New O(3) Transition in Three Dimensions

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(Received 4 February 1993; revised manuscript received 9 July 1993)

A three-dimensional lattice of Heisenberg spins with nearest-neighbor interactions is studied by numerical simulation under the constraint that no free topological singularities (hedgehogs) are allowed. Only nearest-neighbor pairs of oppositely charged hedgehogs are permitted in the sum over configurations. A disordering transition with exponents different from the usual Heisenberg transition is found and tentatively identified as a pure spin wave disordering transition.

PACS numbers: 75.10.Jm

The relationship between topological effects and phase transitions has been a fruitful area of research ever since the seminal work of Kosterlitz and Thouless [1]. The unbinding of pairs of vortices in the two-dimensional XY model drives the transition between a power-law correlated phase and an exponentially correlated disordered phase. This transition would not be possible without the vortices. Topological objects have been studied in three dimensions as well, examples being the vortex loops of the XY model [2] and tunneling events in two-dimensional quantum antiferromagnets [3]. In analogy with the two-dimensional XY model, one can ask what role the hedgehogs [4] of the O(3) Heisenberg model play in the three-dimensional disordering transition. This question has been studied, but not fully answered, due primarily to the fact that there seems to be no simple decoupling between the "spin waves" and the hedgehogs in the three-dimensional O(3) model [5], as there is in the two-dimensional XY model. Analytical work based on extrapolations from two dimensions [6] suggest that hedgehogs should be important in the O(3) transition.

The present paper is inspired by the work of Lau and Dasgupta (LD) [7], who studied the Heisenberg model with a variable suppression of hedgehogs numerically. They considered the partition function

$$Z_h=\sum_{\{\mathbf{S}_i\}}\exp\left(-\beta J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-\lambda_h\sum_I|Q_I|\right), \tag{1}$$

where $\mathbf{S}_i$ are O(3) spins on a cubic lattice with sites labeled by i, β is the inverse temperature, J is the nearest-neighbor Heisenberg coupling, I stands for a dual lattice site, and Q_I is the topological charge at that dual site. The term multiplied by λ_h suppresses hedgehogs for $\lambda_h>0$. The Heisenberg model is reproduced for $\lambda_h=0$. LD found that if λ_h is sufficiently large, there is a nonzero magnetization even at infinite temperature. They also found oppositely charged hedgehogs with arbitrary separation as the transition is approached. This result suggests that the analogy with the two-dimensional XY model holds and that the unbinding of pairs of oppositely charged hedgehogs drives the O(3) Heisenberg transition in three dimensions.

In order to study whether the unbinding of pairs is necessary to disorder the magnet we allow nearest-neighbor pairs (or close pairs) to exist (with variable chemical potential $2\lambda_p$), but no free hedgehogs. We consider the partition function

$$Z_p=\sum_{\{\mathbf{S}_i\}}{}'\exp\left(-\beta J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-2\lambda_p\sum_{\langle IJ\rangle}|D_{IJ}|\right), \tag{2}$$

where the prime on the sum indicates the absence of free hedgehogs and D_{IJ} corresponds to a topological dipole with charges at the nearest-neighbor dual lattice sites I and J. We use a geometric definition of the hedgehog number inside a cube [7,8]. To carry out the numerical approximation to the partition sum we use a Metropolis algorithm [9] in which a randomly chosen spin is updated every time step in conjunction with the histogram method [10]. After the update the configuration of hedgehogs is recomputed. If the new configuration also has only close pairs, it is accepted with a probability specified by the Hamiltonian of Eq. (2). To calibrate our results we first performed simulations for the model of LD, the Hamiltonian of Eq. (1).

Let us summarize our results: Figure 1 shows the phase diagram for the LD model based on our simulations (upper dashed line). We performed simulations only on the axes. We find the critical chemical potential at infinite temperature to be $\lambda_h=2.7$. Using the histogram method we are able to obtain good estimates for the critical exponents via a standard finite-size scaling analysis [11]. We find that the exponents of the infinite temperature fugacity transition are indistinguishable from Heisenberg exponents ($\nu_H=0.66\pm0.05$, $\beta_H=0.33\pm0.05$). This is a new result, although hardly unexpected. Figure 2 shows the data collapse for lattice sizes 6, 8, 10, and 12.

