Effects of solitons in the critical behavior of an anisotropic Heisenberg model in two dimensions

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Monte Carlo calculations for the classical ferromagnetic Ising-like Heisenberg model suggest that solitons may play an important role in driving the phase transition in that model.

There is a large class of classical spin models that has the interesting feature of supporting topological excitations. For instance, for the classical XY model in $d=2$ dimensions it has been shown by Kosterlitz and Thouless[1] that a phase transition takes place due to a mechanism of vortex-antivortex pair dissociation as the temperature T increases through T_{KT}. Recently, Kohring, Shrok, and Wills,[2] using Monte Carlo (MC) techniques, have shown that vortex strings are responsible for the phase transition in three-dimensional planar models. For the pure ideal two dimensional (2D) Heisenberg system [$O(3)$ symmetry] it is accepted that there is no phase transition at all;[3] topological excitations are responsible for the long-range-order destruction for all temperatures. If we add an easy-axis anisotropy (Ising-like) to the isotropic Heisenberg model, the spin-wave spectrum acquires a gap and the system becomes metastable.[4] The decay of such a state cannot occur uniformly. Inhomogeneous fluctuations, such as kinks, which are not sharply bounded domains open the path to the true ground state. In fact, as pointed out by Einhorn, Savit, and Rabinovici,[5] it is possible to understand the phase transition of the 2D Ising model in terms of topological excitations, which are the domain boundaries between islands of aligned spins. For the weakly coupled magnetic chains constituting 3D classical ferromagnets with easy-axis anisotropy, Holyst and Sukiennicki[6] have shown that the phase transition connected with the disappearance of the 3D magnetic ordering is induced by static solitons obtained for 1D systems. The above findings have motivated us to investigate the effect of topological excitations in connection to phase transitions in a two-dimensional easy-axis classical Heisenberg model. As far as we know, there is no critical theory for the 2D easy-axis classical Heisenberg model that takes into account topological excitations. Series expansions and renormalization-group techniques predict critical exponents,[7] but they make no direct reference to the effect of solitons in its critical behavior.

Nonlinear topological excitations in a 2D system may be divided between two types;[8] namely, (i) small topological excitations (droplets) and (ii) large domain walls that are nearly straight on a small scale, but meander on a large scale and may eventually cross the entire system. The stability of round droplets in a 2D ferromagnet with uniaxial anisotropy was investigated by Kosevich, Ivanov, and Kovalev.[9] They defined a topological charge ν, which takes integer values, and corresponds to the amount of vorticity of the droplet. It measures the degree of mapping of the magnetic plane onto a unit sphere. The $\nu=0$ droplet differs from the $\nu>0$ one in that it is topologically equivalent to the ground state and does not contain vorticity.

Since droplets with $\nu=1$ are believed to play an important role in the physics behind the order-disorder phase transition in the 2D Ising system,[8] we have calculated the density of droplets in the model here studied. From now on we will refer to a droplet with $\nu=1$ as a soliton.

To determine the topological charge ν within a curve of length l we have followed a procedure similar to the one used by Tobochnik and Chester[10] in their study of vortices and computed the change in angle from one spin to the next, being sure to define the angle difference between neighboring spins to lie within $-\pi$ and π. To compute the soliton density we calculate the number of solitons in the system by computing the vorticity around every square in the lattice with side length equal to one lattice spacing. The soliton density d is defined as the sum of solitons divided by the lattice volume. We have also checked, starting in the center of a soliton and following a radial direction, if the spins have changed by π along that direction. This completely characterizes a soliton.[11]

In this paper we report MC results for the 2D easy-axis classical ferromagnet which explicitly show that soliton excitations are consistent with the transition being driven by them. The Hamiltonian describing our model is

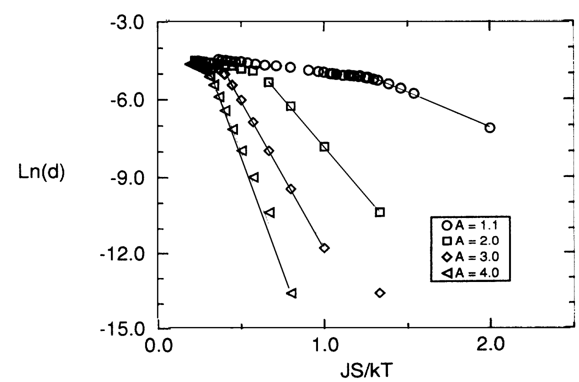

FIG. 1. Logarithm of soliton density as a function of the inverse of temperature (in reduced units) for some values of the anisotropy. Solid lines are fits as defined in the text.

