

Hausdorff Dimension of Critical Fluctuations in Abelian Gauge Theories

J. Hove, S. Mo, and A. Sudbø

Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway
(Received 30 March 2000)

The geometric properties of the critical fluctuations in Abelian gauge theories such as the Ginzburg-Landau model are analyzed in zero background field. Using a dual description, we obtain scaling relations between exponents of geometric and thermodynamic nature. In particular, we connect the anomalous scaling dimension η of the dual matter field to the Hausdorff dimension D_H of the critical fluctuations, which are fractal objects. The connection between the values of η and D_H , and the possibility of having a thermodynamic transition in finite background field, is discussed.

PACS numbers: 74.60.-w, 74.20.De, 74.25.Dw

Anderson has proposed the breakdown of a generalized rigidity associated with proliferation of defect structures in an order parameter as a general means of characterizing phase transitions [1]. In the context of three-dimensional superfluids and extreme type-II superconductors, such ideas have recently been put on a quantitative level [2,3]. It has been explicitly demonstrated that in three spatial dimensions Abelian gauge theories, such as the Ginzburg-Landau theory describing type-II superconductors, suffer a continuous phase transition driven by a proliferation of topological defects in the order parameter, which are closed loops of quantized vorticity [3]. These loops are induced by *transverse* phase fluctuations in a complex scalar order parameter. Such fluctuations are prominent, for instance, in doped Mott-Hubbard insulators [2–4].

In this paper, we investigate the nontrivial geometric properties of these critical fluctuations and give a geometric interpretation of the anomalous scaling dimension of the condensate order parameter both for a charged and a neutral condensate. In addition, we discuss the connection between the geometric properties of the zero-field critical fluctuations and the possibility of having a thermodynamic finite-field phase transition involving unbinding of loops of quantized vorticity.

We emphasize that the main results to be presented are quite general and apply to the static critical sector of any theory of a complex scalar matter field coupled to a fluctuating gauge field in *three spatial dimensions* [2,3,5], provided that the symmetry group of the theory is Abelian.

The Hamiltonian for the system is given by

$$H(q, u_\phi) = m_\phi^2 |\phi|^2 + \frac{u_\phi}{2} |\phi|^4 + |D_\mu \phi|^2 + \frac{1}{4} F^2, \quad (1)$$

where $F^2 = F_{\mu\nu} F^{\mu\nu}$, $F_{\mu\nu} = \partial_\mu h_\nu - \partial_\nu h_\mu$, $D_\mu = \partial_\mu - iqh_\mu$, and $\phi = |\phi| \exp(i\theta)$ is a complex matter field coupled to a massless gauge field \mathbf{h} with coupling constant q . The $|\phi|^4$ term mediates a short-range repulsion, while the gauge field \mathbf{h} mediates long-range interactions. m_ϕ is the *mass parameter* for the ϕ field, and u_ϕ is a self-coupling.

Consider Eq. (1) representing a 3D condensate with charge $q \neq 0$ sustaining stable topological objects in the form of closed vortex loops. Then the theory with $q = 0$ is a field-theoretical description of the ensemble of these stable topological objects, constituting a dual description of the original theory [5]. The theory with $q = 0$ is also a direct field-theoretical description of a neutral condensate. Thus, in 3D, the gauge theory $H(q \neq 0, u_\phi)$ describing a *charged* condensate has a field-theoretical description of its critical fluctuations or topological defects in terms of a theory isomorphic to $H(q = 0, u_\phi)$ describing a similar but *neutral* condensate, and vice versa [5]. In this sense, a charged condensate has neutral vortices with only short-ranged steric interactions, while a neutral condensate has charged vortices with long-ranged interactions. In the former case, the long-ranged interactions between vortex segments are rendered short ranged by fluctuations of the gauge field in the original theory; i.e., the dual gauge field is massive with mass given by the charge of the original problem [5]. A limiting case we consider as a benchmark is the Gaussian theory $H(q = 0, u_\phi = 0)$ which is a field-theory description of (noninteracting) random walkers, but not a field-theoretic description of the critical sector of any gauge theory.

The anomalous dimension η for the ϕ field is defined via the relation

$$G(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}) \phi^\dagger(\mathbf{y}) \rangle = \frac{\mathcal{G}(|\mathbf{x} - \mathbf{y}|/\xi)}{|\mathbf{x} - \mathbf{y}|^{d-2+\eta}}, \quad (2)$$

where $\mathcal{G}(z)$ is some scaling function, and d is the spatial dimension of the system. Particle-field duality dictates that this correlation function has a geometric interpretation, yielding the probability amplitude of finding any particle path connecting \mathbf{x} and \mathbf{y} . A particular example is the *disorder theory* for a set of interacting chains [6]. In the present work, the particle trajectories correspond to vortex lines.

