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LETTER TO THE EDITOR

Role of topological defects in the phase transition of the three-dimensional Heisenberg model

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Abstract. A numerical study of the role of topological point defects in the phase transition of the classical ferromagnetic Heisenberg model in three dimensions strongly suggests that the defects play an essential role in this phase transition. We find that the transition from the ordered to the disordered phase is accompanied by a proliferation and unbinding of pairs of oppositely charged defects. If configurations containing defects are not allowed, then the system appears to remain ordered at all temperatures.

In recent years, theories [1] based on the statistical mechanics of topological defects have been very successful in explaining the critical behaviour near phase transitions in a large class of two-dimensional systems (for a review, see [2]) including the superfluid transition in thin ^{4}He films, the superconducting transition in thin metallic films and the melting transition in two dimensions. In these theories, the transition from the ordered to the disordered phase corresponds to an unbinding of pairs of point defects (vortices in superfluids and superconductors, dislocations and disclinations in crystals) carrying topological charges of opposite sign. It has also been shown recently that the superfluid ([3] and references therein) and superconducting ([4] and references therein) transitions in three dimensions and the nematic to smectic-A transition [5] in liquid crystals can be understood in terms of the statistical mechanics of interacting defect lines and loops. In view of the success of these theories, it is interesting to inquire about the role of topological defects in phase transitions of other systems (for a review see [6]). In this letter, we consider this aspect of the magnetic phase transition in the ferromagnetic classical Heisenberg model in three dimensions. This model is used widely to describe the behaviour of a large number of magnetic systems. It is known that the topological defects in the three-dimensional (3D) Heisenberg model are point singularities (the so-called 'hedgehogs'). This is a consequence of the fact that the second homotopy group $\pi_2(S^2)$ is non-trivial (for a review of the classification of topological defects, see [7]). These point defects carry integer-valued topological charges of both positive and negative sign. For example, a singularity of charge +1 occurs at a point if all the spins around it are directed radially outward from it. The energies associated with a single defect and with a pair of defects with equal but opposite charge have been calculated [8, 9]. It is known [9] that the energy of a defect pair increases linearly with the separation. However, the statistical mechanics of a system of these defects has not been worked out. In particular, the question of whether the defect system exhibits an unbinding transition remains unanswered. Although the critical behaviour of the 3D Heisenberg model has been

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studied extensively by using series expansion, numerical simulations and renormalisation group methods, no information is available at present about the behaviour of the defects near the phase transition. There have been some speculations on the role of defects in this phase transition. A few years ago, Cardy and Hamber [10] used a set of approximate renormalisation group equations near $n = d = 2$ (n is the number of components of the order parameter and d is the dimension of space) to argue that the topological defects must be explicitly taken into account for a correct description of the critical behaviour of the 3D Heisenberg model ($n = d = 3$). We have recently performed a real space renormalisation group calculation [11] which tends to support this conclusion. Halperin [6] has presented qualitative arguments suggesting that the defects are essential for the ferromagnetic to paramagnetic transition to occur in the continuum model. These arguments, if correct, would have important implications on the present theoretical understanding of this phase transition. In particular, one would then have to conclude that the non-linear σ model [12] in which singular defects are not allowed because the spin field is constrained to have a fixed magnitude at all points in space does not provide a correct description of the 3D Heisenberg transition. An understanding of the behaviour of the defects in this system would also be relevant to a class of gauge field theories in which point singularities of a similar nature (monopoles) are known to occur [13].

In this letter, we report the results of a numerical study of the role of topological defects in the phase transition of the 3D Heisenberg model. We find that the number density of defects increases sharply and defect pairs with separations comparable to the system size appear as the temperature is increased through the transition. Simulations in which spin configurations containing defects are not allowed do not show any indication of a transition to the disordered phase. These results strongly suggest that the defects play an essential role in this phase transition.

We consider the classical Heisenberg model on a 3D cubic lattice, defined by the reduced Hamiltonian

$$\mathcal{H} = -K \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

where $\boldsymbol{S}_i$ are three-dimensional vectors of unit length, $\langle ij \rangle$ represents distinct nearest-neighbour pairs of lattice sites and $K = J/k_B T$, $J > 0$. We set $J = k_B = 1$, so that $K = 1/T$ in our notation. For a study of the behaviour of the defects in this model, we need a definition of the topological charge on a lattice. The topological charge Q of a point defect represents the number of times and the sense in which the spins on a closed surface surrounding the defect cover the surface of a unit sphere in spin space. We define this quantity for the lattice system by using a prescription similar to one used by Berg and Lüschere [14] to classify instanton configurations in the 2D Heisenberg model on a lattice. For each unit cube of the lattice, we divide the six faces into twelve triangles, two for each face. Let $\boldsymbol{S}_1(i)$, $\boldsymbol{S}_2(i)$ and $\boldsymbol{S}_3(i)$ be the three spins at the corners of the triangle i, where the sequence 1, 2, 3 is chosen such that the circuit $1 \to 2 \to 3 \to 1$ corresponds to a counterclockwise rotation along the outward normal to the surface of the triangle. We then calculate the area, $\Delta(i)$, of the spherical triangle formed by the three spins on the surface of a unit sphere. The sign associated with $\Delta(i)$ is $\operatorname{sgn}[\boldsymbol{S}_1(i) \cdot (\boldsymbol{S}_2(i) \times \boldsymbol{S}_3(i))]$. The topological charge Q enclosed by the unit cube is then given by

