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KOSTERLITZ-THOULESS TRANSITIONS IN SIMPLE SPIN-MODELS WITH STRONGLY VARYING VORTEX DENSITIES

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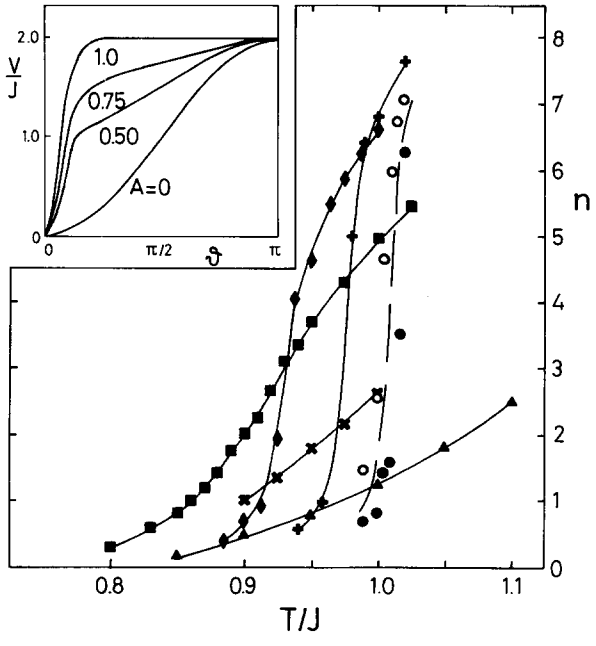
A generalized XY-model, consisting of a family of nearest neighbour potentials of varying shape, for classical planar spins on a two-dimensional square lattice is analysed by a combination of Migdal-Kadanoff real-space renormalization and Monte Carlo simulations on a sequence of finite lattices of up to 256×256 spins. For all potential shapes, Kosterlitz-Thouless transitions are found with the same universal features as in the pure XY-model, whereas the density of vortices in the transition region depends strongly upon the shape of the potential.

The seminal work of Kosterlitz and Thouless[1], more than a decade ago, has led to qualitative understanding of the nature of phase transitions in low-dimensional systems that involve topological excitations. Since then, such transitions have been found to play an important role in a variety of physical systems[2]. Their universal features have often been understood quantitatively, primarily within the framework of dilute Coulomb gas renormalization group equations[3], which are applicable as long as the density of topological excitations is sufficiently low. In addition, computer simulations have yielded a wealth of information on specific (finite) systems, that do not lend themselves to analytic treatment[4]. However, sofar relatively little attention has been paid to rather simple systems in which the density of topological excitations in the transition region can be varied systematically, with an aim at clarifying the importance of their precise behaviour for a complete description of the phase transition, with inclusion of its non-universal aspects.

An important case in point is a two-dimensional (square) lattice of classical planar spins subject to a family of nearest neighbour potentials whose shape can be varied continuously[5,6,7]. In this work we consider a family of such potentials, V(θ), of the form

$$V(\theta) = 2J[(1-A)(1-\cos^2\tfrac{1}{2}\theta)+A(1-(\cos^2\tfrac{1}{2}\theta)^p)] \quad , \quad (1)$$

where $\theta \equiv \theta_i - \theta_j$ is the difference in orientation of nearest neighbour spins <i,j>, J>o (ferromagnetic coupling). The parameter A is varied between A=o (pure XY-model) and A=1; p=50 in all the following[8]. As a result, V takes on shapes depicted in figure 1 (inset). This system is studied by means of real-space Migdal-Kadanoff (MK) style renormalization group (RG) equations[9] and by conventional Monte Carlo simulations[10]. Like the pure XY-model (A=o), all these potentials are expected to support (anti)vortices, and, indeed, upon variation of A, marked differences in the temperature dependence of the vortex-antivortex pair density are observed from the MC-data (figure 1), together with substantial variations of the