For a random walk of length N in $d = 3$, the probability of going from \mathbf{x} to \mathbf{y} is given by [7]

$$P(\mathbf{x}, \mathbf{y}; N) = \left(\frac{3}{2\pi N} \right)^{3/2} \exp \left[-\frac{(\mathbf{x} - \mathbf{y})^2}{2N} \right]. \quad (3)$$

The correlation function $G(\mathbf{x}, \mathbf{y})$ of the corresponding

Gaussian field theory is found by summing up $P(\mathbf{x}, \mathbf{y}; N)$ for all N ,

$$G(\mathbf{x}, \mathbf{y}) = \sum_N P(\mathbf{x}, \mathbf{y}; N) \propto \frac{1}{|\mathbf{x} - \mathbf{y}|}. \quad (4)$$

Comparing this with Eq. (2), we find $\eta = 0$, as expected. The random walker traces out a fractal path with Hausdorff dimension D_H . Moreover, in general, the distance between two points \mathbf{x} and \mathbf{y} N walks apart is given by

$$\langle |\mathbf{x} - \mathbf{y}|^2 \rangle \propto N^{2\Delta}, \quad (5)$$

where Δ is the wandering exponent which for the Gaussian 3D case is $\Delta = 1/2$. Inverting Eq. (5), we find that the total length of the random walker scales with linear size as $L^{1/\Delta}$; hence the Hausdorff dimension of the random walker is given by $D_H = 1/\Delta$. If we set $\mathbf{x} = \mathbf{y}$ in Eq. (3) we find that the unnormalized distribution $D(N)$ of loops of perimeter N is given by

$$D(N) \propto \frac{1}{N} \sum_{\mathbf{x}} P(\mathbf{0}; N) \propto N^{-\alpha}, \quad (6)$$

with $\alpha = 5/2$ for purely random walkers. The extra factor N^{-1} in Eq. (6) comes from the arbitrariness in defining the starting position along the loop. Hence, for the case of strict random walkers in 3D, described by a Gaussian field theory $H = m_\phi^2 |\phi|^2 + |\nabla \phi|^2$, the corresponding set of values for the two geometric and one thermodynamic exponents is given by $(\Delta, \alpha, \eta) = (1/2, 5/2, 0)$.

The loop distribution function $D(N)$ contains an exponential factor suppressing large loops for $T < T_c$,

$$D(N) \propto N^{-\alpha} e^{-\beta \varepsilon(T) N}, \quad (7)$$

where $\varepsilon(T)$ is an effective line tension. We are considering the vortex tangle *at the critical point* where $\varepsilon(T)$ has vanished, such that the system has suffered a *vortex-loop blowout* [2,3,5].

Beyond the Gaussian case, exact exponents cannot be obtained analytically; however, we will derive scaling relations for them. When Eq. (5) is invoked, a generalized probability function $P(\mathbf{x}, \mathbf{y}; N)$ may be written on the form

$$P(\mathbf{x}, \mathbf{y}; N) \propto \frac{1}{N^\rho} F\left(\frac{|\mathbf{x} - \mathbf{y}|}{N^\Delta}\right), \quad (8)$$

where $F(x)$ is a scaling function, and normalizability of P implies $\rho = d\Delta$. From Eq. (6), we find that $P(\mathbf{x}, \mathbf{y}; N)$ should scale with N as $N^{1-\alpha}$, which yields the scaling relation $\rho = \alpha - 1$. Conversely, summing over all N in Eq. (8) to find the correlation function $G(\mathbf{x}, \mathbf{y})$, we obtain

$$G(\mathbf{x}, \mathbf{y}) = \sum_N P(\mathbf{x}, \mathbf{y}; N) \propto \frac{1}{|\mathbf{x} - \mathbf{y}|^{\rho-1/\Delta}}, \quad (9)$$

giving the scaling relation $\eta = \frac{\rho-1}{\Delta} + 2 - d$. Combining the above, we find

$$\eta + D_H = 2, \quad D_H = \frac{d}{\alpha - 1}. \quad (10)$$

A computation of the *geometric* exponent α yields the *thermodynamic* exponent η and the Hausdorff dimension

