A vortex description of the first-order phase transition in type-I superconductors

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Using both analytical arguments and detailed numerical evidence we show that the first order transition in the type-I 2D Abelian Higgs model can be understood in terms of the statistical mechanics of vortices, which behave in this regime as an ensemble of attractive particles. The well-known instabilities of such ensembles are shown to be connected to the process of phase nucleation. By characterizing the equation of state for the vortex ensemble we show that the temperature for the onset of a clustering instability is in qualitative agreement with the critical temperature. Below this point the vortex ensemble collapses to a single cluster, which is a non-extensive phase, and disappears in the absence of net topological charge. The vortex description provides a detailed mechanism for the first order transition, which applies at arbitrarily weak type-I and is gauge invariant, unlike the usual field-theoretic considerations, which rely on asymptotically large gauge coupling.

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The role of topological excitations in the dynamics and thermodynamics of gauge field theories is a subject of great promise ranging 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 as the proliferation of topological excitations, each bringing about disorder comparable to its size\textsuperscript{[1]}. This is true in the XY model in two spatial dimensions (2D), which displays a Kosterlitz-Thouless (KT) transition to a disordered state due to vortex pair unbinding\textsuperscript{[2]}. The second order transition in the 2D Ising model can also be formulated in terms of domain wall percolation. Furthermore there is evidence that the second order transition in the 3D XY universality class is associated with vortex string proliferation\textsuperscript{[1][3]}. In this letter we show how a first-order (discontinuous) phase transition in a simple gauge theory can be understood in terms of 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 2D. The Lagrangian density $L$ is

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

where $\phi$ is a complex scalar field, $F^{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength for the gauge potential $A_\mu$, and $D_\mu = \partial_\mu + i e A_\mu$. We focus on the regime where $\hat{e}^2$ is larger than the scalar coupling $\lambda$. This model describes the long-wavelength behavior of an ideal type-I superconductor.

The standard argument\textsuperscript{[4]} 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 $\kappa \equiv \sqrt{N/e} \rightarrow 0$, 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 non-convex and, generally, gauge dependent. Nevertheless $F[\phi]$ yields the correct qualitative picture for certain aspects of the transition. 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 long lived magnetic excitations of $F[\phi]$ at low temperatures. Moreover, arbitrarily low energy excitations can be produced by the superposition of vortices and anti-vortices. These arguments suggest that vortices are relevant degrees of freedom at criticality. In type-I, vortices attract each other independently of the sign of their quantized flux (topological charge)\textsuperscript{[5]}. Thus Abrikosov vortex lattices are not formed in applied magnetic fields. Instead type-I superconductors form a non-extensive multi-winding vortex, restoring the normal phase at its core. Between the normal and superconducting phases type-I superconductors exhibit a first-order transition.

Vortices are radial, static classical solutions obeying

$$\nabla^2 \sigma - \left( e A_\theta - \frac{n}{r} \right)^2 + \frac{\lambda}{2} (\sigma^2 - v^2) \right] \sigma = 0,$$ \hspace{1cm} (2)

$$\nabla \times A_\theta + e^2 \sigma^2 \left( A_\theta - \frac{n}{cr} \right) = 0,$$ \hspace{1cm} (3)
in temporal gauge $A_0 = 0$, where $\phi = \sigma(r) e^{i n \theta}$. $\theta$ is the polar angle, $n$ is an integer, $A_0(r) = n/e r - a(r)/r$, with boundary conditions $\sigma(r = 0) = a(r = 0) = 0$, $\sigma(r \to \infty) = v$, $a(r \to \infty) \to n/e$. 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

\begin{equation}
\sigma(r) = v - f(r); \quad f(r) = a_S v q K_0(m_S r),
\end{equation}
\begin{equation}
A_0(r) - \frac{n}{e r} = -a_G v m K_1(m_G r),
\end{equation}

where $m_S = \sqrt{\lambda v}, m_G = ev$, $a_S$, $a_G$ are dimensionless constants, and $K_i$ modified Bessel functions of order $i$. The profiles correspond to Yukawa (massive) charges in 2D, 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. 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 re-writing 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 $r_i$, $i \in \{1, N\}$

\begin{equation}
\phi(r, r_1, \ldots r_N) = \frac{\phi(r - r_1) \ldots \phi(r - r_N)}{v^{N-1}},
\end{equation}
\begin{equation}
A_i(r, r_1, \ldots r_N) = \hat{A}_1(|r - r_1|) + \ldots + \hat{A}_N(|r - r_N|).
\end{equation}

This ansatz is exact when the vortices are all coincident or all widely separated. Substituting (6-7) into the static equation (5),

\begin{equation}
\rho(x) V_{\phi}(\phi) = \nabla \cdot (\epsilon \nabla \phi) + 2\eta \nabla^2 \phi + \epsilon \phi \nabla \cdot (\epsilon \nabla \phi) + \epsilon \phi^2,
\end{equation}

we get a rough estimate of the vortex gas clustering temperature $T_{cl} \sim \epsilon/2 = 0.019$ where $\epsilon$ measures the strength of the interaction. We estimate $\epsilon$ from (10), by averaging the strength of vortex-vortex and vortex-antivortex pair interactions, $\epsilon = (\epsilon_{vv} + \epsilon_{v\bar{v}})/2$, where $\epsilon_{vv} \simeq 0.62\nu_{eq}$ and $\epsilon_{v\bar{v}} = 3.80\nu_{eq}^2$. Vortex interactions are softened by a small order parameter, $\nu_{eq} = \sigma(T_0^\nu) \simeq 0.13$.

