Predicting the critical density of topological defects in $O(N)$ scalar field theories

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$O(N)$ symmetric $\lambda\phi^4$ field theories describe many critical phenomena in the laboratory and in the early Universe. Given N and $D\leqslant 3$, the spatial dimension, these models exhibit topological defect classical solutions that in some cases fully determine their critical behavior. For $N=2$ and $D=3$, it has been observed that the defect density is seemingly a universal quantity at T_c. We prove this conjecture and show how to predict its value based on the universal critical exponents of the field theory. Analogously, for general N and D we predict the universal critical densities of domain walls and monopoles, for which no detailed thermodynamic study exists, to our knowledge. Remarkably this procedure can be inverted, producing an algorithm for generating typical defect networks at criticality, in contrast with the usual procedure [Vachaspati and Vilenkin, Phys. Rev. D **30**, 2036 (1984)], which applies only in the unphysical limit of infinite temperature.

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$O(N)$ symmetric scalar field theories are a class of models describing the critical behavior of a great variety of important physical systems. For example, for $N=3$ they describe ferromagnets; for $N=1$ they describe the liquid vapor transition and binary mixtures; and for $N=2$ they describe superfluid ^{4}He and the statistical properties of certain polymers. In the early Universe $N=2$ describes the phase transition associated with the breakdown of Peccei-Quinn symmetry, and models of high energy particle physics may belong to the universality class of $O(N)$ scalar models, whenever the mass of the Higgs bosons is larger that of the gauge bosons. $O(N)$ scalar models are also invoked in most implementations of cosmological inflation and topological defects scenarios [1].

One of the fundamental properties of $O(N)$ $\lambda|\phi|^4$ field theories is the existence, for $N\leqslant D$, of static nonlinear classical solutions (domain walls, vortices, and monopoles) that we will refer to henceforth as topological defects. At sufficiently high temperatures, topological defects can be excited as nonperturbative fluctuations. Their dominance over the thermodynamics, due to their large configurational entropy, is known to trigger a phase transition in $O(2)$ in three and two dimensions, and their persistence at low energies prevents the onset of long range order in $O(2)$, $D\leqslant 2$, and in $O(1)$ in one dimension.

It is therefore natural that universal critical exponents characterizing the phase transition in terms of defects and through the behavior of field correlators must be connected. This connection is made more quantitative whenever one can construct dual models, field theories which possess these collective solutions as their fundamental excitations [2]. In the absence of supersymmetry rigorous mappings between the fundamental models and their dual counterparts exist only in very special cases [2,3]. Duality has been suggested and empirically observed to be a much more general phenomenon, though.

In this paper we explore the duality between the critical behavior of the two-point field correlation function and defect densities at criticality. We will show that this leads to the result that the critical density of vortex strings, observed in recent nonperturbative thermodynamic studies of $O(2)$, is a universal number. Among other insights [4] this shows that the phase transition in $O(2)$ in three dimensions occurs when a critical density of defects is reached, connecting directly the familiar picture of the Hagedorn transition in vortex densities to the more abstract critical behavior of the fields. We also extend our procedure to different N and D, making predictions for the values of the universal densities of domain walls and monopoles, in two and three dimensions.

Finally, but very importantly, the inversion of this procedure allows us to easily generate typical field configurations at criticality. This is of fundamental practical importance. Recent experiments in ^{3}He [5], and large scale numerical studies of the theory [6] have lent quantitative support to the ideas, due to Kibble [7] and Zurek [8], that defects form at a second order phase transition due to a critical slowing down of the fields response over large length scales, in the vicinity of the critical point. The defect networks hence formed have densities and length distributions set by thermal equilibrium at $T=T_c^+$ (note that this picture could change considerably for a first order phase transition).

In contrast most realizations of defect networks used, e.g., in cosmological studies are generated using the Vachaspati-Vilenkin [1] (VV) algorithm. This relies on laying down random field phases on a lattice and searching for their integer windings along closed paths. The absolute randomness of the phases corresponds to the $T\to\infty$ limit of the theory. More fundamentally it yields defect networks that are quantitatively distinct from those in equilibrium at criticality, i.e., at formation.