D_H . Note that both η and D_H are sensitive functions of α , $\partial \eta / \partial \alpha = -\partial D_H / \partial \alpha = d/(\alpha - 1)^2$, such that a precise determination of η and D_H requires great precision in the determination of α . The above reinforces the statement that a geometric transition of the vortex tangle at criticality of the gauge theory Eq. (1) can be assigned a genuine thermodynamic order parameter via a dual formulation of the original theory *in three spatial dimensions* [2,3]. The random walker is represented by a Gaussian theory, Eq. (1) with $(u_\phi = 0, q = 0)$, for which $\eta = 0$. This corresponds to $D_H = 2$, such that the random walker in three dimensions traces out a path that precisely fills a cross-sectional area of the system. *Note that $D_H < 2 \leftrightarrow \eta > 0$, while $D_H > 2 \leftrightarrow \eta < 0$.*

The Hamiltonian equation (1) with $(u_\phi \neq 0, q \neq 0)$ has a dual field theory corresponding to Eq. (1) with $q = 0$ describing the neutral vortex tangle of a charged superconductor [5]. The $|\phi|^4$ term in Eq. (1) represents a *steric repulsion*, i.e., the vortex loops cannot overlap, leading to a random walk problem with self-avoiding *links* (but not necessarily self-avoiding sites), in the sense that parallel vortex segments repel, perpendicular vortex segments can cut [8], while antiparallel vortex segments can annihilate. Hence, this is not a standard self-avoiding path problem. However, we expect $\Delta > 1/2$ or equivalently $D_H < 2$, since steric repulsion should result in a vortex-loop tangle packing space less densely than for the noninteracting case, so that $\eta > 0$. The repulsive interaction between parallel vortex segments also leads to a more efficient suppression of long loops than for the noninteracting case, so that $\alpha > 5/2$.

Consider next Eq. (1) with $(u_\phi \neq 0, q = 0)$ for $d = 3$, which has a dual field theory corresponding to Eq. (1) with $q \neq 0$ describing the charged vortex tangle of a neutral condensate [5]. A long-ranged (anti) Biot-Savart interaction is mediated by the gauge field. This is a relevant perturbation, in renormalization group sense, to a steric contact repulsion [9]. The geometric properties of the charged vortex tangle are a result of a balance between attractive forces mediated by the gauge field, and the steric repulsion. As the numerical simulations show, we find $\Delta < 1/2$, corresponding to $D_H > 2$, which means that the vortex tangle is more compact than the ensemble of pure random walkers, due to the fact that an attractive long-ranged Biot-Savart interaction between oppositely oriented vortex segments overcompensates the steric repulsion so as to contract the vortex-loop tangle not only compared to the pure $|\phi|^4$ case, but even compared to the noninteracting case. The tangle thus packs space so that it more than fills a cross-sectional area of the system.

The fluctuation-dissipation theorem provides a bound on η via the susceptibility $\chi_\phi = \int d^d x G(x) \sim \xi^{2-\eta}$, which is bounded by the volume L^d of the system, $L^{2-\eta} = L^d L^{2-d-\eta} < L^d$, so $\eta > 2 - d$. Equation (10) gives a geometric interpretation of this bound. Specializing to $d = 3$, $\eta = -1$ corresponds to topological excitations

with $D_H = 3$, an upper limit, and a value of $\alpha \geq 2$, guaranteeing normalizability of $D(N)$.

For $d = 3$, the continuous phase transition in a superfluid or extreme type-II superconductor has recently been *demonstrated* to be driven by a proliferation of vortex loops [3,5]. From the above, $\eta = -1$ means that a single vortex loop at T_c packs space completely, i.e., its perimeter N scales as $N \propto L^3$, implying that the vortex-tangle collapses on itself, rendering the transition discontinuous. This may be seen from the standard scaling relation $\beta = \nu(d - 2 + \eta)/2$ for critical exponents. Formally, this implies that the limit $\eta \rightarrow (2 - d)^+$ corresponds to the limit $\beta \rightarrow 0^+$, characteristic of a discontinuous transition. More informally, a collapse of a vortex tangle may be viewed as mediated by an effective attractive vortex interaction, a situation akin to what is known in type-I superconductors. Deep in the type-I regime, it is known that superconductors suffer a weakly discontinuous transition [10].

