The \textit{XY} Model and the Berezinskii-Kosterlitz-Thouless Phase Transition

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Abstract

In statistical physics, the \textit{XY} model in two dimensions provides the paradigmatic example of phase transitions mediated by topological defects (vortices). Over the years, a variety of analytical and numerical methods have been deployed in an attempt to fully understand the nature of its transition, which is of the Berezinskii-Kosterlitz-Thouless type. These met with only limited success until it was realized that subtle effects (logarithmic corrections) that modify leading behaviour must be taken into account. This realization prompted renewed activity in the field and significant progress has been made. This paper contains a review of the importance of such subtleties, the role played by vortices and of recent and current research in this area. Directions for desirable future research endeavours are outlined.

1. PHASE TRANSITIONS

Phase transitions are amongst the most remarkable and ubiquitous phenomena in nature. They involve sudden changes in measurable macroscopic properties of systems and are brought about by varying external parameters such as temperature or pressure. Familiar examples include the transitions from ice to water, water to steam, and the demagnetization of certain metals at high temperature. These dramatic phenomena are described mathematically by non-analytic behaviour of thermodynamic functions, which reflect the drastic changes taking place in the system at a microscopic level. Besides materials science, phase transitions play vital roles in cosmology, particle physics, chemistry, biology, sociology and beyond; The universe began in a symmetric manner and went through a series of phase transitions through which the particles of matter with which we are familiar (electrons, protons, the Higgs boson, etc.) materialised. More mundane examples include traffic flow (where there is a transition between jammed and free-flowing states), growth phenomena and wealth accumulation (where there may be a transition to a condensation phase, for example). While the latter examples refer to non-equilibrium systems, the emphasis in this article is on a famous transition which exists in equilibrium systems.

The mathematical physics which describes such phenomena belongs to the realm of equilibrium statistical mechanics, one of the most beautiful, sophisticated and successful theories in physics. Equilibrium statistical physics is based on the following premise: the probability that a system is in a state $S$ with energy $E$ at a temperature $T$ is

$$P(S) = \frac{e^{-\beta E(S)}}{Z_L(\beta)},$$

where $\beta = 1/k_BT$ and $k_B$ is a universal constant, and $Z_L(\beta)$ is a normalising factor known as the partition function,

$$Z_L(\beta) = \sum_S e^{-\beta E(S)}.$$  \hspace{1cm} (2)

Here, the subscript $L$ indicates the linear extent of the system.

A related fundamental quantity is the free energy, $f_L(\beta)$, given by

$$f_L(\beta) = \frac{1}{T^d} \ln Z_L(\beta),$$  \hspace{1cm} (3)

where $d$ is the dimensionality of the system. Phase transitions can only occur when the system under consideration has an infinite number of states in which it can exist – for example, in the thermodynamic limit $L \to \infty$.

In the modern classification scheme, such phase transitions are categorised as first-, second- (or higher-) order if the lowest derivative of the free energy that displays non-analytic behaviour is the first, second (or higher) one. Transitions of infinite order break no system symmetries. The most famous of these is the Berezinskii-Kosterlitz-Thouless (BKT) transition in the two-dimensional \textit{XY} model \cite{1,2}.

2. THE TWO-DIMENSIONAL \textit{XY} MODEL

The model is defined on a two-dimensional regular lattice, whose sites are labeled by the index $i$, each of which is occupied by a spin or rotator $\vec{s}_i$. These two-dimensional unit vectors have $O(2)$ or $U(1)$ symmetry. The energy of a given configuration is

$$E = -\sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j,$$  \hspace{1cm} (4)

where the summation runs over nearest neighbouring sites or links. This model is used to study systems such as films of superfluid helium, superconducting materials, fluctuating surfaces, Josephson-junctions as well as certain magnetic, gaseous and liquid-crystal systems.