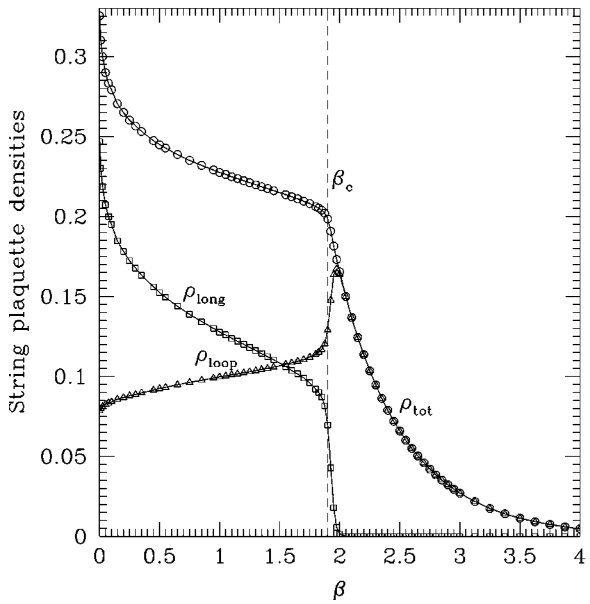

FIG. 1. The string densities, total, loops, and long string, as a function of inverse temperature β. At β_c, the densities display derivative discontinuities, signaling a second order phase transition. $\rho_{\rm tot}(\beta_c)$ coincides for different studies, leading to the conjecture that it is a universal number.

Figure 1 shows the behavior of a system of vortex strings at a second-order phase transition, for $O(2)$ in three dimensions. The data were obtained from the study of the nonperturbative thermodynamics of the field theory [9]. At T_c the total density of string $\rho_{\rm tot}$ displays a discontinuity in its derivative, signaling a second order phase transition.

A disorder parameter can be constructed in terms of string quantities by dividing the string population into long string (typically string longer than $\sim L^2$, where L is the size of the computational domain) and loops, comprising of shorter strings. The corresponding densities are denoted by $\rho_{\rm long}$ and $\rho_{\rm loop}$. In Fig. 1 we can observe that $\rho_{\rm long}$ consistently vanishes below T_c, except for a small range of β where it increases rapidly to a finite critical value. In Ref. [9] we conjectured that in the infinite volume limit $\rho_{\rm inf}$ exhibits a discontinuous transition.

The value of the total string density at β_c, $\rho_{\rm tot}(\beta_c) \simeq 0.20$, coincides with results from studies of different models in the same universality class [9,10]. This fact lead us to the conjecture [9] that $\rho_{\rm tot}(\beta_c)$ is universal.

In order to prove this conjecture we appeal to a well known result, due to Halperin and Liu and Mazenko [11]. Halperin's formula expresses ρ_0, the density of zeros of a Gaussian field distribution in terms of its two-point function. For an $O(N)$ theory the relevant quantity is the $O(N)$ symmetric correlation function $G(x)=\langle \phi(0)\phi(x)^\dagger\rangle$, resulting in

$$\rho_0 \propto \left| \frac{G''(x=0)}{G(x=0)} \right|^{N/2}. \tag{1}$$

Equation (1) measures the density of coincident zeros of all N components of the field at a point. Coincident zeros occur at the core of topological defects. Depending on N and D, coincident zeros can be interpreted as either monopoles, strings, or domain walls. In the particular case of a Gaussian $O(2)$ theory in $D=3$, Halperin's formula allows us to compute the density of vortex strings crossing an arbitrary plane in three-dimensional space, a quantity that is clearly proportional to $\rho_{\rm tot}$.

