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THE ROLE OF TOPOLOGICAL EXCITATIONS AT SECOND-ORDER TRANSITIONS

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The identification of the collective degrees of freedom relevant for the description of a given macroscopic (thermo)dynamic behavior is a broad objective across branches of physics. Statistical models and field theories describing critical phenomena lead to several different kinds of collective excitations. We discuss the role of topological excitations in continuous phase transitions, including recent developments in 3D. The latter allow in principle for the construction of dual descriptions of the phase transitions in terms of these degrees of freedom and help make contact with new experiments aimed at measuring topological defectformation and evolution.

1 Introduction

Topological excitations are features of the spectrum of models describing critical (thermo)dynamics of many important systems. Examples are superfluids and superconductors, (liquid) crystals, magnets and models of high energy particle physics, which predict phase transitions in the early Universe.

Topological defects are collective excitations, largely independent of the microscopic details of the theory. Their nature is instead determined by broad characteristics of the underlying model like its symmetries and dimensionality. Thus they give a convenient mesoscopic description of the system. Qualitatively their importance is that they are in many known cases thermodynamically inexpensive vehicles of long-range disorder. For this reason they are typically associated with order-disorder transitions.

Topological excitations are known to be important in low spatial dimensions, preventing long-range order to set in. In three spatial dimensions they

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were also suggested by Onsager [1] and Feynman [2] as the vehicles of disorder responsible for destroying the superfluid state of liquid ^{4}He. In three spatial dimensions order-disorder transitions in $O(N)$ models are of second order and are well described by renormalization group methods. A description of the critical phenomenon in terms of topological excitations seems therefore unnecessary.

Independently of these considerations topological defects were proposed as a means to solve several cosmological problems [3,4]. In this context, the problem of determining densities and other properties of topological defects lead to the design of experiments that search directly for these quantities. Such experiments have now been performed in a very large range of materials and conditions, including superfluids (^{4}He [5] and ^{3}He [6,7]), high-T_c superconductors [8], liquid crystals [9], and hopefully in the near future nonlinear optical systems [10] and atomic Bose-Einstein condensates.

Motivated by these questions we have been seeking to understand the behavior of topological excitations at second-order transitions. This paper will describe some of our findings together with their relevance for a dual description of the critical phenomena in terms of topological excitation creation and/or proliferation. The dual formulation of critical phenomena in terms of topological excitations received many important contributions by Hagen Kleinert. These issues are reviewed in his book [11], to which the reader is referred.

2 Low-Dimensional Cases: Defects and Long-Range Order

The simplest example of a defect is a domain wall in the Ising model (or in a real $\lambda\phi^4$-field theory). The domain wall divides regions of space where the system is in one of two energetically equivalent minima. The domain wall costs a finite amount of energy per unit area (its tension). In the Ising model there is an exact equivalence between a description of the system in terms of domain walls (i.e. only the sites where neighboring spins anti-align) and directly in terms of the spins themselves. The model has a second-order phase transition for $D \geq 2$.

In 1D, domain walls are so likely thermodynamical that they subsist in the system all the way down to $T = 0$ in the infinite-volume limit. For this reason the system never displays long-range order at finite temperature and a second-order transition never occurs. This is the essence of the Mermin-Wagner theorem.

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In 2D the Ising model can be exactly solved. The system has a second-order transition which is associated with domain wall proliferation. The existence of walls implies local disorder in the sense that at either side of the wall both values of the spin are realized. If a wall is small and closed onto itself this disorder is local and the long-range order of the state will subsist - this situation is therefore characteristic of the symmetry broken phase, below T_c. Conversely, if a wall can be produced that crosses the volume, independently of the size of the system, then long-range order has been destroyed. This is what happens at and above T_c.

Complicating the model so that the magnitude of the spins is also a degree of freedom (resulting in e.g. a $\lambda\phi^4$-model) results in a phase transition of the same universality class - only dimensionful quantities like the value of T_c or of correlation length change but not their functional variation of temperature. The change in critical temperature can be traced back to the change of the wall tension in the new model.