The scenario proposed in seminal papers by Berezinskii and Kosterlitz and Thouless \cite{1,2} is that at a temperature above the critical one ($T > T_c$ or $\beta < \beta_c$) positively and negatively charged vortices (i.e., vortices and antivortices) which are present (see Fig. 1) are unbound (dissociated from each other) and disorder the system. Below the
The fundamental realization of \([9]\) was that the thermal scaling forms \([3\) and \(9\) (and similar formulae for related thermodynamic functions) are inconsistent as they stand. Instead, they must be modified to include logarithmic corrections: \(C_{\infty}(t) \sim s^{-2}(\ln s)^{q} t^{-2}\) with \(q = 6\) and
\[
\chi_{\infty}(t) \sim t^{2-2\eta_c}(\ln \xi_{\infty}(t))^{-2r},
\]
where RG indications implicit in \([2]\) are that \(r = -1/16 = -0.0625\).

Eq. (10) is an analytic prediction, which, since it is based on perturbation theory, requires confirmation through non-perturbative approaches. However, infinite lattices are not attainable using finite numerical resources. Instead, one simulates finite systems, where, at criticality \((t = 0)\), the lattice size \(L\) plays the role of \(\xi_{\infty}\) in this model. The finite-size scaling (FSS) prediction for the susceptibility is then
\[
\chi_{L}(0) \sim L^{2-2\eta_c}(\ln L)^{-2r}.
\]

To verify the BKT scaling scenario then, the thermal formula (10) and/or the FSS formula (11) needs to be confirmed numerically. Sophisticated FSS techniques (involving partition function zeros) were used in \([8, 9]\) to resolve, for the first time, the hitherto conflicting results for \(\nu, \beta_c\) and \(\eta_c\). However, the analysis resulted in an estimate of \(-0.02(1)\) for \(r\), a value in conflict with the RG prediction of \(r = -1/16 = -0.0625\) from \([2]\).

Thus, in recent years, the focus of numerical studies of the XY model shifted to the determination of the logarithm exponent \(r\). Indeed, the FSS analyses of \([10, 11, 12]\), using \([11]\), yielded values compatible with that of \([8, 9]\) but incompatible with \([2]\) (see Table 1). Nonetheless, it was clear that taking the logarithmic corrections into account leads to the resolution of the \(\nu, \beta_c, \eta_c\) controversy. The most precise estimate for the critical temperature in the literature for the XY model with the standard action of \([4]\) is contained in \([13]\) and is \(\beta_c = 1.1199(1)\). This value was obtained by mapping the XY model onto the exactly solvable body centered solid-on-solid model, and thereby circumventing the issue of logarithmic corrections. As demonstrated in Table 1, recent analyses which have included the logarithmic corrections have resulted in estimates for \(\beta_c\) compatible with this value (while keeping \(\eta = 1/4\)). In \([11]\) and \([12]\) respectively, phase transitions in a lattice grain boundary model and a lattice gauge theory are studied. Because these are in the same universality class as the XY model in two dimensions, they have the same scaling behaviour \([11]\). However, the critical temperatures in these models bear no relationship to that of the XY counterpart. Although \([10]\) contains a study of the XY model, it employs the Villain

3. LOGARITHMIC CORRECTIONS

The critical temperature \((T < T_c\) or \(\beta > \beta_c\)) they are bound together and are relevant as dynamical degrees of freedom. There, long-range correlations between spins at sites \(i\) and \(j\) (separated by a distance \(r\), say) exist and are described by the correlation function whose leading behaviour in the thermodynamic infinite-volume limit is
\[
G_{\infty}(r) \sim r^{-\eta(\beta)}.
\]

The correlation length (which measures to what extent spins at different sites are correlated) diverges and this massless low-temperature phase persists, with the system remaining critical with varying \(\eta(\beta)\), up to \(\beta = \beta_c\) at which \(\eta(\beta_c) = \eta_c\). Above this point, correlations decay exponentially fast with leading behaviour
\[
G_{\infty}(r) \sim e^{-r/\xi_{\infty}}.
\]

Here \(\xi_{\infty}(t)\) is the correlation length, and \(t = T/T_c - 1 > 0\) measures the distance from the critical point.