Monte Carlo simulations have been performed on the lattice version of Eq. (1) in the phase-only approximation to determine precise values of α , both for $q = 0$ and $q \neq 0$. We have also performed simulations on pure random walkers described by the theory $H(q = 0, u_\phi = 0)$. They reveal that a determination of α is less fraught with finite-size effects than a determination of D_H . Thus, we have focused on determining α . The model we consider is

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j - q_C h_{ij}) + \frac{1}{2} (\nabla \times \mathbf{h})^2, \quad (11)$$

where the site variable θ_i is the phase of the complex matter field $\phi = |\phi| \exp(i\theta)$ of Eq. (1), when the system is discretized, J is essentially a bare phase stiffness, and the link variable $h_{ij} = \int_i^j d\mathbf{l} \cdot \mathbf{h}$. The charge q_C is the (original) charge entering in the simulations. Up to this point we have considered a general charge q irrespective of whether it couples to the original condensate or the resulting vortex tangle. The numerical simulations are performed on the phase of the condensate; hence the concept of *original* and *dual* are fixed in terms of the numerical simulations. Consequently we introduce the charges q_C for the condensate and q_V for the vortices, with the understanding that $q_C \neq 0 \Rightarrow q_V = 0$ and vice versa.

From the phase distributions of the matter field we can extract vortex loops [3]. These loops have charge q_V and are described by the field theory $H(q_V, u_\phi)$ [5]. Hence, we can study the critical properties of the charged field theory $H(q_V, u_\phi)$ by considering the geometric properties of the thermally excited vortex-loop tangle at the critical temperature in the 3D XY model. Conversely, the geometric properties of the vortex tangle with $q_C \neq 0$ yield the critical properties of the neutral field theory $H(q_V = 0, u_\phi)$ of Eq. (1).

The simulations with $q_C = 0$ are described elsewhere [3], while for $q_C \neq 0$ the simulations proceed as follows.

For every site on the lattice a phase change $\theta_i \rightarrow \theta'_i$ is attempted, and accepted or rejected according to the Metropolis algorithm. Then a change in $h_{ij} \rightarrow h_{ij} + \delta h$ is attempted, and accepted or rejected according to the Metropolis algorithm. When updating h_{ij} we update all the link variables on a randomly oriented elementary plaquette containing h_{ij} as one of its four edges. Updating of \mathbf{h} in this fashion guarantees that the gauge-fixing condition $\nabla \cdot \mathbf{h} = 0$ is enforced at all times. For $q_C = 0$, the simulations were performed for a system of size $L \times L \times L$ with $L = 180$, while those for $q_C \neq 0$ were performed with $L = 64$.

During the simulations we have sampled the distribution function $D(N)$, Eq. (7), obtaining α . The results are shown in Fig. 1 and listed in Table I. The value of α obtained for $q_C \neq 0$ (dual neutral), which is the hardest system to simulate, gives a value for η in good agreement with high-precision results for η of the pure ϕ^4 theory [11]. This serves as a useful benchmark on our method of extracting η . For $q_C = 0$ we have simulated much larger systems than for $q_C \neq 0$. The deviation from the Gaussian value $\alpha = 5/2$ is substantial, and of opposite sign compared to $q_C \neq 0$. Given the size of the system we consider for $q_C = 0$, it is unlikely that this is a finite-size artifact. An $\alpha < 5/2$ guarantees $\eta < 0$ for the $q_C = 0$ (dual charged) case, contrary to the value of $\eta > 0$ for