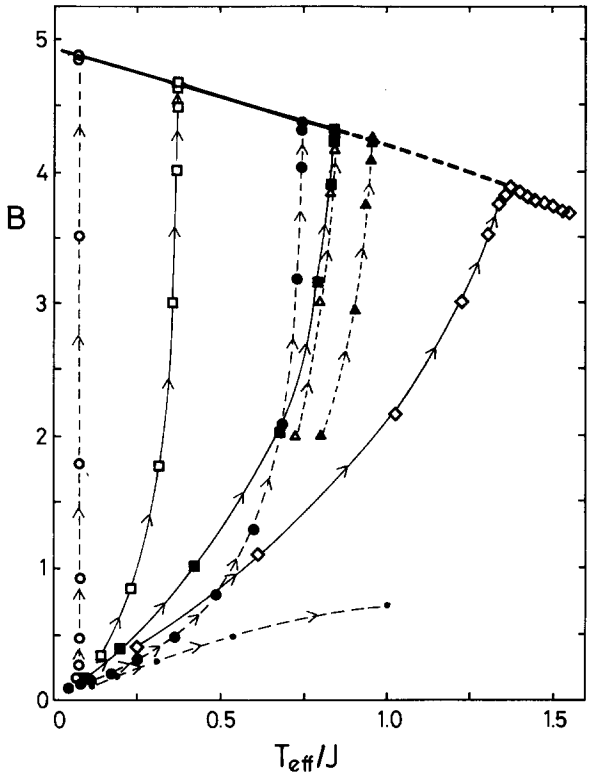


1. Density n (per site ×10^2) of vortex-antivortex pairs as a function of temperature for potentials as shown in the inset. Triangles (A=o), tilted crosses (A=0.25), squares (A=0.50), diamonds (A=0.75), crosses (A=0.90), circles (A=1). Curves are drawn to guide the eye.

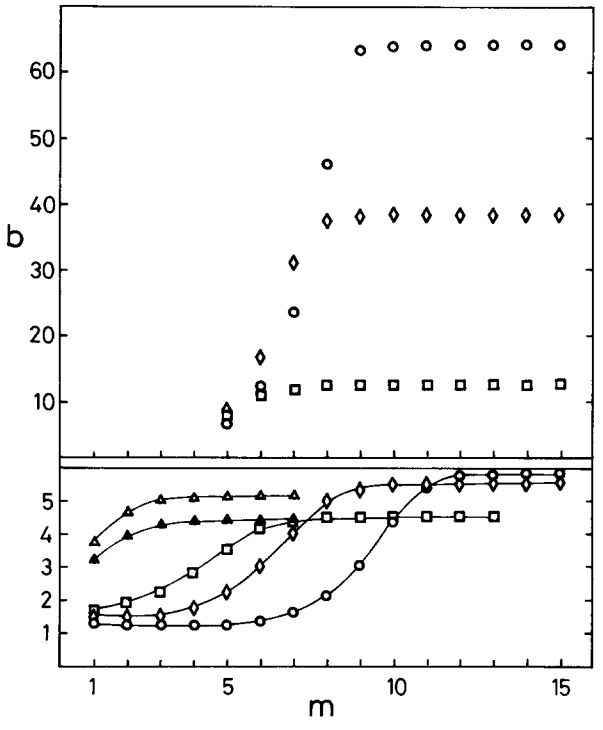
transition temperature (figure 4). The latter is obtained from MC-data on the specific heat and helicity modulus[6]. Notice the apparent hysteresis of the A=1 data in figure 1, which will be discussed later.

A complete picture of the RG behaviour of the system can be inferred from figures 2 and 3. We have used the RG transformation applied in ref. 9 to the pure XY-model, namely

$$\exp(v^{(m+1)}(s_1)) = \{\sum_{s=-\infty}^{+\infty} \exp(v^{(m)}(s)+v^{(m)}(s_1-s))\}^2/D \quad , \quad (2)$$



2. RG flow of B, T_{eff} according to (2). Heavy black line: approximate fixed line. Data are successive iterations. A=1, circles connected by dashed lines; A=0.50, squares with full lines; A=o, triangles.



3. Bare barrier height b versus number of iterations m, for an initial temperature close to T_{MK} (lower part), and for 10% lower temperature (upper part; except empty triangles (A=o) which fall into lower part). Meaning of symbols same as in fig. 1.

m designates the mth iteration; exp(v(s)) is the fourier transform of exp(v(θ)), and $v(\theta) \equiv -\beta V(\theta)$ ($\beta=1/T$). The denominator D equals the sum over s_1 of the expression in the numerator. This is clearly the most transparent way of studying the system, since it shows directly how V(θ) behaves under renormalization. At each stage of the renormalization, the potential is characterized by only two parameters, an effective "temperature"