The phase diagram for the model with close pairs only is also plotted in Fig. 1 (lower dashed line), where the critical $\lambda_p=0.6$ at infinite temperature. For $\lambda_p=0$ the model disorders at about $T_c(\text{pair})=3$, higher than the Heisenberg transition temperature of about $T_c(\text{Heis})$

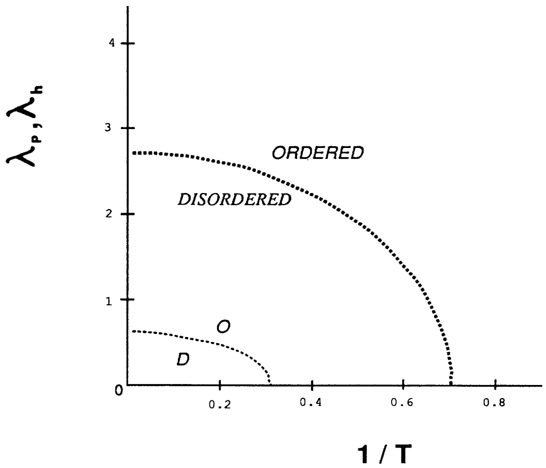

FIG. 1. The phase diagrams of the Lau-Dasgupta model (upper dashed line) and the model with close pairs only (lower dashed line). Simulations were carried out only along the axes. The ordered and disordered phases are marked for both models.

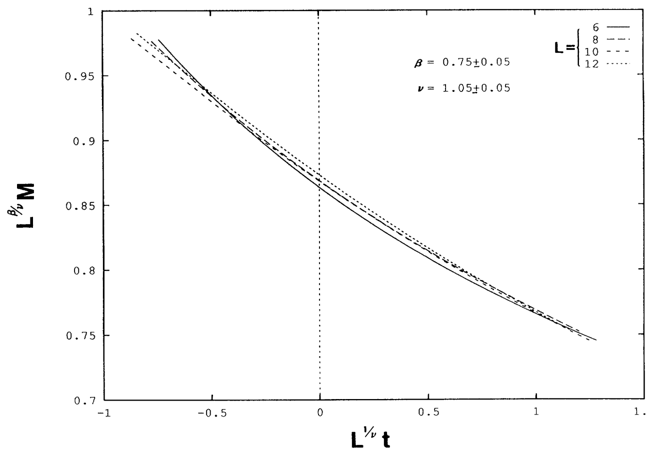

FIG. 3. A typical data collapse for the model with close pairs only where the notation is as before. The estimates for the exponents are very different from the Heisenberg exponents.

=1.5. This result demonstrates that free hedgehogs are not necessary for disordering the magnet. Figure 3 shows a typical data collapse for this model (at $\lambda_p=0$), which seems to be of slightly poorer quality than the data collapse for the LD model. The surprise is in the values of the critical exponents, which we estimate to be $\nu=1.05\pm0.05$ and $\beta=0.75\pm0.05$. These are different by much more than numerical error from the Heisenberg exponents. Numerical error was estimated by comparing the results of different runs, and also by visually inspecting the finite size scaling for different assumed values of the exponents. The infinite temperature transition in this model also belongs to the new universality class.

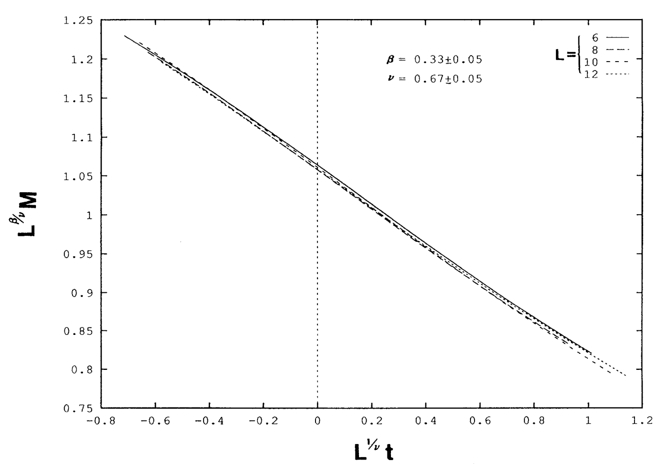

FIG. 2. A typical finite size scaling data collapse for the Lau-Dasgupta model for lattices of 6^3, 8^3, 10^3, and 12^3 sites. Here $t=(T-T_c)/T_c$ and M is the average magnetization. The estimates of the exponents based on the best data collapse are within numerical error of the Heisenberg exponents.

