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Phase transitions in three dimensional generalized xy models

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Abstract. Generalized xy lattice spin models consist of three-component unit vectors, associated with a D-dimensional lattice (say $\mathbb{Z}^D$), parameterized by usual spherical angles (θ_k, ϕ_k), and interacting via a ferromagnetic potential restricted to nearest neighbours, of the form $W_{jk} = -\epsilon(\sin\theta_j \sin\theta_k)^p \cos(\phi_j - \phi_k)$, $p \in \mathbb{N}$, $p \geq 1$; here ϵ is a positive quantity setting energy and temperature scales. The models were recently introduced, and proven to support an ordering transition taking place at finite temperature when $D = 3$; in turn, this transition had been investigated by different techniques for $p = 2, 3, 4$, and found to belong to the same universality class as the xy model (i.e. $p = 1$). More recently, it was rigorously proven that for sufficiently large p the transition becomes first order. Here we present a detailed analysis of the transitional properties of this class of models for selected values of p. For $p = 8$ simulation results showed a second order phase transition belonging to the xy class of universality; they suggested tricritical behaviour for $p = 12$, and gave evidence of first-order transitions for both $p = 16$ and $p = 20$.

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1 Introduction and potential models

The critical behaviour of statistical mechanical lattice spin models depends upon a few features such as lattice dimensionality, number of spin components, functional form (especially range and symmetry) of the interaction potentials; over the years, such models have been deeply and extensively studied for their own sake, as well as used to describe, in a way both comparatively simple and reasonably adequate, a variety of physical situations such as solid solutions, magnetically ordered systems, nematic and sometimes cholesteric liquid crystals, adsorption phenomena. The simplification resulting from the neglect of translational degrees of freedom had made it possible to obtain rigorous mathematical results [1,2] entailing existence or absence and sometimes type of a phase transition, and, on the other hand, to study it by a whole range of techniques, such as Mean Field and Cluster Mean Field treatments, high-temperature series expansion of the partition function, Renormalization Group and computer simulations. For a review on the critical behaviour of the simplest of these models see reference [3] and references therein.

Other, more elaborate potential models involve (in some combination or other) isotropic or anisotropic linear couplings between spin components, sometimes higher powers of scalar products among the interacting spins, multipolar (usually dipolar) interactions, Dzyaloshinski-Moriya terms, single-site anisotropy fields; in some specific favourable cases one has even been able to match the model and its potential parameters with the experimental system [4]. The nature of the magnetic ordering transition observed experimentally in the absence of an external field can be of both second (more frequently) or first order. This might, for example, result from doping by nonmagnetic impurities, anisotropy of interactions in spin space, or coupling to the lattice (for extensive reviews see [5,6]).

This paper addresses some recently introduced lattice spin models, defined by [7]:

$$W_{jk} = -\epsilon(\sin\theta_j \sin\theta_k)^p \cos(\phi_j - \phi_k), \ p \in \mathbb{N}, \ p \geq 1. \quad (1)$$

where ϵ is a positive quantity setting energy and temperature scales (i.e. $T = k_B t/\epsilon$, where t denotes the absolute temperature). Here we consider three-component spins (unit vectors) parameterized by usual spherical angles (θ_k, ϕ_k), and coupled by a ferromagnetic interaction potential restricted to nearest neighbours; notice that the case $p = 1$ corresponds to the usual xy model. On the other hand, the planar rotator (PR) model involves

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two-component spins, parameterized by polar angles φ_j, and the interaction reads

$$U_{jk} = -\epsilon \cos(\varphi_j - \varphi_k); \tag{2}$$

this interaction potential can also be recovered as a limiting case of equation (1), by setting $p = 0$. In this case the θ-dependence only survives in the free-spin measure.