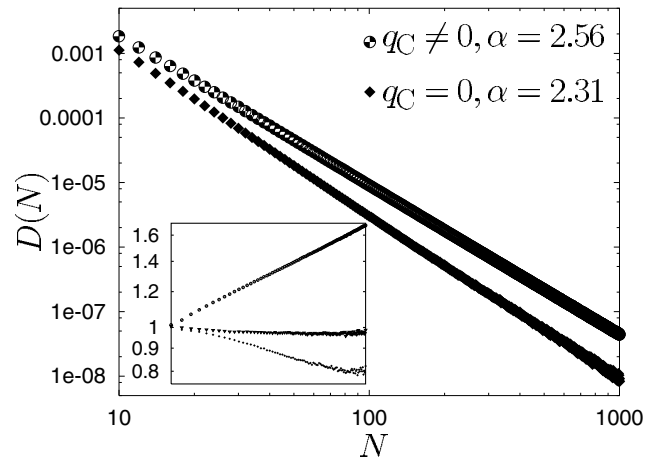


FIG. 1. The vortex-loop distribution function $D(N) \sim N^{-\alpha}$ as a function of loop perimeter N , at the critical point for the charged ($q_C \neq 0, q_V = 0$) and neutral ($q_C = 0, q_V \neq 0$) cases. Numerical results for the exponents $(\alpha, D_H, \Delta, \eta)$ are given in Table I. The system size is $L \times L \times L$, with $L = 180$ for $q_C = 0$, and $L = 64$ for $q_C \neq 0$. The inset shows *simulation results* for $N^{5/2}D(N) \sim N^{5/2-\alpha}$ on a double-logarithmic scale. Top: $q_C = 0, L = 180$ (dual charged). Middle: Noninteracting vortex loops (Gaussian case), $L = 64$. Bottom: $q_C \neq 0, L = 64$ (dual neutral). The results demonstrate that $5/2 - \alpha > 0$ for $q_C = 0$ (dual charged), while $5/2 - \alpha < 0$ for $q_C \neq 0$ (dual neutral). Hence, by Eq. (10), $D_H > 2, \eta < 0$ for $q_C = 0$, while $D_H < 2, \eta > 0$ for $q_C \neq 0$. The latter agrees with other high-precision results for η ; see Ref. [11]. Note that the Gaussian result $\alpha = 5/2$ is obtained to high precision, for $L = 64$.

TABLE I. The loop distribution exponent α , as determined from Monte Carlo simulations. The remaining exponents have been determined from Eq. (10). Symbols are explained in the text.

Exponent	Gaussian	$q_C = 0, q_V \neq 0$	$q_C \neq 0, q_V = 0$
α	5/2	2.312 ± 0.003	2.56 ± 0.03
D_H	2	2.287 ± 0.004	1.92 ± 0.04
Δ	1/2	0.437 ± 0.001	0.52 ± 0.01
η	0	-0.287 ± 0.004	0.08 ± 0.04

$q_C \neq 0$ [3,11]. In particular, the inset in Fig. 1 lends strong support to the proposition that $\eta(q_C \neq 0) > 0$, while $\eta(q_C = 0) < 0$.

The value $\eta < 0$ obtained for the original neutral, dual charged case, is significant: It implies that $D_H > 2$ for this case. *Whether $D_H > 2$ or $D_H < 2$ is of great import to the possibility of having a genuine phase transition driven by a vortex loop unbinding even in the presence of a finite background field such as magnetic induction in type-II superconductors.* A vortex system accesses configurational entropy more easily if it is compressible than if it is incompressible. For the charged case the gauge-field fluctuations render the system compressible. In the neutral case, the system expands screening strings of closed vortex loops to a larger extent than for the charged case, as substitutes for the gauge-field fluctuations. This is why $D_H(q_C = 0) > D_H(q_C \neq 0)$. There is an infinitely larger amount of screening vortex strings in the neutral case (dual charged) than for the charged case (dual neutral), which is the true significance of the fact that η is smaller for $q_C = 0$ than for $q_C \neq 0$. The possibility of the zero-field vortex-loop blowout transition surviving the presence of a finite field is much greater in a neutral superfluid or an extreme type-II superconductor than in a charged condensate with *a priori* good screening.

Given the significance of $D_H > 2$, we elaborate on the fact that for the original neutral (dual charged) case, we find $\eta < 0$. The Lehmann representation of the Fourier transform $\tilde{G}(p)$ of Eq. (2) is sometimes used to argue that η obeys the strict inequality $\eta > 0$. The Lehmann representation of $\tilde{G}(p)$ is given by

$$\tilde{G}(k) = \int_0^\infty d\mu^2 \frac{\rho(\mu^2)}{k^2 + \mu^2}, \quad (12)$$

where $1 = \int_0^\infty d\mu^2 \rho(\mu^2)$, and $\rho(\mu^2) = Z\delta(\mu^2 - m_\phi^2) + \sigma(\mu^2)$. The propagator for the Gaussian case would be $\tilde{G}(k) = 1/(k^2 + m_\phi^2)$, where m_ϕ^2 refers to the bare mass parameter in Eq. (1). Thus, $\eta > 0$ follows if $0 < Z < 1$, which holds for a uniformly positive $\rho(\mu^2)$. However, in theories with a *local gauge symmetry*, the two-point correlation function is a gauge-dependent quantity. Hence, we cannot interpret $\rho(\mu^2)$ as a positive definite observable spectral weight. In particular, $\sigma(\mu^2)$ may in principle be made negative for certain values of μ by a gauge transformation. This invalidates the reasoning leading to the strict inequalities $Z < 1$ and $\eta > 0$. Finally, we mention that a

negative η , as found here and in other simulations [3,5] all representing exact results, is in agreement with an early one-loop ϵ expansion [10] and also with recent nonperturbative renormalization group calculations [12].