$$Q = \sum_{i=1}^{12} \Delta(i). \tag{2}$$

This procedure corresponds to an interpolation of the spin field along geodesic lines on a unit sphere in spin space. Apart from a set of 'exceptional' configurations [14] of measure zero, this prescription yields well defined integral values for Q. Also, this definition of Q ensures that the net topological charge is always equal to zero in a system with periodic boundary conditions.

In our Monte Carlo (MC) study of the equilibrium behaviour of the defects near the phase transition, we used the standard Metropolis algorithm. Typically, 1000–2000 MC steps per spin were used for equilibration and 4000–8000 steps per spin were used for calculating averages. The simulations were performed for samples with linear dimension $L=8$, 12 and 16 using periodic boundary conditions. As a test of the simulation procedure, we calculated the internal energy per spin (E), the specific heat (C) and the averages of M, M^2 and M^4, where M is the magnitude of the magnetisation:

$$M = \left| 1/N \sum_i \boldsymbol{S}_i \right| \tag{3}$$

and $N = L^3$ is the total number of spins. Since the MC updating procedure generates uniform rotations of the whole spin system, a calculation of the MC average of $\boldsymbol{M}$ is not meaningful. From finite-size scaling analyses of the observed temperature and sample-size dependence of C, $\langle M \rangle$, $\langle M^2 \rangle / \langle M \rangle^2$ and $\langle M^4 \rangle / \langle M^2 \rangle^2$ (the brackets $\langle \ldots \rangle$ denote a MC average), we find that the phase transition occurs at $K_c = 0.69 \pm 0.01$ ($T_c = 1.45 \pm 0.02$) and the critical exponents have the values $\beta = 0.36 \pm 0.04$, $\nu = 0.71 \pm 0.01$. These results are in good agreement with the currently accepted values [15, 16]. At regular intervals along the MC evaluation of the system at a fixed temperature, we examined the spin configurations and determined the topological charge Q associated with each unit cube of the sample. The magnitude of the non-zero charges was almost always equal to unity. Only a few defects with $Q = \pm 2$, and none with $|Q| > 2$ were found. The observed temperature dependence of the average defect pair density $\langle n \rangle$ (n = number of defect pairs/N) is shown in figure 1. The density of defects is found to increase sharply as T is increased through T_c. The rapid increase of $\langle n \rangle$ near T_c can be seen more clearly in the insert of figure 1 where we have plotted the numerically calculated derivative $\mathrm{d}\langle n \rangle / \mathrm{d}T$ against T for two sample sizes. The temperature at which $\mathrm{d}\langle n \rangle / \mathrm{d}T$ peaks is identical within error bars to the T_c determined from the thermodynamic data. The peak of $\mathrm{d}\langle n \rangle / \mathrm{d}T$ increases in height and becomes sharper as L is increased, suggesting that $\mathrm{d}\langle n \rangle / \mathrm{d}T$ diverges at T_c in the thermodynamic limit. A finite-size scaling analysis of the data is consistent with a divergence of the form

$$\frac{\mathrm{d}\langle n \rangle}{\mathrm{d}T} \simeq |(T - T_c)/T_c|^{-\Psi} \tag{4}$$

with $\Psi \simeq 0.65$. The temperature dependence of $\langle n \rangle$ for $T < T_c$ is well described by the activated form, $\langle n \rangle \propto \exp(-\Delta E / T)$, whereas deviations from this form are observed for $T > T_c$. The value of ΔE obtained from a fit to the data is $\Delta E = 12.7 \pm 0.7$, which is close to 4π, the value expected [9] for the energy of a defect pair separated by unit distance in the continuum limit. At low temperatures, we find that defects with opposite charges are closely bound together, the separation being just one lattice spacing for most pairs. As T approaches T_c from below, the number of defects increases sharply, and the pairing-up of defects with opposite charges in an unambiguous way becomes difficult. However, careful examination of the defect configurations shows that defect