The last key observation is that in the critical domain of a second order transition, all $O(N)$ theories are effectively approximately Gaussian, but with nontrivial critical exponents. In particular renormalization group analysis shows that the mass and quartic coupling vanish at T_c [12,13]. Higher order polynomial terms (e.g. $\propto \phi^6$) may be generated but are small. Hence in the critical domain the field two-point function can be written as

$$G(\mathbf{x}) \propto \int d^D\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^{2-\eta}}. \tag{2}$$

$\eta \ll 1$ is the universal critical exponent taking into account deviations from the mean-field result (cf. Ref. [14]).

Thus the effective Gaussianity of the theory allows the use of Eq. (1) to compute the critical value of $\rho_{\rm tot}(\beta_c)$. Modulo renormalization, the final result depends *only* on η establishing, as conjectured, that $\rho_{\rm tot}(\beta_c)$ is a universal quantity. Substituting, Eq. (2) into Eq. (1), we obtain

$$\rho_{\rm tot} \propto \left(\frac{\eta+1}{\eta+3} \right) \frac{k_{\rm max}^{3+\eta} - k_{\rm min}^{3+\eta}}{k_{\rm max}^{1+\eta} - k_{\rm min}^{1+\eta}}, \tag{3}$$

where we have introduced upper and lower momentum cutoffs $k_{\rm max}$ and $k_{\rm min}$. In the case of a lattice of size L and lattice spacing a, we take $k_{\rm min}=2\pi/L$ and $k_{\rm max}=2\pi/a$ which leads to

$$\rho_{\rm tot} \propto \frac{1}{a^2} \left(\frac{\eta+1}{\eta+3} \right) \frac{1-(a/L)^{3+\eta}}{1-(a/L)^{1+\eta}}. \tag{4}$$

For large enough lattices, $a/L \ll 1$, and we obtain

$$\rho_{\rm tot} \propto \frac{1}{a^2} \left(\frac{\eta+1}{\eta+3} \right). \tag{5}$$

Note that $\rho_{\rm tot}$ is given in units of 1/area. In the regime of validity of Eq. (2), $a^2\rho_{\rm tot}$ the defect density per lattice plaquette is independent of the lattice spacing. The defect-defect mean separation length is then given by $\xi \propto a\sqrt{(\eta+3)/(\eta+1)}$. In addition, the form of the spectrum [Eq. (3)] is only valid for small k. We must therefore adopt a physical ultraviolet cutoff that renders Eq. (5) sensible. This scale is the defect's width. Our statements about the *universality* of $\rho_{\rm tot}$ rest upon this choice.

In order to generate quantitative predictions we need to determine the exact proportionality factor in Eq. (5). This can be achieved by invoking the other instance when the interacting theory becomes Gaussian. In the high temperature limit $\beta \rightarrow 0$, the effective interaction becomes irrelevant: on the lattice, fields at different points will be completely uncorrelated. This situation corresponds to the VV algorithm where a field is thrown randomly at each lattice site and a network of strings is built by identifying phase windings. Figure 1 shows the agreement of the densities at $\beta=0$ with the well known VV result of $\rho_{\rm VV}=1/3$ (in lattice units), with 75% long string.[1] Since the totally uncorrelated field corresponds to a flat power spectrum $G(k)\sim k^0$ we normalize Halperin's expression by imposing $\rho_{\rm tot}=\rho_{\rm VV}$ for $\eta=2$,

$$\rho_{\rm tot}=\frac{5}{3}\left(\frac{\eta+1}{\eta+3}\right)\rho_{\rm VV}. \qquad (6)$$

This expression is valid for general lattices, given the corresponding $\rho_{\rm vv}$. For a cubic lattice and setting $\eta\simeq0.035$, the value corresponding to the universality class of the $O(2)$ model in three dimensions [12], we obtain $\rho_{\rm tot}=0.190$. This is close to the value $\rho_{\rm tot}\simeq0.2$ observed both in the $\lambda\phi^4$ [9] and XY [10] studies in three dimensions.