As we have seen in the Ising model the description of the critical phenomenon in terms of the proliferation of walls or directly in terms of spins is exact. This ceases to be true in more general circumstances.

The next important example is the Kosterlitz-Thouless (KT) transition. It deals with the $O(2)$ model in 2D. As we have seen above this model allows for vortex solutions, in addition to other collective degrees of freedom such as spin waves and quasi-particles. Kosterlitz and Thouless [12] and Berezinskii [13] suggested that the transition in this model (between a disordered state at high temperature and a state with algebraic order at low temperature) proceeds by vortex pair separation, which, as we discussed above, leads to long-range disorder.

At long distances, vortex solutions in 2D behave as unscreened point charges, i.e. they have a $\log(r/a)$ potential. By mapping the vortex charge to the electric charge one can establish the equivalence between a gas of vortices and the Coulomb gas in 2D. In this process the remaining excitations of the model were neglected. Thus the statement that the Coulomb gas describes the transition in the $O(2)$ model is equivalent to the statement that other degrees of freedom are irrelevant in the critical region. This is a much stronger statement than the equivalence between the domain wall and the spin description in the Ising model.

The Coulomb gas has a well-known transition between an insulator and a conductor state. Conduction is associated with the presence of free charges in the plasma whereas the insulator state is characterized by dipole bound

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states.

At low temperatures there is an energetic suppression of vortices. These can only occur as bound pairs, which cost a vanishing amount of energy with separation. As the temperature is increased pairs become bigger and more frequent. As a result, screening of charges becomes more and more effective. This process continues as the temperature is increased until a critical temperature is reached such that pairs of any size can be created and the system becomes conducting.

This effect can be seen by estimating the free energy of vortices. Start below the KT transition and estimate the free energetic cost of adding a new charge dipole of a given separation R to the system. The bare interaction can be written as

$$V(R) = 2\pi\rho_s \log(R/a). \tag{1}$$

On the other hand, the number of states Ω available to the pair is $\Omega = 2\pi V R/a$, where the volume V accounts for all places where the first charge of the pair can be placed and the perimeter factor arises for all the sites the second charge can take, at a distance R from the first in 2D. Thus the free energy F for the new pair is estimated to be

$$F(R) \simeq V(R) - k_B T \log(\Omega). \tag{2}$$

There is always a temperature $T_{\mathrm{KT}} = 2\pi\rho_s/k_B$ at which it becomes possible to create a pair of arbitrary separation. Of course, in rigorously computing T_{KT} one needs to take into account the interaction between the charges of the pair and those of the existing plasma. This can be done rigorously via the Kosterlitz-Thouless recursion relations which account for the screening of the interaction of the new pair due to the polarizable medium. This effect makes the potential weaker than the bare one, as can be expected on general grounds. Thus the Coulomb gas together with the original models connected to it by duality can in fact be solved analytically. Their predictions have been confirmed with great success, e.g. in ^{4}He films and 2D superconductors [14].

We end this section by noting the fundamental role of the topological excitations in the examples considered above in bringing about the critical phenomenon. Moreover the description in terms of these excitations is simpler, which made it possible to solve the resulting dual models analytically.

In what follows we will discuss whether these advantages generalize to 3D. In 3D, $O(N)$ models always display second-order transitions, at which

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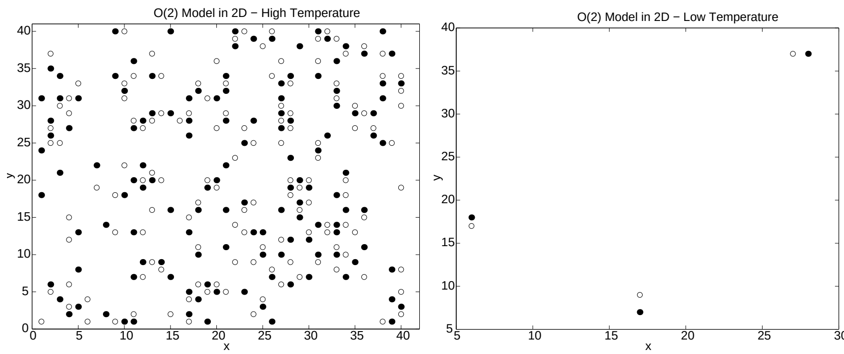