This is corroborated by a simple calculation on Eq. (1). At the critical point, amplitude fluctuations are irrelevant, and the important fluctuations are *transverse* phase fluctuations, or vortices [2,3,5]. Ignoring amplitude fluctuations yields an effective zeroth order Hamiltonian governing the transverse θ fluctuations, whose Fourier transform \mathcal{F} we denote by \mathbf{S}_k , $\mathcal{F}((\nabla\theta)_T) = \mathbf{S}_k = -2\pi i(\mathbf{k} \times \mathbf{n}_k)/k^2$, where \mathbf{n}_k is the Fourier transform of the *local vorticity*. We find, after integrating out the transverse gauge field, that $H = \Xi^2(k)\mathbf{S}_k \cdot \mathbf{S}_{-k}$, where $\Xi^2(k) = k^2/(k^2 + 2q^2)$. (When $q \neq 0$, longitudinal phase fluctuations may be gauged away.) For $q = 0$, we have $\Xi^2(k) = 1$, while $\lim_{k \rightarrow 0} \Xi^2(k) \sim k^2$ for $q \neq 0$. The coupling to a fluctuating gauge field *softens* the transverse phase fluctuations, providing the effective phase stiffness with an extra power k^2 compared to the $q = 0$ case. Thus, $\tilde{G}^{-1}(k, q = 0) = k^2 + \Sigma(k)$ and $\tilde{G}^{-1}(k, q \neq 0) = k^4 + \Sigma(k)$. In both cases, the $k \rightarrow 0$ limit of the self-energy $\Sigma(k)$ is given by $\Sigma(k) \sim k^{2-\eta}$. We thus have $\lim_{k \rightarrow 0} \tilde{G}^{-1}(k) \sim k^{2-\eta}$ provided that $\eta > 0$ for $q = 0$ and, when invoking the absolute lower bound, $\eta > -1$ for $q \neq 0$. Note that for $q = 0$, a pure $|\phi|^4$ theory, we do expect the Lehmann representation coupled with positive definiteness of $\rho(\mu^2)$ to hold.

This work was supported by the Norwegian Research Council via the High Performance Computing Program and by Grant No. 124106/410 (S.M. and A.S.). J.H. thanks NTNU for support. Communications with F.S. Nogueira and Z. Tešanović are gratefully acknowledged.

- [1] P.W. Anderson, *Basic Notions in Condensed Matter Physics* (Benjamin/Cummings, Menlo Park, CA, 1984); see also P.G. de Gennes, in *Proceedings of the Nobel Symposium* (Academic Press, New York, 1973), Vol. 24, p. 112.
- [2] Z. Tešanović, Phys. Rev. B **59**, 6449 (1999).
- [3] A.K. Nguyen and A. Sudbø, Phys. Rev. B **60**, 15 307 (1999); Europhys. Lett. **46**, 780 (1999).
- [4] V.J. Emery and S.A. Kivelson, Nature (London) **374**, 434 (1995); see also H. Kleinert, Phys. Rev. Lett. **84**, 286 (2000).
- [5] J. Hove and A. Sudbø, Phys. Rev. Lett. **84**, 3426 (2000).
- [6] H. Kleinert, *Gauge Fields in Condensed Matter* (World Scientific, Singapore, 1989), Vol. 1.
- [7] D. Austin *et al.*, Phys. Rev. D **49**, 4089 (1994).
- [8] A. Sudbø and E.H. Brandt, Phys. Rev. Lett. **67**, 3176 (1991); C. Carraro and D.S. Fisher, Phys. Rev. B **51**, 534 (1995).
- [9] C. Dasgupta and B.I. Halperin, Phys. Rev. Lett. **47**, 1556 (1981).
- [10] B.I. Halperin *et al.*, Phys. Rev. Lett. **32**, 292 (1974).
- [11] M. Hasenbusch and T. Török, J. Phys. A **32**, 6361 (1999).
- [12] I.F. Herbut and Z. Tešanović, Phys. Rev. Lett. **76**, 4588 (1996); **78**, 980 (1997); I.D. Lawrie, *ibid.* **78**, 979 (1997).