As this critical point is approached, the leading scaling behaviour of the correlation length, the specific heat and the susceptibility (which respectively measure the response of the system to variations in the temperature and application of an external magnetic field) are
\[
\xi_{\infty}(t) \sim e^{bt^{-\nu}},
\]
\[
C_{\infty}(t) \sim \xi_{\infty}^{-2},
\]
\[
\chi_{\infty}(t) \sim \xi_{\infty}^{-2-\eta_c},
\]
in which \(b\) is a non-universal constant. This exponential behaviour is known as essential scaling, to distinguish it from more conventional power-law scaling behaviour (in which, for example, \(\xi_{\infty}(t) \sim t^{-\nu}\)). In summary, the BKT scenario means a transition which (i) is mediated by vortex unbinding and (ii) exhibits essential scaling.

Besides the two-dimensional XY model, transitions of the BKT type exist in certain models with long-range interactions \([3]\), antiferromagnetic models \([4]\), the ice-type \(F\) model \([5]\) and in string theory \([6]\) amongst others. Thus a thorough and quantitative understanding of the paradigmatic XY model is crucial to a wide breadth of theoretical physics.

For many years Monte Carlo and high-temperature analyses of the XY model sought to verify the analytical BKT renormalisation-group (RG) prediction that \(\nu = 1/2\) and \(\eta_c = 1/4\) and to determine the value of \(\beta_c\). Typically \(\beta_c\) was determined by firstly fixing \(\nu = 1/2\). Subsequent measurements of \(\eta_c\) yielded a value incompatible with the BKT prediction. Because of the elusiveness of its non-perturbative corroboration, the essential nature of the transition was questioned \([7]\). See Table 1 of \([8]\) for an extensive overview of the status of the model up to that point.
Table 1: Estimates for $\beta_c$ and $r$ for the XY model from a selection of recent papers with indications of the method used to obtain them (RG related, FSS or thermal scaling).

| Authors          | Year | Method   | $\beta_c$   | $r$     |
|------------------|------|----------|--------------|---------|
| Kosterlitz, Thoulless | 1973 | RG       | $-0.0625$    |         |
| Irving           | 1997 | FSS      | $1.113(6)$   | $-0.02(1)$ |
| Kenna            | 1996 | thermal  | $0.077(46)$  |         |
| Patrasciou      | 1997 | FSS      | $1.1158(6)$  | $0.042(5)$  |
| Seiler          | 1997 | thermal  | $1.120(4)$   | $-0.027(1)$ |
| Campostrini et al | 2005 | FSS      | $-0.056(7)$  |         |
| Hasenbusch, Pinn | 1997 | RG       | $1.1199(1)$  |         |
| Jaster, Hahn    | 1999 | FSS      | $-0.0233(10)$|         |
| Dukovski et al  | 2002 | FSS      | $1.120(1)$   |         |
| Chandrasekharan, Strouthas | 2003 | FSS      | $-0.035(10)$|         |
| Hasenbusch      | 2005 | FSS      | $-0.056(7)$  |         |

While large scale simulations were required to resolve these puzzles, a different technique, not requiring extensive simulations was used in [15]. A conformal mapping was used to switch from a confined $L \times L$ lattice to the semi-infinite half plane. In this way, $\eta(\beta)$ could be deduced from the correlation function at any value of $\beta \geq \beta_c$. In particular, $\eta_c = 1/4$ is accurately recovered at the transition temperature and clear evidence for existence of logarithmic corrections in the correlation function $G(r)$ is presented.

4. VORTEX UNBINDING

The vortex-binding scenario is crucial to the BKT phase transition in the two-dimensional XY model. Because the energy of a single vortex increases with the system size as $\ln L$, at low temperature they can only occur in vortex-antivortex pairs. Mutual cancelation of their individual ordering effects means that such a pair can only affect nearby spins and cannot significantly disorder the whole system. Topological long-range order exists in the system at low temperature. However at high temperature, the number of vortices proliferates and the distance between erstwhile partners becomes so large that they are effectively free and render the system disordered.