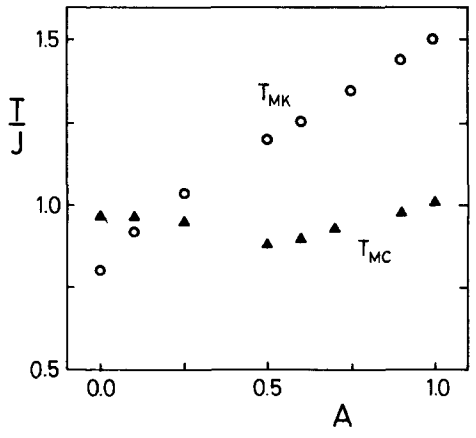
$$T_{eff}^{-1} \equiv -\frac{d^2 v(\theta)}{d\theta^2}\Big|_{\theta=o} = \sum_s s^2 e^{v(s)} \Big/ \sum_s e^{v(s)} \qquad (3)$$

(whose initial value at temperature T is given by $T_{eff}^{-1} = T^{-1}(1-A+pA)$), and a bare "barrier" height b, or scaled height B, given by

$$b \equiv v(\theta=o) - v(\theta=\pi) \; ; \; B = b\, T_{eff} \; . \qquad (4)$$

A plot of B versus T_{eff} (figure 2) reveals, that for all A the system is characterized by the same fixed line, with the same end point, as in the pure XY-model[11]. Only the flow towards this fixed line is vastly different as one varies A. As A approaches unity, the entire fixed line is sampled over an increasingly narrow range of temperatures, which is reflected by the behaviour of the vortex-antivortex pair density (fig. 1). E.g. at A=0.50 results shown are at T/J = 1.08, 1.19 and 1.25, at A=1 at T/J = 1.3698, 1.50150 and 1.50157. Nevertheless, the renormalized fixed potentials, at given T, are extremely different, as one can see in figure 3, where the barrier b is plotted as a function of the number of RG steps m. The lower part shows b(m) at a temperature close to T_{MK}, the temperature mapped onto the (approximate) end point of the fixed line and identified with the transition temperature (see fig. 4). The upper part shows b(m) at a 10% lower T (same as in fig. 2) for various values of A: $b_\infty = \lim_{m\to\infty} b(m)$ is seen to increase rapidly with A, which is again consistent with the behaviour of the vortex-antivortex pair density. One is therefore temped to conclude from these RG results, that all these potentials exhibit a Kosterlitz-Thouless transition characterized by the dissociation of vortex-antivortex pairs, despite the completely obscure way in which the Migdal-Kadanoff scheme treats the vortices. (And, indeed, not all predictions of this scheme are at least qualitatively correct, e.g. the transition temperatures (fig. 4). One may argue, however, that this is a non-universal feature.)

For the case A=1, and variable p, the above observation has first been made in ref. 7, on the basis of sample MK style renormalization, using an indirect representation of the potential. And, as a result, the first order nature of the transition at A=1, p=50, found in ref. 5 and 6, has been questioned in ref. 7. The above complete MK renormalization for the family of potentials (1), in the spirit of ref.

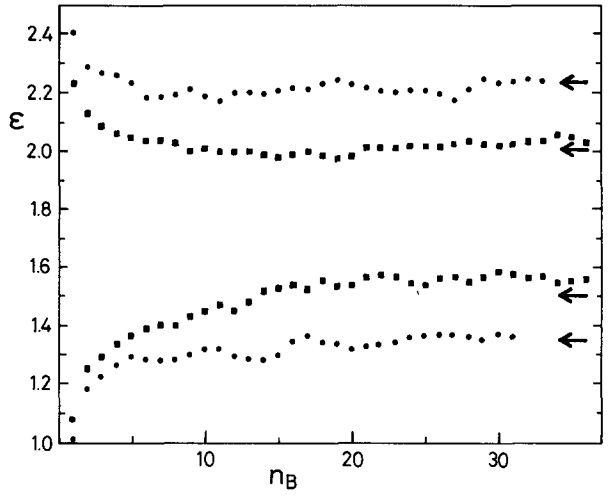


4. Approximate transition temperatures as a function of A, from MK renormalization (T_{MK}) and MC simulation (T_{MC}).

9, underscores this point. However, lingering doubts about the ability of the MK scheme to reflect the correct behaviour of vortices upon renormalization, call for more direct evidence. This is presented here in the form of very long MC simulations on a (very) large, judiciously chosen system.