Before we can identify the new critical point as a new universality class with O(3) symmetry, we have to deal with some subtleties. Consider once again the updating process, which is potentially nonlocal, as demonstrated by Fig. 4, which shows two configurations of pairs. Figure 4(a) shows a long chain of pairs, where the two oppositely charged hedgehogs in the center (circled) cannot annihilate, since that would leave two free charges. However, in Fig. 4(b) they can, since the remaining hedgehogs can now be repaired with no free charges. Thus, the allowed phase space of a spin may depend (in certain configurations) upon the state of a spin far away. To avoid this nonlocality, which would make the time required for each update prohibitive, we keep track of the pairs as they form. If an update annihilates two

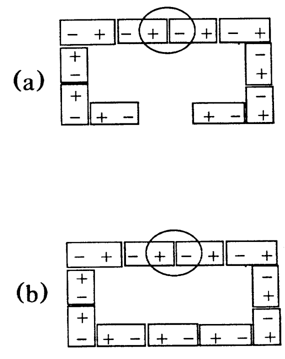

FIG. 4. Two possible configurations of close pairs. In (a) the oppositely charged hedgehogs cannot annihilate since that would leave two unpaired hedgehogs. In (b) they can since the remaining hedgehogs can be repaired leaving only close pairs.

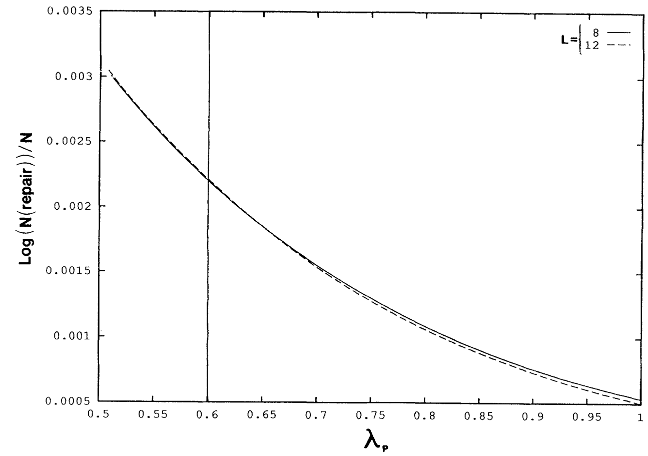

FIG. 5. A plot of $\langle\log(N_{\text{repair}})\rangle/N$ versus λ_p at $T=\infty$, where N_{repair} is the average number of distinct repairings of close pairs and N is the number of sites in the lattice for 8^3 and 12^3 lattices. The vertical line marks the transition. The number of repairings is small and smoothly varying, indicating that loops do not proliferate near the transition.

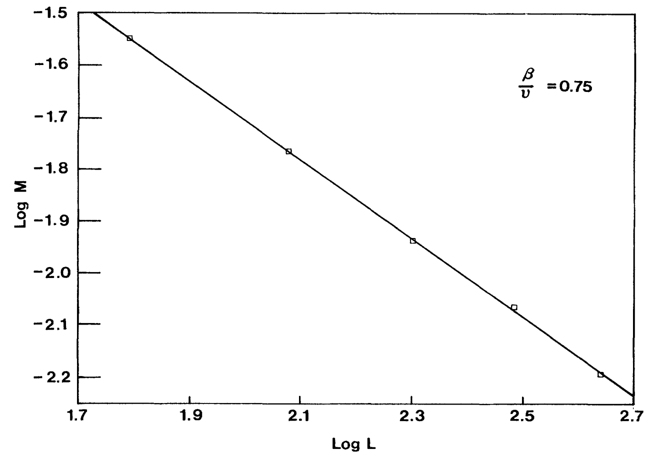

FIG. 6. A plot of $\log[M(T_c)]$ vs $\log(L)$ for the pair transition. The points represent $L=6,8,10,12,14$. The slope is consistent with the β and ν found previously and shows no tendency to change.

hedgehogs belonging to different pairs, we look for a local repairing (within 2 lattice units). If no such local repairing is found, the update is not accepted. However, it is easy to see that all permissible spin configurations are reached by this procedure. The price we pay for making the Hamiltonian local is that we now have an extra degree of freedom on the faces of the cubes, and perhaps a longer equilibration time.

It is important to address whether the above nonlocality plays any role in the transition we have discovered. The extra variable introduced above to mark the close pairs can be coarse grained to a variable length vector (say **v**). Integrating out this vector would leave a model with only O(3) spin variables, but with nonlocal interactions which depend on the correlations of **v**. As long as there is no second order transition in the **v** variables, their correlations will be exponential, and the O(3) model can be considered effectively local [12].