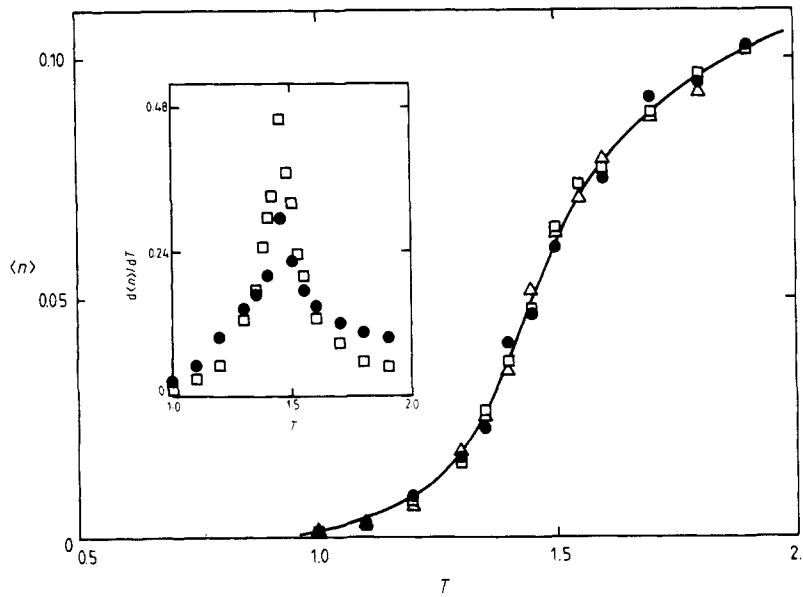

Figure 1. Variation of the equilibrium defect-pair density $\langle n \rangle$ with temperature T. The full curve is a guide to the eye. The insert shows the temperature dependence of $d\langle n \rangle / dT$ for two sample sizes. ●, $8 \times 8 \times 8$; △, $12 \times 12 \times 12$; □, $16 \times 16 \times 16$.

pairs with separations comparable to $L/2$ appear at temperatures close to or above T_c. In the $L = 16$ sample, for example, all defect pairs have separations less than $\sqrt{7}$ units for $T \leqslant 1.3$ whereas the distribution of pair separations extends up to 9 units at $T = 1.6$. All these features are qualitatively very similar to those found in simulations [3, 17] of 2D and 3D XY transitions which are known to be mediated by topological defects. Our results, therefore, suggest that the 3D Heisenberg transition also corresponds to an unbinding of defect pairs.

To investigate further the role of defects in this phase transition, we carried out MC simulations with a modified reduced Hamiltonian [3]

$$\mathcal{H}' = -K \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \lambda \sum_{\text{cubes}} |Q|. \tag{5}$$

For $\lambda > 0$, the new term in $\mathcal{H}'$ suppresses configurations containing defects. We first considered the limit $\lambda \to \infty$, which corresponds to restricting the ensemble to states with no defects. This restriction was imposed by using the following MC updating procedure. We started with a configuration containing no defects (e.g. the fully aligned ferromagnetic ground state). Every update attempt was then checked to determine whether it would create a defect pair. If it did, then the attempted change was rejected; otherwise, it was accepted or rejected according to the usual Metropolis algorithm. With this procedure, we simulated the thermodynamics of samples with $L = 6$, 8 and 12. The observed behaviour did not show *any* indication of a transition from the ordered to the disordered phase at *any* temperature. The thermodynamic quantities E, C and $\langle M \rangle$ were found to change smoothly with temperature at all temperatures up to $T \to \infty$ ($K = 0$). The ratios $\langle M^2 \rangle / \langle M \rangle^2$ and $\langle M^4 \rangle / \langle M^2 \rangle^2$ showed an N dependence that is characteristic of the ordered phase at all temperatures. The results for $\langle M \rangle$ shown in figure 2 indicate that the magnetisation remains finite at all temperatures.