A similar exercise permits the computation of the critical density of domain walls for $O(1)$ and monopoles in a $O(3)$ theory at the critical temperature in three dimensions. The density of domain walls per link is

$$\rho_{\rm tot}=\left(\frac{5}{3}\right)^{1/2}\left(\frac{\eta+1}{\eta+3}\right)^{1/2}\rho_{\rm VV}. \qquad (7)$$

For a cubic lattice the density in the high-temperature limit is $\rho_{\rm VV}=1/2$ and at the critical temperature we obtain, with $\eta=0.034$ [12], $\rho_{\rm tot}\simeq0.38$. For monopoles, for the flat-spectrum case we will take $\rho_{\rm VV}\simeq0.1$. A better estimate can be obtained from a tetrahedral discretization of the sphere, resulting in $\rho_{\rm VV}=3/32$. Using

$$\rho_{\rm tot}=\left(\frac{5}{3}\right)^{3/2}\left(\frac{\eta+1}{\eta+3}\right)^{3/2}\rho_{\rm VV}, \qquad (8)$$

with $\eta=0.038$ [12] we obtain the critical value $\rho_{\rm tot}=0.040$. Finally for domain walls in two dimensions, the density per link at β_c is

$$\rho_{\rm tot}=\sqrt{2}\left(\frac{\eta}{\eta+2}\right)^{1/2}\rho_{\rm VV}. \qquad (9)$$

Taking $\eta=0.26$ [12] and $\rho_{\rm VV}=1/2$, we obtain $\rho_{\rm tot}=0.24$.

Remarkably the present procedure can be inverted to generate a typical defect network at criticality. The approximate Gaussianity of the field theory at T_c implies that the statistical distribution of fields, $P[\phi]$ is given by

$$P[\phi]=\mathcal{N}e^{-\int d^3k|\phi_k|^2/G(|k|)}. \qquad (10)$$

This distribution can be sampled by generating fields as

$$\mathrm{Re}(\phi_k),\mathrm{Im}(\phi_k)=\frac{R}{\sqrt{2}}\sqrt{G(|k|)}, \qquad (11)$$

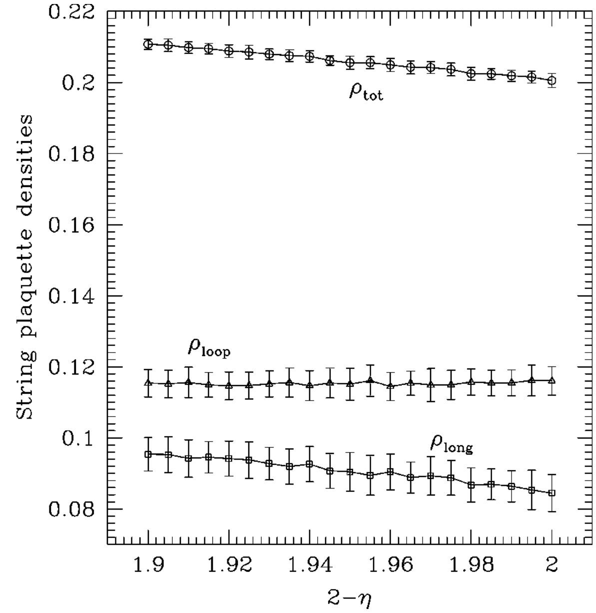

FIG. 2. The string densities from the 50 Gaussian realizations as a function of η for a lattice with $N_{\rm lat}=64$. Error bars indicate the standard deviation from the mean.

where R is a random number from a Gaussian distribution, with zero mean and unit variance. The field can then be Fourier transformed to coordinate space, its phases identified at each site, and vortices found in the standard way. We will employ the lattice form of $G(|k|)$:

$$G(|k|)^{-1}=\left[\sum_{i=1}^{D}2[1-\cos(k_i)]\right]^{(2-\eta)/2}\sim_{|k|\to0}|\mathbf{k}|^{2-\eta}. \qquad (12)$$

We have performed several tests on the algorithm, by comparing it to the results of the nonperturbative thermodynamics of the fields at criticality. We used lattices of size $N_{\rm lat}^3$ with $N_{\rm lat}=16$, 32, 64, and 128. All results are averages over 50 samples obtained from independent random realizations. Figure 2 shows the string densities for values of η between 0 and 0.1, including all reasonable values of η in three dimensions.