The xy model can be regarded as an extreme case of a general anisotropic Heisenberg model. Actually, the terminological convention adopted here as well as by other Authors is not always followed, and the name "xy model" is sometimes used in the Literature to indicate planar rotators; on the other hand, both models are known to produce the same universality class. The two named models have a rich variety of applications in condensed matter physics [8]; they describe magnetic films with planar anisotropy, but also thin-film superfluids or superconductors, or two-dimensional solids. In Statistical Physics, they were also extensively studied for fundamental reasons, as describing, for example, classical Coulomb gas or fluctuating surfaces and the roughness transition; although no exact solution exists for them, many of their essential properties are known from different approaches [9].

As for the rôle of p in equation (1), notice also that it could be taken to be a real positive number, say ranging between 0 and 1 (and hence continuously interpolating between PR and xy models); on the other hand, larger values of p reinforce the out-of-plane fluctuations; this makes it possible to widely vary the anchoring of spins with respect to the horizontal plane which might have direct experimental relevance; as for the model, this change of anchoring is ultimately reflected by the significant changes in transition behaviour, as explained below.

As discussed in reference [7], on the basis of the known behaviour of the planar rotator model [1,2,10] and of available rigorous inequalities (i.e. Ginibre's inequalities [11–14], and Wells' inequality together with its generalizations to continuous spins [15–18]), one can conclude that, when $D = 2$ and for all values of p, the named potential models produce orientational disorder at all finite temperatures, and support a Berezinskiĭ-Kosterlitz-Thouless(-like) (BKT) transition [15–17]; this result was already known for the xy model (see, e.g., Ref. [10]). On the other hand, when $D = 3$, these models support ordering transitions taking place at finite temperatures; in both cases, the transition temperatures are bounded from above by the corresponding values for the planar rotator counterpart. Notice, however, that the mathematical results in reference [7] did not fully specify the nature of the transition.

For $D = 3$ a Mean Field (MF) approach as well as its Two-Site Cluster (TSC) refinement have been used in reference [7] to estimate transition temperatures for $p = 2, 3, 4$. Notice also that $(\sin\theta)^p$, and hence the absolute value of the interaction potential, decrease with increasing p, and this aspect is reflected by the p-dependence of the estimated transition temperature. Models defined by $D = 3$ and $p = 2, 3, 4$ have been studied via extensive Monte Carlo (MC) simulations in reference [19]. The phase transition was found to be of the second order, and the model to belong to the xy universality class. Furthermore, it has been found that the p-dependence of critical temperature follows a power-law decay, at least for the values used there.

The Authors of reference [20] had estimated transition temperatures by other techniques as well, i.e. by self-consistent harmonic approximation (SCHA), both for $D = 2$ and $D = 3$, and found that the transition temperature is decreasing against p. In this case however we do not have the power-law decay found for the above mentioned methods [19]. Moreover, a study of the models in their continuum limits, carried out by the same Authors [20], also showed that out-of-plane fluctuations, and consequently the magnon density, decrease with increasing p. Models defined by $D = 2$ and $p = 2, 3, 4, 5$ have been studied by MC simulations in reference [21], and found to produce a BKT-(like) transition, possibly changing to a first-order transition for larger p, due to the large number of vortices and strong out-of-plane fluctuations.

More or less simultaneously with the above study, a somewhat similar situation, involving interactions isotropic in spin space and suitable polynomials in the scalar product, had been investigated in references [22,23], where the possible existence of first-order transitions had been proven rigorously, thus justifying previous conjectures based on simulation evidence. More precisely, the named models have the form (possibly within numerical factors)

$$V_{jk} = -\epsilon(2^{-p})\,(1+\tau)^p, \tag{3}$$

where $\tau = \tau_{jk}$ denotes the scalar product between the two interacting 2- or 3-component spins; it was proven [22,23] that a first-order transition takes place for $D = 2, 3$ and sufficiently large p, and that this behaviour is independent of the nature of the low-temperature phase. Simulation evidence of this behaviour had first been produced some twenty years ago for $D = 2$ and the 2-component case [24,25], and various objections were raised against this interpretation (e.g. Ref. [26]); Evidence of a first-order transition for $D = 2$ and 3-component spins was reported a few years ago [27]; see also references [22,23] for a more detailed bibliography.