It was for a long time believed that altering the energetics of the XY model to disable the vortex-binding scenario may lead to a transition different to the Berezinskii-Kosterlitz-Thouless one [19]. The step model is obtained from the XY model by replacing the Hamiltonian [4] by

$$E = -\sum_{\langle i,j \rangle} \text{sgn}(\vec{s}_i \cdot \vec{s}_j).$$

The energy associated with a single vortex for this system is expected to be independent of the lattice size. Therefore, on the basis of this argument, vortices could exist at all temperatures, disordering the system. I.e., there was expected to be no vortex-driven phase transition in the step model – if there is a phase transition, it was expected not to be of the BKT type. Indeed, early studies supported this assertion [19].

However, in [8,9], very strong numerical evidence was presented that (i) there is a phase transition in the step model and (ii) it is of the BKT type (with even the corrections to scaling being the same as those for the XY model). Given the very different vortex energetics for the two models, this came as a surprise.

The issue was further addressed in [20], where evidence for the existence of a BKT transition in the step model was again proffered. The approach of [20] focused on numerical analyses of the helicity modulus, which experiences a jump at the transition. A similar approach to the XY model is contained in [21]. The main idea of [20], which explains the occurrence of the BKT transition in the step model, is that while the energy associated with a single fixed vortex in the system remains finite, the free energy grows as $\ln L$. This fact inhibits proliferation of free vortices in the low-temperature phase. It further implies that the harmonic properties of the interaction [4] do not form a necessary condition for a BKT transition. Consequently, and as pointed out in [20], the BKT phase transition may...
be an even more general phenomenon than hitherto recognised.

5. FUTURE DIRECTIONS

Asymptotic freedom of \( d = 2 \) \( O(N) \) models: It is generally believed that there are differences of a fundamental nature between abelian and nonabelian models. The \( XY \) model has an \( O(2) \) symmetry group and is abelian, while all \( O(N) \) models with \( N > 2 \) are nonabelian. The Mermin-Wagner theorem states that a continuous symmetry of the \( O(N) \) type cannot be broken in two dimensions \[22\]. Thus there cannot be a transition to a phase with long-range order in either of the \( N = 2 \) or \( N > 2 \) scenarios there. However, in a two-dimensional theory, topological defects of dimension \( m \) can exist if the \((1-m)^{th}\) homotopy group, \( \pi_{1-m} \), of the order parameter space is non-trivial. For \( O(N) \) models, this space is the hypersphere \( S^{N-1} \). The only non-trivial group is \( \pi_1(S^1) \) which is isomorphic to the set of integers under addition. This is the condition that gives rise to point defects (vortices) with integer charge in the \( N = 2 \) case (the \( XY \) model). The binding of these vortices at low temperatures is the mechanism giving rise to the BKT phase transition \[11, 22\].

For \( N > 2 \), conditions are not supportive of the existence of topological defects of this type and the widely held belief is that there is no phase transition, there being no distinct low-temperature phase. Perturbation theory predicts that the \( N > 2 \) models are asymptotically free. There is, however, no rigorous proof to this effect. This belief has been questioned and \[14, 22\] have given numerical evidence for the existence of phase transitions of the BKT type in these models as well as heuristic explanations of why such transition could occur and a rigorous proof that this would be incompatible with asymptotic freedom.

Perturbative and Monte Carlo calculations for the \( N = 3 \) and \( N = 8 \) models have been performed in \[23\], which do not support the existence of such a BKT-like phase transition there and instead are in agreement with perturbation theory and the asymptotic freedom scenario. Nonetheless, the controversy has not entirely gone away \[23, 24, 25\], and one may argue that inclusion of logarithmic considerations could help for a precise unambiguous resolution.