Figure 1. Typical vortex (full circles) and antivortex (open circles) configurations at high and low temperatures in the 2D XY model. At low temperatures all vortices are in pairs and the material is an insulator. The transition to a conductor proceeds by the nucleation of unpaired vortices.

the characteristic length scale diverges. Then a scaling hypothesis together with renormalization group methods allows us to compute critical exponents, which stand in excellent agreement with experiments. The description of the transition in terms of topological excitations seems therefore superfluous unless it can generate new information not easily describable in terms of field correlators.

Recently it has become clear that the existence of a description of the critical phenomena in terms of topological excitations can indeed be investigated quantitatively.

3 What Happens in Three Spatial Dimensions?

The exploration of the role of topological excitations in 3D has recently received much attention [15-18]. While it is still too early to form the complete picture, many properties of the model for $N = 2$ are now known. This section especially comprises a cursory description of this recent progress.

Very much independent of the details of the theory of second-order transitions questions arose in cosmology, first formulated by Kibble [3,4], about the possibility of forming topological defects at cosmological phase transitions. Motivated by these questions several experiments in condensed matter systems were developed to test topological defect formation in the laboratory. Defect densities can be related to the size of the correlation length in the vicinity of the critical point. But where do topological defects come from

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and why is it possible that almost no defects are formed if the system is cooled from $T < T_c$?

It is actually quite easy to answer these questions, at least in the context of specific models. Consider for example ^{4}He, one of the systems where defect formation experiments have been performed [5]. The superfluid transition is excellently described by an $O(2)$ model in 3D. This model has a simple partition function which can be readily sampled. One can then identify and characterize topological excitations in this model as a function of, say, temperature. The results are shown below. The model is also relevant for extreme type II superconductors such as all high-T_c materials.

To gauge our expectations let us follow the simple argument [19] used above to derive the conductor-insulator transition in the Kosterlitz-Thouless case. We will do so with a twist: it is extremely difficult to account for the detailed interaction between string segments because of the many configurations a string of a given size can take. We will therefore neglect them, but consider a simple string that has a given finite energy per unit length (a tension), which we call σ. The partition function is

$$Z = \mathcal{N} \int dE \; \Omega(E) e^{-\beta E}, \tag{3}$$

where $\Omega(E)$ is the number of configurations with a given energy E. Since we are considering non-interacting strings we only need to consider the number of configurations of a string of length $l = E/\sigma$.

To proceed we observe that a free string is equivalent to a gas of Brownian random walks. Furthermore we require that all string loops are closed. We regularize the problem by taking the step size to be of a given length a, which should be at least of the order of the string's core size. Then the number of configurations $\Omega(l)$ is

$$\Omega(l) = \frac{V}{a^3} A \left(\frac{l}{a}\right)^{-3/2} \left(\frac{l}{a}\right)^{-1} z^{l/a}, \tag{4}$$

where we purposefully separated several different contributions. From left to right, the first factor accounts for the number of possible starting points, the second for the probability that the string will return to its origin in l/a steps, the third removes overcounting since any point along the string is a legitimate starting point, and the forth and final accounts for the number of configurations of a walk of l/a steps, given that each step has access to z states (z is, for example, the coordination number of the lattice).