Even more recently [28] the two lines of research were so to speak joined: it was proven that, also for the generalized xy model (Eq. (1)), the transition turns first order for large p, both in $D = 2$ and $D = 3$. One has a BKT low-temperature phase in the two-dimensional case, and ferromagnetic order in the three-dimensional one.

A simple but telling physical interpretation of the above mathematical theorems can be obtained by considering the density of states for the pair potentials in equations (1) and (3), and especially the fractions corresponding to their minimum and shallow regions, respectively. Numerical estimates of the density of states were worked out by calculating the pair potential over a rather fine grid of points, uniformly spaced with respect to $\cos\theta$ and $(\phi_j - \phi_k)$, and collecting the results into a potential energy hystogram; more precisely, the minimum region (and hence the minimum fraction ρ_{min}) were defined by

Table 1. Estimates of ρ_{min} and ρ_{sha} for different values of p and for the families of models defined by equations (1) and (3).

	Models (1)		Models (3)	
p	ρ_{min}	ρ_{sha}	ρ_{min}	ρ_{sha}
4	0.0170	0.2174	0.0694	0.3136
8	0.0087	0.4606	0.0353	0.5596
12	0.0059	0.5955	0.0237	0.6790
16	0.0044	0.6776	0.0178	0.7480
20	0.0035	0.7323	0.0143	0.7927

the pair potential being smaller than $-(3\epsilon/4)$, whereas the shallow region (and hence ρ_{sha}) were defined by the potential being smaller than 0.01ϵ in magnitude. For both families of models this procedure (Tab. 1) showed that, upon increasing p, the minimum fraction kept decreasing, and the shallow one kept increasing. As for the isotropic models, such a result could be anticipated from the plots of V_{jk} versus τ, but no such simple visualization is possible for the anisotropic ones.

The above mathematical theorems do not yield sharp estimates for the threshold value of p where the first order transition sets in, and this kind of result has to be determined by numerical approaches. Thus the goal of this letter is to characterize their ordering transitions by means of MF and TSC treatments, as well as MC simulation, for different values of the exponent $p = 8,\ 12,\ 16$, and $p = 20$. Furthermore the critical behaviour of the models is to be discussed.

2 Computational aspects

MF and TSC calculations were carried out as discussed in reference [7], for $5 \leq p \leq 12$, and then $p = 16, 20$. In both cases we found that, upon increasing p, the transition changes from second to first order; the two treatments exhibited different thresholds, i.e. between 5 and 6 for MF, between 10 and 11 for TSC; as remarked above, the exponent $p > 0$ can, but need not, be restricted to an integer number; thus we treated p as real positive number, and determined the tricritical points where the transition changes its order (see Ref. [29] for a detailed review on the properties of tricritical points); this analysis yielded $p = 5.1229$, $T_{tri} = 1.0966$ for MF, and $p = 10.8602$, $T_{tri} = 0.8695$ for TSC, respectively. An investigation of the properties of the Landau expansion for the two expressions of the thermodynamic potential relevant to MF and TSC (see Ref. [7]) showed that the tricritical points are stable.

Extensive simulations were carried out for $p = 8, 12, 16, 20$, on periodically repeated cubic samples, consisting of $\mathcal{N} = L^3$ sites, where $L = 10, 16, 20, 24, 30$ for $p = 8, 12$, and $L = 10, 20, 30$ for $p = 16, 20$; some additional simulations were carried out for $p = 12,\ L = 36, 40$ and $p = 16,\ L = 36$. Equilibration runs took between 25 000 and 250 000 cycles, and production runs took between 250 000 and 1 000 000; macrostep averages for evaluating statistical errors were taken over 1000 cycles. Simulations were mostly run in cascade, in order of increasing temperature; for $p = 12, 16, 20$ and $L = 30$, additional runs were carried out in order of decreasing temperature, so as to look for evidence of hysteresis. Calculated observables (potential energy U, specific heat C_V, in-plane magnetic order parameter M and associated susceptibilities χ_1 and χ_2), as well as simulation methodology, closely followed the lines of our previous paper [19].