The values for the densities depend on the size of the lattice, converging to finite values for large $N_{\rm lat}$. In Fig. 3 we can see the scaling of $\rho_{\rm tot}$ with box size for two choices of the critical exponent, the mean field value $\eta=0.$ and the theoretical result for the $O(2)$ universality class in three dimensions: $\eta=0.035$. We can predict the form and the power of this scaling through Eq. (4). Writing $a/L=1/N_{\rm lat}$, the number of points in the lattice, and expanding Eq. (4) in powers of $1/N_{\rm lat}$ we see that Halperin's result converges to its infinite volume limit according to

$$\rho_{\rm tot}(\infty)-\rho_{\rm tot}(N_{\rm lat})=\frac{1}{N_{\rm lat}^{1+\eta}}+O(1/N_{\rm lat}^2) \qquad (13)$$

[1]This is the result for a field with a continuous phase—in their original paper [1] Vachaspati and Vilenkin used a discretized phase which leads to a smaller value of about 0.29 for the total density.

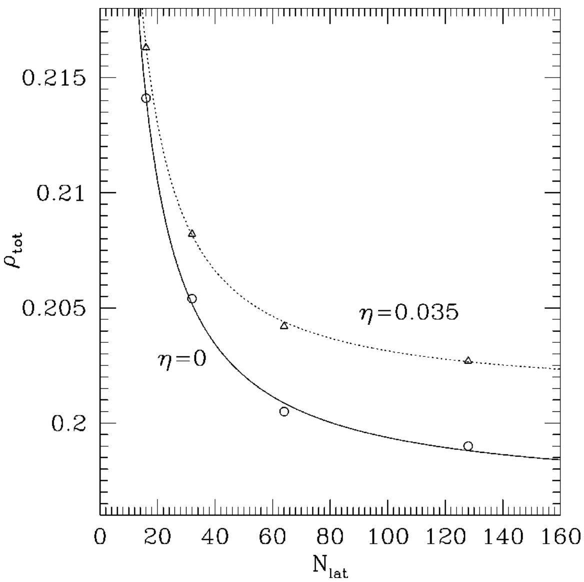

FIG. 3. The total string density for two values of η for $N_{lat}=16$, 32, 64, and 128 and respective fits to a power law. Statistical errors are much larger than the deviation of the points to the fits.

To check these scalings we fitted the data of Fig. 3 to a power law of the form

$$\rho_{tot}(N_{lat})=\rho_{tot}(\infty)+\frac{A}{N_{lat}^{\alpha}} \qquad (14)$$

For $\eta=0$ and $\eta=0.035$, we found

$$\eta=0.0, \quad \rho_{tot}(\infty)=0.1969, \quad A=0.3259, \quad \alpha=1.060,$$

$$\eta=0.035, \quad \rho_{tot}(\infty)=0.2012, \quad A=0.3422, \quad \alpha=1.124.$$

These values of α are indeed close to 1, with a larger correction for $\eta=0.035$ as expected from Eq. (13).

In Ref. [9] for a lattice of size $N_{lat}=100$ we measured $\rho_{tot}(\beta_c)=0.198\pm0.004$. For a Gaussian field with $\eta=0.035$ we obtain $\rho_{tot}=0.203\pm0.003$. The agreement of the two results is very satisfactory.

The results for ρ_{long} and ρ_{loop} using these two different methods are also in good agreement. In this case we were not able to find a reasonable scaling expression. The results for $N_{lat}=100$, using $\eta=0.035$ are $\rho_{long}=0.080\pm0.004$ and $\rho_{loop}=0.121\pm0.004$. These compare well with the nonperturbative results $\rho_{long}=0.076\pm0.005$, $\rho_{loop}=0.120\pm0.004$. Even more impressive is that the string length distribution at criticality can also be reproduced by our Gaussian field algorithm. This distribution can be successfully fitted to an expression of the form [9]

$$n(l)=Al^{-\gamma}e^{-\beta\sigma l}. \qquad (15)$$

The fit to the results of the Gaussian field algorithm shows a small variation of the parameters A,γ, and σ for $\eta\sim0.0$–0.1. σ is consistently zero, reflecting the fact that the spectrum is always scale invariant. The value of γ varies between 2.34 and 2.40. For the critical exponent $\eta=0.035$ we obtained $\gamma\simeq2.35$. Once again this is in good agreement with the result from the lattice nonperturbative thermodynamics at T_c [9], $\gamma\simeq2.36$.