It is very difficult to study correlations in finite size systems. Instead we look at loops of close pairs, which are essential for any nonlocality. If this nonlocality drives the transition, we expect the loops to proliferate near the transition. Each disjoint loop of close pairs can be paired in two distinct ways. We compute the number of distinct ways of pairing the close pairs and take the logarithm to estimate the importance of loops. Specifically, let us consider the infinite temperature limit, in which the demagnetization transition occurs as λ_p is reduced. We compute the average of the logarithm of number of independent pairings [$\langle\log(N_{\text{repair}})\rangle/N$, where N is the number of lattice sites] and its variance in the system numerically. As shown in Fig. 5, in the critical region the number of pairings is small and smoothly varying. We have also considered the quantity

$$R_1(\text{loop}) = \frac{\langle(\log N_{\text{repair}})^2\rangle}{\langle(\log N_{\text{repair}})\rangle^2}\,. \tag{3}$$

If the loops proliferate in a phase transition, we expect a crossing of the R_1 curves for different lattice sizes [11]. There is no such crossing in the critical region. Faced with this absence of evidence linking loops of pairs to the demagnetization transition, we tentatively conclude that the nonlocality induced by loops of pairs has nothing to do with the transition. Furthermore, alerted by a previous example of the relevance of the percolation of topological objects [13], we have computed the probability of finding a percolating cluster of close pairs. In the critical region the density of close pairs is too small to percolate (at criticality only 12% of the sites are occupied by hedgehogs). Also, the peak of $dP/d\lambda_p$, which reliably marks the percolation threshold [14], occurs far from the demagnetization transition. For the finite temperature transition at $\lambda_p=0$ the pairs percolate very close to the demagnetization transition. However, since the exponents are the same at all temperatures, the infinite temperature results show that percolation cannot have anything to do with the demagnetization transition. Thus, the pairs are well behaved in the critical region of the demagnetization transition. Loops of pairs do not proliferate and pairs do not percolate.

It is also important to check for any evidence of a crossover. Figure 6 shows a plot of $\log[M(T_c)]$ versus $\log(L)$. From standard finite size scaling, the slope of the line should be β/ν. We find a slope consistent with the β and ν found previously. Also, there is no tendency for the slope to change for higher L, which we interpret as absence of evidence for a crossover. We emphasize that there could be a crossover at much larger L, but we see no evidence of it.

These results have led us to tentatively espouse the following position: Since the introduction of a small amount of hedgehog suppression into the Heisenberg model merely shifts the critical temperature and does not alter the exponents, the hedgehog suppression term is an irrelevant operator (as one can conclude immediately from the dimension of the perturbation in the continuum). As one coarse grains the system, it renormalizes the spin stiffness and disappears. However, the Heisenberg fixed point has a finite basin of attraction for the irrelevant operator, and beyond a certain λ_h one leaves this basin of attraction and the transition disappears. The pair transition we have discovered belongs to a different universality class (assuming no crossover at large L). Since there are no free hedgehogs in the pair model, and the pairs do not proliferate, we can speculate that the disordering is caused entirely by spin waves. It is believed that the $2+\epsilon$ expansion [15-17] does not include the effects of hedgehogs, and should therefore produce the exponents of a pure spin wave disordering transition. However, there are recent fundamental objections [18] to the validity of the $2+\epsilon$ expansion which may make its results moot. If the above identification is correct, spin waves disorder the magnet in a second order phase transition belonging to a hitherto unknown universality class, but the introduction of free hedgehogs drives the system into the Heisenberg universality class. This is in agreement with earlier generic considerations about the effects of free hedgehogs in an already disordered magnet [19]. The situation is in stark contrast to the two-dimensional XY model, where the spin waves alone cannot disorder the magnet. We emphasize that our numerical results do not prove this identification but merely suggest it.

Numerical simulations of a model in which pairs of larger size are allowed, but free hedgehogs are still absent would serve as a good test of the hypothesis made above. If this model disorders with different exponents than the pair model of this paper the hypothesis will have been considerably weakened. We have been unable to do this because the time for each Monte Carlo update increases enormously if one allows larger pairs. The other interesting question is the stability of this new transition with respect to the introduction of free hedgehogs. Unfortunately, the crossover effects in finite systems would make this effect very difficult to see numerically.

In summary, we have numerically investigated a model of O(3) spins on a lattice where only close hedgehog-antihedgehog pairs are allowed. We find a disordering transition with new exponents, belonging to a hitherto unknown three-dimensional O(3) universality class (assuming no crossover at large L), which we tentatively identify as the class corresponding to pure spin wave disordering. The results also suggest that nontrivial topology in the form of free hedgehogs, though not necessary to disorder the magnet, is an essential feature of the Heisenberg transition. Many open questions remain, including results on the stability of the dipole transition to free hedgehogs and a verification of the physical basis of disordering.

We are grateful to Professor B. I. Halperin, Professor D. Rokhsar, and Dr. Gilles Zumbach for illuminating discussions. We also thank Professor Joan Adler and the hospitality of the Technion. M.K. is supported by an NSF graduate fellowship.

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