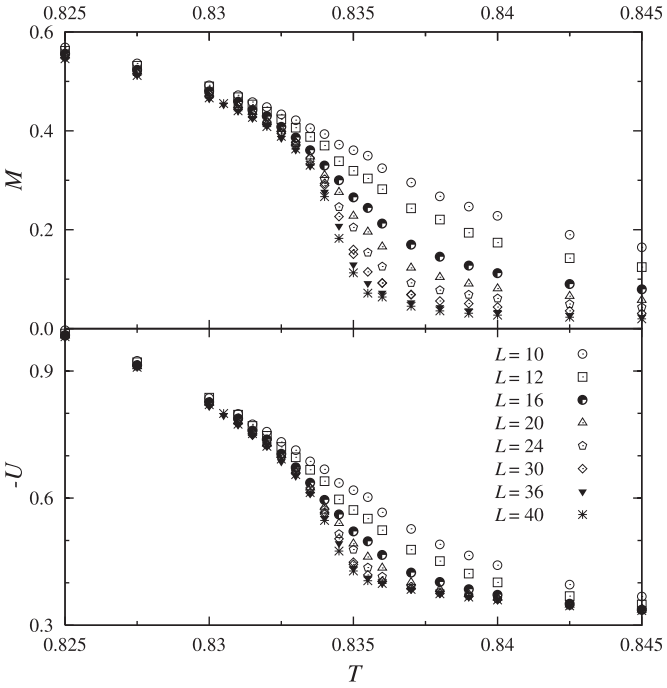

Fig. 1. Simulation results for the mean energy per spin U and the in-plane magnetization M obtained with different sample sizes for $p = 12$. Here and in following figures, the statistical errors are smaller than symbol sizes.

3 Simulation results

Simulation results for $p = 8$ (not shown) yielded evidence of a second-order transition with significant growth of orientational fluctuations, similarly to the simulation results reported in reference [19] for $p = 2, 3, 4$; simulation results were analysed by finite-size scaling theory [19,30] generally considered more reliable than the extraction of exponents by fits to the data obtained for a fixed lattice size, and yielded the transition temperature $T_c = 0.920 \pm 0.001$, and critical exponents in the xy universality class ($\nu = 0.67,\ \beta = 0.35,\ \gamma = 1.32$, within statistical errors ranging between 0.01 and 0.02) [3].

Simulation results for $p = 12$ are plotted in Figure 1; upon increasing L, both C_V and χ_1 showed sharpening peaks at $T \approx 0.834$: changes of both U and M around

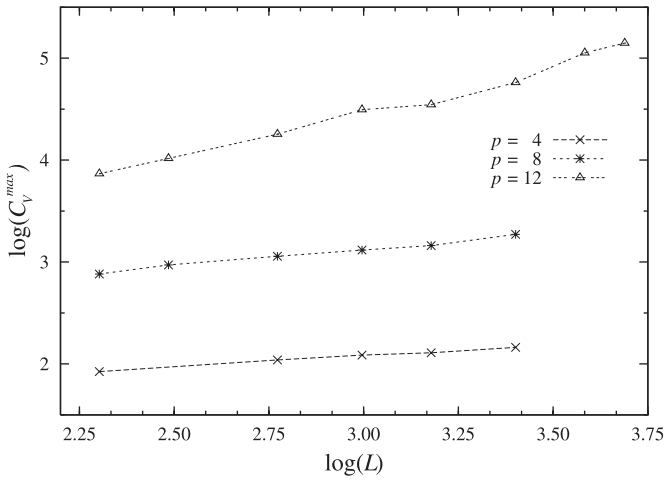

Fig. 2. Specific heat maxima versus system size on logarithmic scales. The curves serve to only guide the eye. The cases $p = 4$ and $p = 8$ correspond to a second order phase transition, while the slope of the curve $p = 12$ suggests a tricritical behaviour.

this temperature became steeper and steeper, although without any hint of a discontinuity. The data obtained via MC simulation were first analysed by the usual finite size-scaling theory relevant to second order phase transitions, and a violation of the this theory showed up for this value of p. Thus, as mentioned above, some additional simulations were started just above the transition and carried out in cooling order, and their results were found to coincide with their counterparts produced in heating order, to within associated statistical errors. Thus no sign of hysteresis was found indicating the absence of a strong first-order transition as well.