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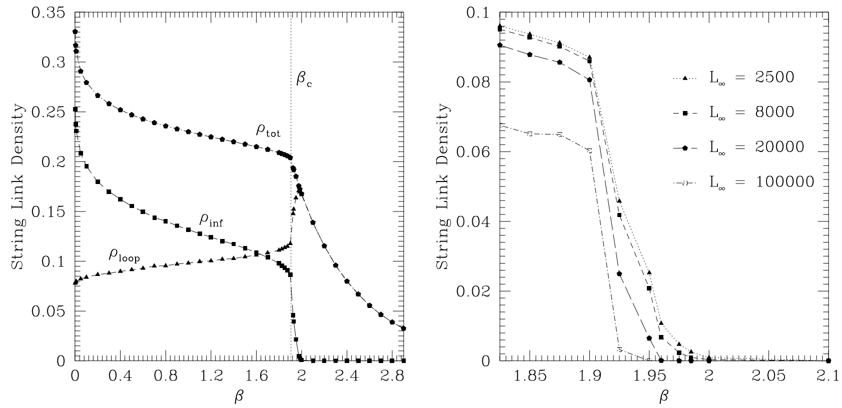

Figure 2. String densities as a function of inverse temperature β (left), for long strings $\rho_{\rm inf}$, short loops $\rho_{\rm loop}$, and total $\rho_{\rm tot}$. The transition proceeds by the creation of long strings. The long string density jumps (right) at $T = T_c$, as the length scale is taken to be larger.

The present exercise is also valid for domain walls in 2D. Walls unlike most strings experience short range interactions and for them the Brownian walk approximation is actually much better.

Notice that the number of configurations is enormous: it grows exponentially with the string's length. It is the extraordinary configurational entropy of extended topological excitations that makes them likely thermodynamically. The partition function can therefore be written as

$$Z = \mathcal{N} \sum_{L/a=1}^{\infty} \Omega(l/a) e^{-\beta l} = A' \sum_{L/a=1} \left(\frac{l}{a}\right)^{-5/2} e^{-\beta L \sigma_{\rm eff}}, \tag{5}$$

where

$$\sigma_{\rm eff} = \sigma - \frac{T \ \log(z)}{a} \equiv \sigma \frac{T_H - T}{T_H} \tag{6}$$

is the effective tension or free energy of the string per unit length. Notice that strings are exponentially suppressed at low temperatures because of their energetic cost. Thanks to the entropic contribution, however, there is a critical (Hagedorn) temperature $T_H = \sigma a / \log(z)$, at which the string length distribution becomes scale invariant and long strings are no longer exponentially suppressed.

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This transition is analogous to both the conductor insulator transition in the Kosterlitz-Thouless picture (the interacting nature of strings will be discussed below) and the wall percolation transition in the 2D Ising model.

Notice that the argument for a defect transition *per se* does not tell us the order of the transition (between analytic or second order). If a defect percolates the volume, it is clear that fluctuations of the field modulus can occur over arbitrarily large length scales - the transition must therefore be associated with a diverging length scale and be second order.

Non-interacting strings are rare. They exist e.g. at critical coupling in the Abelian Higgs model. What happens when strings do interact? The simplest case to discuss is again the vortex string in the $O(2)$ model. As discussed above, these interact with long-range $\log(R/a)$ potential between any two segments. The interaction is attractive if segments have opposite orientations (the analog of a vortex-antivortex pair) and repulsive otherwise. Consequently strings will try to minimize their energetic cost by aligning themselves in the most favorable configuration. Strings in the $O(2)$ scalar model are therefore in general self-seeking as we shall see below in more detail. The analog of a conductor insulator transition in 3D must therefore occur when string segments become free. Then the resulting strings loose their self-seeking character and should become Brownian random walks.

These qualitative expectations are realized for vortex string excitations in a complex $\lambda\phi^4$-theory. To see this we have sampled the model's partition functio n and characterized its string vortex excitations at different temperatures. The results are shown in Figs. 2 and 3.

Figure 2 shows the string densities as a function of $\beta = 1/T$. Strings cease to be exponentially suppressed at $T = T_c$ (with T_c measured via field correlators). In that case the derivative of the string densities has a discontinuity. At this same point long strings appear in the system.