Finally the predictions for ρ_{tot} from Halperin's formula, when compared to the accuracy of the Gaussian algorithm, seem rather poor. The expression is meant to apply for continuum distributions, while all other values of ρ_{tot} were obtained on the lattice. A straight substitution of the lattice correlator [Eq. (12)] into Eq. (1) increases ρ_{tot} to 0.21 from 0.19, covering our full range of results. To perform a precise comparison however Halperin's formula should be rederived for a field theory on the lattice. Despite these shortcomings Halperin's formula has the merit of being the only analytical way of estimating the critical densities of defects in theories where nonperturbative thermodynamic results are scarce.

We have therefore established the connection between the universal critical exponent characterizing the behavior of the $O(N)$ field two-point correlator and the critical density of defects. This relation implies that defect densities at T_c for a system undergoing a second order phase transition are universal numbers. Their physical values can be obtained by specifying the defect's width. We predicted them for several $O(N)$ models in two and three dimensions. Based on these insights we proposed an algorithm for generating networks of defects at the time of formation. In particular, we have shown that this algorithm reproduces accurately all the features of a string network in three dimensions at criticality. This procedure, instead of the more usual algorithm of Ref. [1], should be used to generate typical defect networks at the time of their formation.

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[1] T. Vachaspati and A. Vilenkin, Phys. Rev. D **30**, 2036 (1984).
[2] H. Kleinert, *Gauge Fields in Condensed Matter Physics* (World Scientific, Singapore, 1989).
[3] R. J. Baxter, *Exactly Solvable Models in Statistical Mechanics* (Academic Press, London, 1982).
[4] G. A. Williams, Phys. Rev. Lett. **82**, 1201 (1999).
[5] C. Bäuerle *et al.*, Nature (London) **382**, 332 (1996); V. M. H. Ruutu *et al.*, *ibid.* **382**, 334 (1996).
[6] N. D. Antunes, L. M. A. Bettencourt, and W. H. Zurek, Phys. Rev. Lett. **82**, 2824 (1999), and references therein.
[7] T. W. B. Kibble, J. Phys. A **9**, 1387 (1976).
[8] W. H. Zurek, Nature (London) **317**, 505 (1985); Acta Phys. Pol. B **24**, 1301 (1993).
[9] N. D. Antunes, L. M. A. Bettencourt, and M. Hindmarsh, Phys. Rev. Lett. **80**, 908 (1998); N. D. Antunes and L. M. A. Bettencourt, *ibid.* **81**, 3083 (1998).
[10] G. Kohring, R. E. Shrock, and P. Wills, Phys. Rev. Lett. **57**, 1358 (1986).

[11] B. I. Halperin, in *Physics of Defects*, Proceedings of Les Houches Summer School, Vol. 35, 1980, NATO ASI, edited by R. Balian, M. Kléman, and J.-P. Poirier (North-Holland, Amsterdam, 1981), p. 816; F. Liu and G. F. Mazenko, Phys. Rev. D **46**, 5963 (1992).

[12] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon Press, Oxford, 1996).

[13] C. Wetterich, in *Electroweak Physics and the Early Universe*, edited by J. C. Romão and F. Freire (Plenum, New York, 1994), p. 338, and references therein.

[14] General power laws were considered by J. Robinson and A. Yates, Phys. Rev. D **54**, 5211 (1996); R. J. Scherrer and A. Vilenkin, *ibid.* **56**, 647 (1997).