In order to determine the order of the phase transition for this value of the exponent p, we analysed the outcome of the simulations using finite-size scaling theory for a few values of p. More precisely, we investigated the behaviour of the specific heat maxima as a function of L (see Fig. 2). Recall that the specific heat maxima should obey the finite-size scaling relation

$$C_V^{max}(p, L) \sim L^{2y-3}, \tag{4}$$

with $y = 1/\nu$ for a second-order phase transition [30], and $y = 3$ for a first-order one [31]. The results for $p = 4$ and $p = 8$ were found to be consistent with $y = 1/\nu$ ($\nu = 0.67$ is the critical exponent of the xy universality class), whereas for $p = 12$ we found that y ranges between 1.95 ± 0.03 (when data for all sample sizes are included) and $y = 2.00 \pm 0.05$ (when the smallest sample sizes corresponding to $L = 10$ and $L = 12$ are excluded). Next we have tried to check the scaling behaviour by using scaling forms relevant to a tricritical point. In this case one has $C_V \sim L\sqrt{\ln L}$ see reference [29] for details. We were not able to capture the logarithmic dependence of the specific heat on L, but conclude that the transition for this value of the exponent p is most likely to be a tricritical point. Our simulation estimate of the transition temperature T_c for the named case is 0.834 ± 0.001; here the error bars

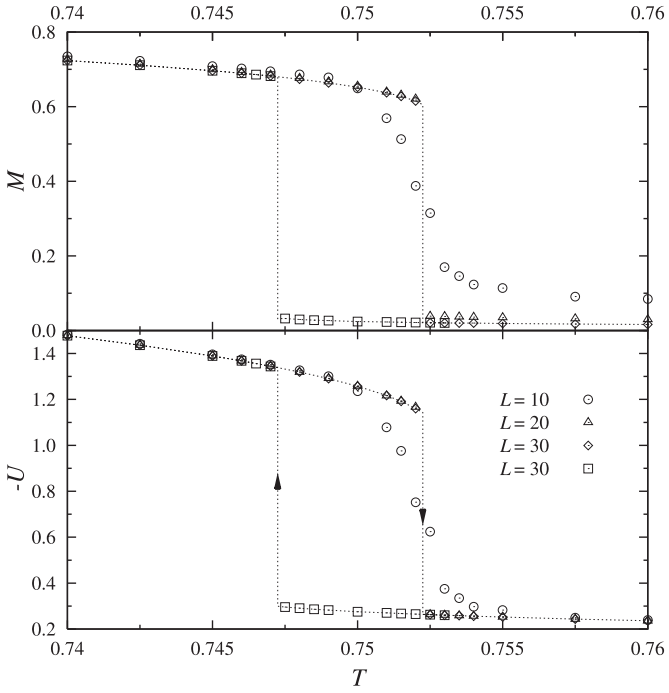

Fig. 3. Simulation results for the mean energy per spin U and the in-plane magnetization M obtained with different sample sizes for $p = 20$. Diamonds denote simulation results obtained in heating order, whereas squares denote cooling order; vertical dotted lines and arrows mark the jumps obtained in heating (right-hand segment) and in cooling order (left-hand segment), respectively.

are conservatively taken to be twice the temperature step used in the transition range.

Simulation results obtained with $p = 16$ (not shown), as well as with $p = 20$ (Fig. 3), exhibited for $L = 30$ recognizable jumps of U and M, taking place over a temperature range of 0.0005; on the other hand, both C_V and the susceptibility χ_1 (not reported here) showed a peak about the same temperature.