What is then the quantitative character of individual strings as the temperature is changed? To proceed we will assume and confirm *a posteriori* that the length distribution of strings assumes the same functional form as Eq. (5) but with temperature dependent coefficients. Thus we take the loop length distribution to be

$$n(l) = A l^{-\gamma} e^{-\beta \sigma_{\rm eff} l}, \tag{7}$$

where l is in units of a and A, γ, and $\sigma_{\rm eff}$ will be computed numerically. The behavior of γ and $\sigma_{\rm eff}$ is shown in Fig. 3, together with the distance

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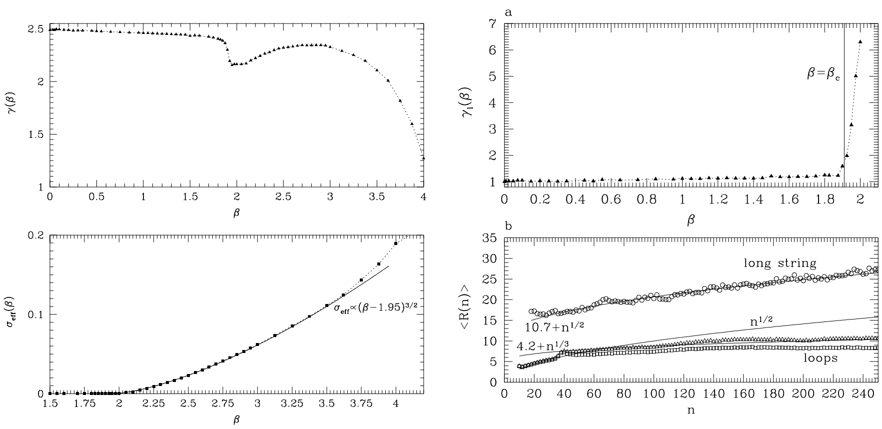

Figure 3. The critical behavior of the string tension (bottom left) and the exponent γ (top left). The long string formed at the transition is approximately Brownian. The exponent $\gamma \simeq 1$ (top right) for long strings is the correct Brownian value in a periodic domain. The Brownian character of long strings can be seen directly by plotting the distance *vs.* number of steps (bottom right), while short string loops remain self-seeking.

between two string segments as a function of length. Detailed study of these quantities indicates that strings below the transition are self-seeking, but that long strings, when produced at $T = T_c$, appear essentially as random walks.

Critical exponents measured directly in terms of strings can be related in turn to those of the field correlators [20]. This suggests that there is a dual model in terms of interacting strings that describes the system just as well as the original one based on the fields. At present it is of course still more cumbersome to compute most quantities based on such a model, in contrast to the canonical resolution of the problem in terms of scaling and the renormalization group.

Thus we have shown that for a $\lambda\phi^4$ $U(1)$ model the second-order transition is accompanied by the proliferation of strings. Results by Nguyen and Sudbø [17] and by Kajantie *et al.* [18] have confirmed the same picture for the type II Abelian Higgs model and the XY magnet, which are all in the same universality class.

The remaining question is whether the phase transition in terms of strings can somehow be seen to be more or less fundamental than that in terms of fields directly. This is certainly a difficult question. To answer it one would need to construct a statistical model in the same universality class, where one

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of the degrees of freedom (the strings or the fields) would be absent.

4 Conclusions and Discussion

We discussed how topological excitations are linked to critical phenomena in several important models. In particular the numerical investigation of models with a proven track record in terms of critical exponents has recently revealed that the phase transition there is accompanied by critical behavior in terms of topological excitations.

In 3D for $O(N)$ models, the renormalization group description of the transition is sufficient to yield thermodynamic predictions but, as we have shown, it is a generic feature of the transition that it is accompanied by topological excitation percolation, at least in the best studied cases for $N = 1, 2$. It remains unclear if either of these two perspectives for the transition is more fundamental than the other. Depending on the experimental observable either can become more advantageous.

The advantage of topological defects and other collective excitations is that they provide us with a mesoscopic description of the relevant degrees of freedom involved in the critical phenomenon. In doing so we are allowed to disregard microscopic details of the underlying theory and obtain a simpler effective description.

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