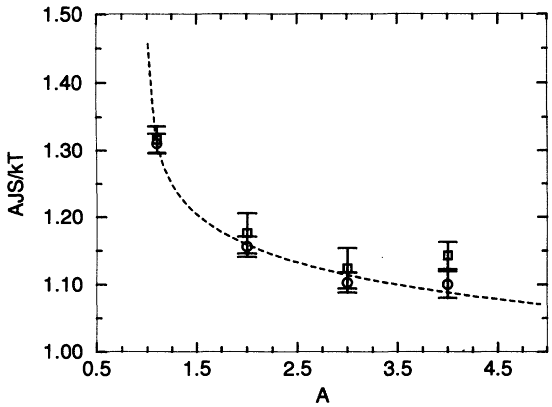

FIG. 2. Inverse of temperatures T_c (circles) and T^* (squares) as a function of the anisotropy. The dashed line is the function defined by Eq. (3).

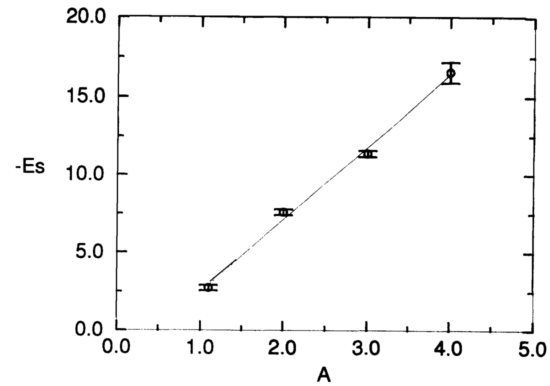

FIG. 3. Soliton energy as a function of the anisotropy. Solid line is the curve $E_s = 4A - 1$.

$$H = -\sum_{\langle ij \rangle} J[S_i^x S_j^x + S_i^y S_j^y + A S_i^z S_j^z] , \tag{1}$$

where J is the exchange constant and A characterizes a uniaxial anisotropy ($J, A > 0$). We will calculate the critical temperature T_c and the soliton density d as a function of the anisotropy A. The simulations were performed using standard Metropolis techniques for $L \times L$ lattices with periodic boundary conditions, with L up to 40. For each simulated point we used between 1×10^4 and 2×10^5 MC steps, depending on L and T, in order to thermalize the system. Averages were taken over 2000 initial configurations for all temperatures. To estimate the critical temperature T_c, we determined the position of the maxima of the specific heat and susceptibility for four lattices sizes ($L = 10,20,30,40$) and then used finite-size scaling[12] to obtain T_c. The soliton density d was determined for each of the four lattices: we found that the result did not change substantially with L. In Fig. 1 we plot the logarithm of d as a function of the inverse of T for several values of A. We found out that our simulated results are well fitted by the function (represented by solid lines)

$$d = Ce^{-B/T} , \tag{2}$$

C and B being constants which assume different values below and above a certain temperature T^*. From our data we calculated T^* as a function of A and the results are shown in Fig. 2 (represented as squares) together with the results for T_c (represented by circles). As we can see, the agreement between these two calculations is very good, suggesting that soliton excitations should play an important role in driving the phase transition. In Fig. 2 we show as a dashed line a fit of the function

$$f = \frac{[a - \ln(A-1)]}{b} , \tag{3}$$

with $a = 6.00$ and $b = 5.88$. We remark that this functional form agrees with early results for T_c performed by Binder and Landau[13] for a similar model.

The coefficient of the exponential in Eq. (2) can be interpreted as the soliton energy E_s, at least in the low-temperature region. In Fig. 3 we show $E_s = B$ as a function of A (circles). The solid line is a best fit given by

$$E_s \approx 4.7A - 2.0 . \tag{4}$$

Our results suggest that topological excitations might play an important role in driving the phase transition in the model described by Eq. (1) and by extension of the universality argument in those which have the same order-parameter symmetry. Thus more theoretical work is necessary in order to get more understanding of the effects of soliton excitations in the phase transition of the 2D classical Ising-like model.

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