The diluted \( XY \) model: An interesting current topic of research has been the question of the role of impurities in the \( XY \) model \[28\]. The presence of impurities brings the model closer to real systems, where such physical defects are present. Impurities are modeled by randomly diluting the number of sites (or bonds) on the lattice. Clearly, if the dilution is so strong as to inhibit the percolation of spin-spin interactions across the lattice (such that it is effectively broken into finite disconnected sets) no phase transition can occur for any model. Thus moderate dilution generally is expected to decrease the location of the transition temperature. However, the special additional feature of the \( XY \) model is the presence of vortices and the fact that they drive the transition. Vortices are attracted to and, to some extent, anchored by impurities and the vortex energy is reduced at such a vacancy. Therefore with increasing dilution, more vortices can be formed and the amount of disorder in the system is increased. This effect may enhance the lowering of the critical temperature to such an extent that it vanishes before the percolation threshold is reached.

This is the issue addressed in \[28, 29, 30, 31\]. The percolation threshold occurs when the density of site vacancies is \( \rho = 0.41 \). The critical vacancy density is identified by the vanishing of the critical temperature, which in turn is identified as being the location at which \( \eta(\beta) = 1/4 \). In \[29\] the critical temperature was reported to vanish above the percolation threshold at vacancy density \( \rho \approx 0.3 \). However, in \[30\] it was suggested that the critical density is, in fact, closer to the percolation threshold. Support for the latter result recently appeared in \[31\]. If this is true, it means that the vortices do not, in fact, strongly enhance the lowering of the critical temperature.

From the collective experience with the pure \( XY \) model as reported above, it is clear that a more precise identification of the critical temperature through \( \eta(\beta) = 1/4 \) would require taking account of the logarithmic corrections, although ignoring them may suffice as first approximation. Indeed, ignoring these corrections in the pure model also leads to an estimate for the critical temperature which is higher than accurate values \[31\].

Besides the value of the critical temperature in a diluted model, one is also interested in the scaling behaviour of the thermodynamic functions at the phase transition there. The Harris criterion predicts that disorder does not change the leading scaling behaviour of a model if the critical exponent \( \alpha \) associated with the specific heat of the pure model is negative \[32\]. This is the case for the \( XY \) model in two dimensions. However, it is unclear what effect dilution can have on the quantitative nature of the exponents of the logarithmic corrections in such a case. This would be an interesting avenue for future research, and the \( XY \) model (which has negative \( \alpha \)) offers an ideal platform upon which to base such pursuits.

Other models with logarithmic corrections: Logarithmic corrections to scaling also exist in other important models. While their existence has been unambiguously verified in \( d = 4 \) \( O(N) \) models \[33, 34\], this is not so in most cases \[35\]. In particular, Kim and Landau applied FSS techniques to the four-state \( d = 2 \) Potts model \[36\]. Again, FSS behaviour could only be described if the logarithmic corrections are included. However, here inclusion of the leading multiplicative logarithmic corrections is insufficient and sub-leading additive corrections are required. The puzzle of why unusually large numbers of correction terms are necessary (despite the availability of the exact value of \( \beta_c \) in this model) could, perhaps, now be resolved by an analysis on the scale of \[17\] and this would be another interesting avenue to pursue. Similar problems concerning logarithmic corrections and their detection exist in other two-dimensional models such as the diluted Ising model \[37\]. Theoretical progress on the general issue of logarithmic corrections will be reported elsewhere \[35\].

6. CONCLUSIONS

The issue of topologically driven phase transitions characterized by the two-dimensional \( XY \) model has been revis-
itted and a timely review of the status of scaling at the famous Berezinskii-Kosterlitz-Thouless transition given. After two decades of work, the perturbative renormalization group predictions of \( \nu = 1/2 \) and \( \eta_c = 1/4 \). The recent controversy over the value of the leading logarithmic correction exponent \( r \) (summarized in Table 1) has been re-examined and claims as to its resolution (at least in the context of finite-size scaling) and state-of-the-art calculations summarized [17]. Besides the XY model, such multiplicative logarithmic corrections are manifest in a variety of other models, and their resolution in these contexts is now at the forefront current modern numerical investigations in statistical and lattice physics. A summary of some recent work on such models, as well as likely future directions has been given.

Finally, recent work [20] confirming the vortex-binding scenario as the phase transition mechanism in the XY model has also been reviewed to complete a full account of the current status of one of the most remarkable and beautiful models in theoretical physics.

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