Actually, additional simulations, carried out for $p = 16$, $L = 36$, showed abrupt jumps of both U^* and M taking place over the same temperature range as for $L = 30$; estimates of transitional properties carried out as discussed in references [32,33], also confirmed the results obtained for $L = 30$. The case $p = 16$ showed no evidence of hysteresis. Simulation results for $p = 20$ already exhibited corresponding jumps in U and M for $L = 20$; moreover, for $p = 20$, there was a recognizable sign of hysteresis. Transitional properties for $p = 16, 20$ were estimated by analyzing simulation results for the largest sample size $L = 30$ and in heating order only, as discussed in references [32,33], and are reported in Table 2.

On the other hand, we tried estimating the transition temperatures for $p = 16, 20$ by means of the method, developed in reference [34]. There it is rigorously demonstrated that for finite systems undergoing a first order phase transition the transition temperature can be read

Table 2. Summary of transitional properties obtained by different methods. MC estimates for $p = 16, 20$ were obtained by analyzing results for the largest sample $L = 30$, in heating order, as discussed in references [32,33].

Method	p	T_c	ΔU	M
MF	12	0.8366	1.3140	0.7687
TSC	12	0.8461	0.5437	0.5098
MC	12	0.834 ± 0.001		
MF	16	0.7836	1.5355	0.7836
TSC	16	0.7906	1.0097	0.6721
MC	16	0.784 ± 0.001	0.62 ± 0.05	0.53 ± 0.02
MF	20	0.7486	1.6712	0.8387
TSC	20	0.7549	1.2578	0.7374
MC	20	0.752 ± 0.001	0.90 ± 0.04	0.62 ± 0.02

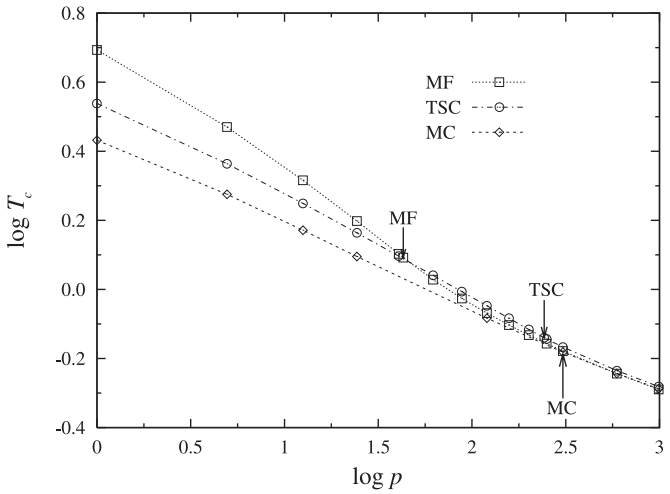

Fig. 4. p-dependence of the transition temperature T_c. The values for $p = 1,\ 2,\ 3$ and 4 are taken from references [19,35]. Locations of tricritical points are indicated by arrows.

off from the intersection temperatures T_i of the magnetization, corresponding to sample sizes L and $2L$, i.e. $M(T_i, L) = M(T_i, 2L)$. The estimated temperature should differ from the bulk critical one only by exponentially small corrections. In the present case we used the sample sizes $L = 10$ and $L = 20$, and results obtained in these two ways were consistent among themselves.

In Figure 4 we present the behaviour of the transition temperature as a function of p for $1 \leq p \leq 20$. Data for $1 \leq p \leq 4$ are taken from references [7,35]. Notice that, for $p \leq 4$, TSC gives better estimates of T_c than MF, then the two roles are exchanged for $p = 8, 12$, and finally the three methods give very similar answers when $p \geq 16$, i.e. where the transition has a pronounced first-order character. Moreover, the p-dependence of $T_{c,MC}$ now seems to be no longer well fitted by an inverse-power law, and a change a slope for larger p can be seen in all the three curves.

To summarize, starting from and complementing some recent mathematical results [28], we have considered potential models defined by larger value of the exponent p in equation (1), associated with a 3-dimensional lattice, and studied them by MF, TSC and MC simulation. MF and TSC yielded a tricritical behaviour with tricritical points having real (non-integer) values of the parameter p. As for simulation results, xy critical behaviour was found for $p = 8$, the case $p = 12$ suggested tricritical behaviour, whereas evidence of first-order transitions was obtained for $p = 16, 20$.

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