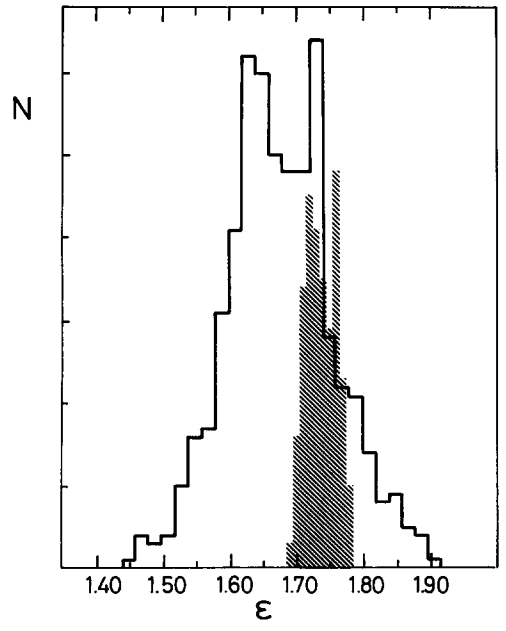
For A=o, it is well known that the system exhibits a continuous transition. For A=1, the transition appears to be first order upon consideration of MC simulations of lattices up to 128×128 spins[5]. In fact, the MC evidence, that supports this conclusion, can be further expanded. Figure 1 shows, that not only the average energy[5], but also the vortex-antivortex pair density exhibits marked hysteresis in a small neighbourhood of T = 1.01, the approximate transition point. The upper branch (open circles) is obtained by thermalization of the system from a completely disordered initial configuration (cooling run), the lower one (full circles) from a completely ordered initial configuration (heating run). Figure 5 shows, that even on lattices of 256×256 spins (the maximum size considered in this work) the average energies per spin for cooling and heating runs do not show the slightest tendency of approaching each other (which would have been an indication for cross-over to a continuous transition). Finally typical configurations, obtained upon cooling the system, reveal highly non-uniform distributions of (anti)vortices; they occur predominantly in rather small pairs, close together, in islands that only fill part of the lattice.

However, we may now return to the RG results once more, in order to deduce a rough estimate of the lattice size, at which a cross-over between first order and continuous transition may be expected to become visible. From fig. 3 (bottom part) we observe that the number of iterations needed to approach the end point of the fixed line rapidly increases with A. Intuitively, we may expect to need at least a lattice of $2^m \times 2^m$ spins in a simulation, with m large enough for the fixed line to have been approached. This means, that, for A=1, we would need a lattice of some $2^{11} \times 2^{11}$ spins, in order

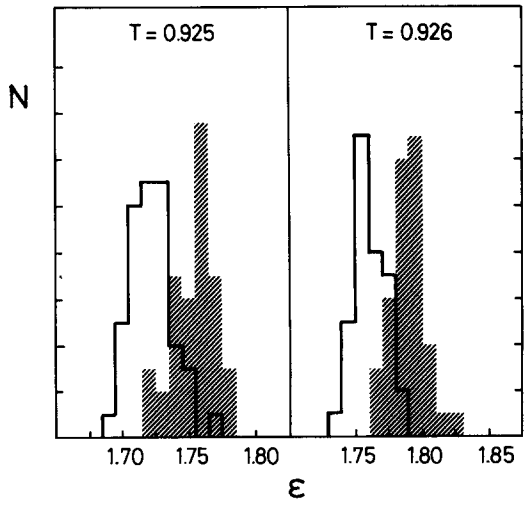


5. Block averaged energies per spin ε versus number of blocks n_B in the course of MC runs on a $2^8 \times 2^8$ lattice. Circles for A=1.0 at T/J=1.01, squares for A=0.90 at T/J=0.975. Upper branches are cooling runs, lower branches heating runs. Arrows indicate approximate location of the two peaks found in the distribution of ε-values on a 60×60 lattice.

for the onset of cross-over to be seen. Since we cannot treat such a lattice here, a smaller value of A has to be considered, for which evidence on a rather small lattice still indicates first order behaviour. For A=0.75, the transition is apparently first order on a 60×60 (and smaller) lattice, while effects of cross-over are visible on a lattice of $2^8 \times 2^8$ spins. The results are summarized in figures 6 and 7. For a 60×60 lattice, at T=0.925, the distribution of average energies shows a clear double peak structure[12]. Unlike in the case A=1, the energy fluctuations clearly limit our ability to resolve the peaks very accurately. For this reason close to 10^6 sweeps through the entire lattice are made, and the second peak at $\epsilon \sim 1.73$-1.74 is persistently present. For a lattice of $2^8 \times 2^8$ spins, where energy fluctuations are much smaller, a distinct double peak structure is present. The separation, however, is definitely not more than half that for the 60×60 lattice, even with allowance for the unprecise location of the peaks on the smaller lattice. The small overall shift of the distribution (fig. 6) with lattice size, at T=0.925, is unimportant, and due to the fact that the energy is a very steep function of temperature (see also fig. 7). In fact, the finite lattice transition temperature has saturated, for a 60×60 lattice, to within limits much smaller than indicated by the size of the data points in figure 4. Nevertheless, in order to be certain that our result is not misleading, because of the possibility of small changes in the finite lattice transition point, we calculated the remnants of hysteresis on a $2^8 \times 2^8$ lattice for different temperatures (fig. 7). The difference in peak locations is found to be equally small. Finally, to be sure, that the differences between heating and cooling runs,