The equation of state for the almost ideal (low density) gas of vortices at high $T$ can be computed by standard cluster expansion methods. For simplicity we model the attractive potential as a square well with a strength $\epsilon$ and an interaction length $l$. Then

\begin{equation}
P \simeq \rho T (1 - \rho B_2), \quad B_2 = \frac{\pi l^2}{2} \left( \exp \frac{\epsilon}{T} - 1 \right),
\end{equation}
where we neglected terms proportional to $\rho^n$, $n \geq 3$. 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 $T_{cl}$:

$$T_{cl} \simeq \frac{\epsilon}{\ln \left(1 + \frac{2}{\rho \pi l^2}\right)}.$$  

Using $\rho \pi l^2 \simeq 0.37 = \sigma(T_c^-) - \sigma(T_c^+)$, and $\epsilon$ as above we obtain $T_{cl} \simeq 0.020$. Both estimates of $T_{cl}$ are compatible with the measured $T_c$ and coincide in the limit $\epsilon / T \ll 1$ and $\rho \pi l^2 \simeq 1$.

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 [12], characterized by different gauge invariant stochastic generators. We choose the simple set $\{\phi^2, E\}$, leading to

$$\partial_t \phi_a = \left[\nabla^2 - \epsilon^2|A|^2 - \frac{\lambda}{2}(|\phi|^2 - 1)\right] \phi_a - 2\epsilon ab A^b \partial_i \phi_b - 2\phi_i \left[\eta_a \partial_i |\phi|^2 + \Gamma_g\right]$$

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

$$\partial_t E_i = (\nabla \times B)_i + J_i, \quad J_i \equiv -\epsilon^2 |\phi|^2 A_i - \epsilon \epsilon_{ij} \phi_j \partial_i \phi_b,$$

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

with $E_i = \partial_t A_i$, $B = \nabla \times A$. 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 2 real components of $\phi$, whereas $i$ is a spatial vector index. $\epsilon_{ij}$ is the totally anti-symmetric rank 2 tensor. The stochastic sources $\Gamma$ obey fluctuation-dissipation relations

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

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

![FIG. 2](image1.png)

**FIG. 2.** a) The probability distribution of $\sigma$ at $T = 0.01844$, in the critical region, showing coexistence of the normal and superconducting phases. b) A hysteresis loop for the vortex density $\rho$ obtained by cooling (triangles) and heating (circles) the system through the critical region.

These estimates of $T_{cl}$ are very qualitative in nature. For our choice of parameters the exact 2-vortex potential is not known. Moreover the virial expansion is notoriously unreliable near a transition, especially in the presence of clustering. We plan to examine the quantitative behavior of the vortex particle ensemble, through a direct thermodynamic study using either the exact intervortex potential or the Yukawa gas interaction of [3].

Nevertheless, a vortex ensemble picture leads to several qualitative predictions i) $\rho$ will behave as a disorder parameter, vanishing discontinuously in the superconducting phase, ii) the vortex ensemble must show signs of a clustering instability in the metastable phase and iii) multi-charged vortices must be visible under sudden nonequilibrium cooling.
disappear when the system transits to the superconducting state, as shown by the spatial average of \( \sigma = |\phi| \). Vortices in the normal phase are identified by their quantized fluxes, a quantity that is manifestly gauge invariant. The probability distribution of \( \sigma \) close to \( T_c \) is shown in Fig. 2. The double peak demonstrates coexistence of the two phases, characteristic of first order transitions. Fig. 2) shows a hysteresis loop in \( \rho \), obtained by slowly heating and then cooling through the critical region.

![Figure 4](image_url)

**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.

The metastability of the vortex ensemble is a consequence of the small probability for the formation of a large vortex cluster. While the free energy is lowered through attractive interactions in the volume, the spatial cluster boundary, where vortices are rarefied, is thermodynamically costly. Thus small 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 the relevant degrees of freedom at criticality, their profiles cannot be clearly observed in the normal phase, because vortices appear there only as transient fluctuations. Below \( T_c \), where they could exist as well defined objects, their ensemble collapses and vortices disappear in the absence of quantized net flux. Fast quenches evading equilibrium in the metastable region do display well defined vortices and show striking evidence of their clustering, see Fig. 4.

In conclusion, we argued for a vortex description of the mechanism underlying the first-order transition in the 2D type-I Abelian Higgs model and provided detailed numerical evidence in support of this picture. Below \( T_{c1} \) the vortex ensemble becomes metastable and eventually collapses to a non-extensive thermodynamic phase and the system becomes a superconductor. The vortex interpretation of the transition is gauge invariant and does not require \( e^2 \gg \lambda \), unlike the field-theoretic 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.

The vortex description must now be subjected to closer quantitative scrutiny by direct studies of particle ensembles. Still, we believe that its qualitative success bodes well for applications to 3D, where point vortices become lines, and may participate in interesting critical phenomena such as crystal melting and in cosmology.

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