal gas for $T \gg T_c$ (short dashed), and a random distribution (long dashed), with the same density as the metastable region. The latter exhibits correlations typical of the subcritical percolation problem. Vortex clustering is maximal in the metastable phase, a premonitory sign of the dynamical clustering instability, and disappears for $T \gg T_c$.

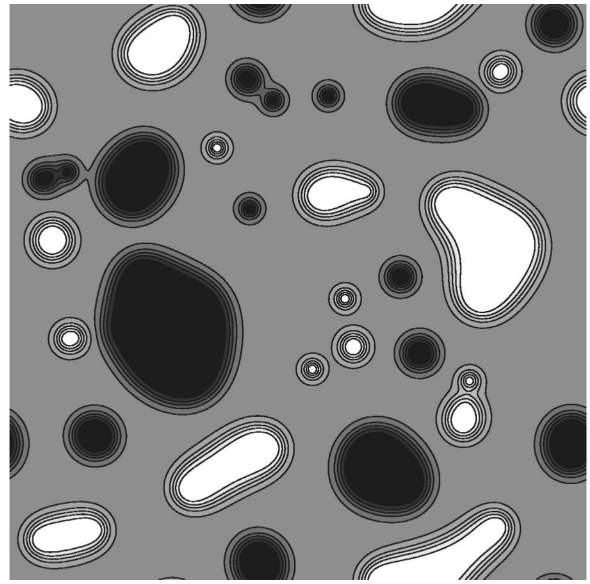

FIG. 4. Contours of magnetic flux after a fast temperature quench, showing the clustering of singly quantized vortices (smallest circular features) into large integer charge bound states. White (black), localized, regions denote (anti)vortices. The total collapse of the vortex ensemble was avoided due to fast cooling, which evaded the metastable region.

with $\langle \Gamma_{s,g} \rangle = 0$. We choose $e = 1.5$, $\lambda = 0.1$, and solve a lattice (noncompact) version of Eq. (12), with $\eta_s = \eta_g = 0.05$, $dt = 0.02$, and $dx = 0.5$.

Figure 1(b) shows that a substantial vortex population $\rho \neq 0$ exists in the symmetric (normal) phase, but that all vortices suddenly disappear, when the system transits to the superconducting state, as shown by the spatial average of $\sigma = |\phi|$, Fig. 1(a). Vortices are identified by their quantized fluxes, a quantity that is manifestly gauge invariant. The probability distribution of σ close to T_c is shown in Fig. 2(a). The double peak demonstrates phase coexistence characteristic of first-order transitions. Figure 2(b) shows a hysteresis loop in ρ, obtained by slowly heating and then cooling through the critical region.

The metastability of the vortex ensemble is a consequence of the small probability for forming a large vortex cluster. While the energy is lowered through attractive vortex interactions in the volume, the spatial cluster boundary, where vortices are rarefied, is thermodynamically costly. Thus, small vortex clusters are subcritical and can exist in the metastable phase without leading to its collapse. Evidence for incipient clustering is shown in Fig. 3, where we plot the radial density of like-charge vortices around another vortex. Clustering is maximal in the metastable region and negligible at higher $T \gg T_c$.

While we argue that vortices are relevant degrees of freedom at criticality, their profiles cannot be easily observed in the normal phase because they appear there only as transient fluctuations in a noisy background. Below T_c, where they could exist as well-defined objects, their ensemble collapses and vortices disappear in the absence of quantized net flux [16]. Fast quenches evading equilibrium in the metastable region do display well-defined vortices and show striking evidence of their clustering, see Fig. 4. This suggests an interesting scenario for defect formation experiments in type-I superconductors where the density of defects may vary *descontinuously* with cooling (or quench) rate. This would be qualitatively distinct from other phase transitions and from the current theoretical arguments of topological defect formation.

In conclusion, we argued for a vortex description of the mesoscopic mechanism underlying the first-order transition in the 2D type-I Abelian Higgs model and provided detailed numerical evidence in its support. Below $T_{\rm cl}$ the vortex ensemble becomes metastable and eventually collapses to a nonextensive thermodynamic phase and the system becomes ordered. The vortex interpretation of the transition is gauge invariant and does not require $e^2 \gg \lambda$, unlike the field-theoretical arguments for a first-order transition. Instead, the attractive nature of the vortex potential is manifest even in the weakest type-I regime, and metastability and collapse are inescapable. Moreover, this description of criticality in type-I 2D Abelian-Higgs model creates interesting links with the statistical mechanics of other attractive particle ensembles.

A full quantitative validation of the vortex description will require direct molecular dynamics studies of particle ensembles. Still, its qualitative success, demonstrated here, bodes well for applications to three dimensions [17], where vortices become lines that may participate in interesting critical phenomena, e.g., in crystal melting and cosmology.

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