6. Number N (arbitrary units) of block-averaged ε-values on a 60×60 lattice, $8.3.10^5$ measurements, and on a $2^8 \times 2^8$ lattice (shaded distribution), $1.3.10^5$ measurements, at T=0.9250.



7. Distribution of block-averages on a $2^8 \times 2^8$ lattice at T=0.9250 and T=0.9260. Results obtained upon heating and cooling (shaded distribution) are shown separately.

small as they are on a $2^8 \times 2^8$ lattice, are not an artifact altogether, we evaluated energy distributions well outside the transition region, at T=0.915 and 0.935, and find perfect overlap between heating and cooling results there.

In conclusion then, for A=0.75 there exists a small amount of energy hysteresis which diminishes with increasing lattice size. This strongly suggests, that the infinite system exhibits a continuous rather than a first order transition. Clearly, one would have liked to observe this feature e.g. at A=1, where it should be far more pronounced. This, however, would involve simulation on a forbiddingly large lattice, as the MK renormalization already indicates. Indeed, on lattices up to $2^8 \times 2^8$ spins, the transition still appears to be beautifully first order; finite size effects seem to have saturated (fig. 5), but, in fact, extremely large lattices have to be considered.

In summary, our main result for generalized XY-models, given by expression (1), is the existence of Kosterlitz-Thouless (continuous) transitions for all potential shapes, with the same universal features as in the pure XY-model (A=o,p=1), but with a strong dependence of the density of vortices, in the transition region, upon the shape of the potential. In the MC simulations, the continuous nature of the transition is inferred from the behaviour of the thermal energy on a sequence of finite lattices, whose maximum size needs to be increased drastically as the shape parameter A approaches unity, in order to establish cross-over from first order to continuous behaviour.

The fact, that the transition is always continuous for potentials of the form (1), or those discussed in ref. 5 and 6, is interesting for at least two reasons. Simulations are widely used to study systems with topological excitations, and, usually, there are no a priori indications as to how large a finite system should be considered. The present work identifies steep variations of the density of topological excitations over a small temperature range, caused here by the shape of the interaction, as one factor that may critically influence the apparent behaviour of finite systems. This is made particularly clear by studying a whole family of simple potentials, rather than one isolated, often complicated interaction. Secondly, it would be interesting to study RG equations directly involving the vortices[3,9], for such strongly varying densities. To achieve this, one would like to represent the model in terms of Coulomb gases, which would form the natural starting point for a renormalization group treatment. Unfortunately, that is not straightforward as soon as $p > 1$ [13].

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10. Measurements are made after each sweep through the lattice. Block-averaged values contain $1.5.10^3$ measurements. Heating and cooling runs occur in about equal numbers. For 60×60 lattices several independent runs of at least 10^5 sweeps are used, and a very conservative 10^4 sweeps are discarded for thermalization. For $2^8 \times 2^8$ lattices one very long run is made, both heating and cooling the system, and typically 2. to 3.10^4 sweeps are discarded for thermalization. Other details not relevant to a selfcontained presentation can be found in: J.E. van Himbergen, J. Phys. C17 (1984) 5039 and in ref. 6.
11. Only selected results are shown in fig. 2. As in the pure XY-model, there is no rigorous fixed line within the MK-scheme; see ref. 9 for a full discussion.
12. Also studied were the distribution of 3.10^5 to 6.10^5 energies at T=0.920 (no structure), T=0.9225 (one large peak at $\epsilon \simeq 1.60$ and a small shoulder at higher ϵ), T=0.9260 (a broad peak at $\epsilon \simeq 1.80$ and a large shoulder at lower ϵ, which cannot be clearly distinguished as a second peak) and T=0.9275 (no structure). This clearly places T=0.9250 in the center of a small apparent hysteresis loop.
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