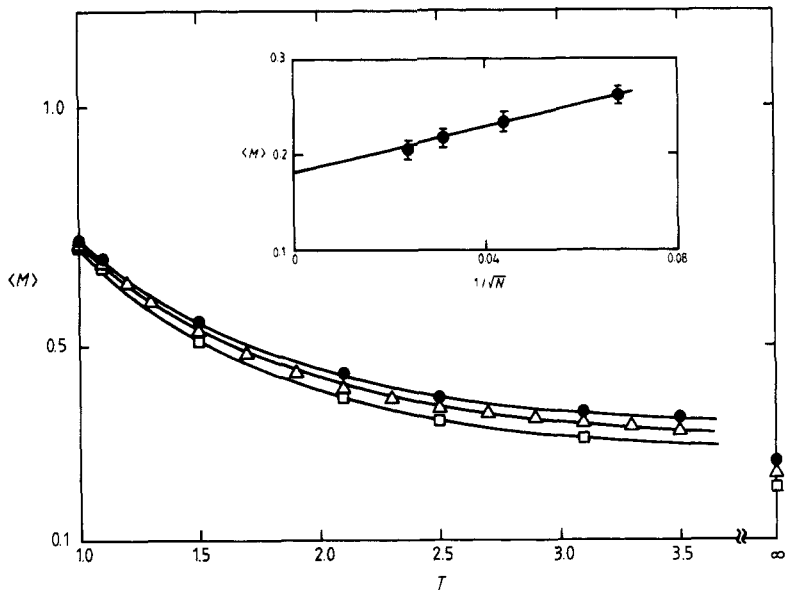

Figure 2. Temperature dependence of the magnetisation $\langle M \rangle$ obtained from simulations in which defects are not allowed. Full curves are guides to the eye. The insert shows a plot of $\langle M \rangle$ at $T \to \infty$ against $1/\sqrt{N}$, N being the number of spins. The straight line is the line of best fit. ●, $6\times6\times6$; △, $8\times8\times8$; □, $12\times12\times12$.

As shown in the insert of figure 2, the sample size dependence of $\langle M \rangle$ at $K = 0$ is well described by the form $\langle M \rangle = M_0 + \alpha N^{-1/2}$ with $M_0 \simeq 0.18$ and $\alpha \simeq 1.2$. This suggests that the observed non-vanishing of $\langle M \rangle$ at $K = 0$ is not a trivial finite-size effect. Since most of our results in the $\lambda \to \infty$ limit were obtained from simulations in which the system was warmed up from the ground state, we have to consider the possibility that the observed behaviour is caused by a trapping of the system in a small region of phase space with non-zero M and is, therefore, an artefact of the updating procedure used by us. To check this possibility, we repeated the simulations at $K = 0$ with two other starting configurations with no defects, one with $M = 0$ and the other with $M = \frac{1}{2}$. As shown in figure 3, all these runs converge to the same value, $\langle M \rangle \simeq 0.23$. This observation confirms that the non-zero values of $\langle M \rangle$ at all temperatures are not caused by a trapping in phase space. We have also simulated the behaviour of the model defined in (5) as a function of λ with $K = 0$. We find a rapid change of $\langle M \rangle$ near $\lambda = \lambda_c \simeq 2$. If λ is appreciably smaller than λ_c, then the N dependence of $\langle M \rangle$ is well described by the form $\langle M \rangle \propto 1/\sqrt{N}$, which is characteristic of the disordered phase. For values of λ somewhat larger than λ_c, the variation of $\langle M \rangle$ with N is similar to that shown in the insert of figure 2. All these results indicate that the system remains ordered at all temperatures if λ is sufficiently large, and configurations containing defects are essential for the transition to the disordered phase to take place. Similar results were obtained in a recent numerical study [3] of the role of vortex loops in the 3D XY transition.

The conclusion that topological defects play a crucial role in the phase transition of the 3D Heisenberg model introduces a completely new approach to a theoretical understanding of this transition. In particular, it raises the possibility of formulating a theory of the critical behaviour at this transition in terms of the statistical mechanics

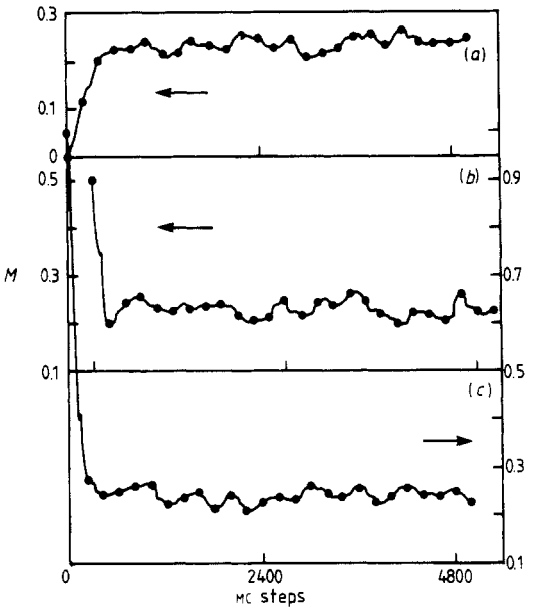

Figure 3. Evolution of the magnetisation M in MC simulations ($L = 8$, $T \to \infty$, no defects) for three different starting configurations (*a*) $M = 0$, (*b*) $M = 0.5$, (*c*) $M = 1.0$.

of the system of point defects. Because of non-linearities arising from the three-dimensional nature of the Heisenberg spins, a description of this transition in terms of defects would, however, be much more complicated than Kosterlitz-Thouless-type theories [1, 2] of defect-mediated transitions. We are currently looking into this question.

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