Ferromagnetic Phase Transition in a Heisenberg Fluid: Monte Carlo Simulations and Fisher Corrections to Scaling

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The magnetic phase transition in a Heisenberg fluid is studied by means of the finite size scaling technique. We find that even for larger systems, considered in an ensemble with fixed density, the critical exponents show deviations from the expected lattice values similar to those obtained previously. This puzzle is clarified by proving the importance of the leading correction to the scaling that appears due to Fisher renormalization with the critical exponent equal to the absolute value of the specific heat exponent α. The appearance of such new corretions to scaling is a general feature of systems with constraints.

Monte Carlo (MC) simulations of finite systems near phase transitions have received considerable attention in recent years [1]. Of notable current interest are continuum spin fluid models [2] which are considered as a first step towards the modeling of ferrofluids [3] and adsorption surface phenomena [4]. Several important results, which have both theoretical and experimental interest, were obtained for such models. For example, it was found that the phase diagrams for spin fluids due to the interplay between spin and translational degrees of freedom are much more complicated [2] than in nonmagnetic liquids. Magnetic ordered phases can exist both in gas and liquid states. By applying an external magnetic field, one can shift significantly the locus of the gas-liquid transition [5] and change the dynamic properties [6]; both the static and dynamic properties in the models discussed show differences from the nonmagnetic fluid and the magnetic lattice model.

One important question in this context is whether the magnetic transition in a Heisenberg fluid belongs to the same universality class as the corresponding transition in the lattice model. On general grounds (annealed systems) [7], the lattice universality class is expected. In Ref. [8] using the MC method, a novel set of critical exponents was found that were in disagreement with the expected results. Similar disagreements were later obtained for two- and three-dimensional (2D and 3D) Ising fluids [9,10], where Fisher renormalized exponents were expected [7]. In all the cases mentioned, a weak *dependence* of universal quantities on the density of particles $n = N/V$ and *systematic deviation* from the predicted critical exponents were observed in the MC simulations. The general conclusion was that computer simulations were strongly affected by *nonlinear crossover* effects, which hide the true asymptotic critical behavior, giving only effective critical exponents.

The goal of the present study is to resolve this puzzle by performing a new series of MC simulations for a Heisenberg fluid, considering larger finite size systems, and to compare the results obtained with the previous data [8].

Contrary to the belief that the true asymptotic critical behavior would be observed, deviations from the expected exponents remained. It is the aim of this Letter to show that a new correction term [7] (Fisher correction term) has to be taken into account in the finite size scaling (FSS) even for very large systems.

Let us consider a classical system, composed of N magnetic particles of mass m and described by the Hamiltonian [6,8]

$$H = \sum_{i=1}^{N} \frac{m\mathbf{v}_i^2}{2} + \sum_{i<j}^{N} [\Phi(r_{ij}) - J(r_{ij})\mathbf{s}_i \cdot \mathbf{s}_j], \quad (1)$$

where $\mathbf{r}_i$ and $\mathbf{v}_i$ denote the position and velocity of particle i carrying spin $\mathbf{s}_i$. In our MC study, the liquid subsystem potential $\Phi(r_{ij})$ was chosen to be of soft-core-like form, $\Phi(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6] + \varepsilon$ at $r < 2^{1/6}\sigma$ and $\Phi(r) = 0$ otherwise, and the exchange integral $J(r_{ij}) > 0$, describing spin interactions, was modeled by the Yukawa function, $J(r) = \epsilon(\sigma/r)\exp[(\sigma - r)/\sigma]$. The function $J(r)$ was truncated at $R = 2.5\sigma$ and shifted to zero at the truncation point (this avoids force singularities during MD calculations [11]). Staying within the classical approach we consider $\mathbf{s}_i$ as a three-component continuous vector with a fixed length $|\mathbf{s}_i| = 1$.

The simulations were carried out in the basic cubic box $V = L^3$ (employing periodic boundary conditions) at the reduced density [12] of $n^* = N\sigma^3/V = 0.6$ for a reduced core intensity of $\varepsilon/\epsilon = 1$. A number of particles N were taken as $N = 125$, 256, 512, 1000, 2048, 4000, 8000, and $16\,384$. The simulations have been performed for five values of reduced temperature T^*, $T^* = k_B T/\epsilon = 2.000$, 2.025, 2.050, 2.075, and 2.100. The system was allowed to achieve equilibrium for $100\,000\,N$ attempted moves. The total number of trial moves per particle (cycles) performed in the equilibrium state was $1\,000\,000$. The canonical averaging over the system was carried out using a biasing scheme [13,14] for sampling orientational degrees of freedom. To minimize computational costs, the cell list

technique [14] was employed in handling the interparticle interactions.

The critical properties of a system in the thermodynamic limit may be extracted from the behavior of finite size systems by examining the size dependence of thermodynamic quantities [1,15]. According to the FSS theory, various thermodynamic quantities can be written in a scaling form $q(L, T) = L^{x_q/\nu} Q(z)$, where L is a linear length of system, x_q is a critical exponent of the quantity q, and $z = tL^{1/\nu}$ is the temperature scaling variable with $t = (T - T_c)/T_c$ (T_c and ν are, respectively, the bulk critical temperature and critical exponent of correlation length ξ). Because we are interested in zero-field properties, only the scaling variable z appears in the scaling function Q.

There are several methods to determine the critical temperature T_c. One of them is the Binder crossing technique [1] formulated for the fourth-order cumulant $U_4 = 1 - M_4/(3M_2^2)$, where $M_l = \langle m^l \rangle$, $m = |\mathbf{m}|$, and $\mathbf{m} = N^{-1} \sum_{i=1}^{N} \mathbf{s}_i$. This method does not need any assumptions about critical exponents, but for small systems the position of intersection points between any two curves U_4, related to systems with lengths L and L', depends usually on L and L', because of corrections to FSS. We have estimated the value of T_c as the average over the cross-section temperatures $T_{\text{cross}}(L, L')$, found for systems with $L = L_i$ and $L' = L_{i+1}$ ($i \geq 3$), giving $T_c = 2.055 \pm 0.001$. Here and below the increasing subscript i denotes increasing numbers of particles N_i from the set $\{N_i\}$ considered. In a similar way, we found $U_4^* = 0.618 \pm 0.003$. The same estimate for T_c has been found by using the crossing technique for the function $\xi(L_i, T)/L_i$ (see, e.g., [16]) within the phenomenological renormalization group scheme. Using a more precise method for extracting T_c [1] from the values $T_{\text{cross}}(L, L')$, obtained for the Binder parameter U_4 with the fixed ratio $L_4/L_1 = L_5/L_2 = L_7/L_4 = L_8/L_5 = 2$, we have obtained $T_c = 2.054 \pm 0.001$ and $U_4^* = 0.619 \pm 0.002$.

An alternative method, proposed in [17], allows one to estimate simultaneously both the critical temperature T_c and the critical exponent ν within the same series of calculations. The main idea of this approach (the scanning technique) is to look for a quantity-independent slope of the set of functions V_l with $l = 1, 2, \ldots, 6$, all of which have similar scaling behavior. These functions are defined via the derivatives $K_l = \partial M_l/\partial \beta$ (see, for details, Ref. [17]). The results are shown in Fig. 1, so that we have $T_c = 2.057 \pm 0.001$ and $1/\nu = 1.396 \pm 0.006$. Note that within the scanning technique, no corrections to scaling have been taken into account.

We have also used other known methods [1] to estimate T_c. One of these (the shifting technique) is based on the analysis of the size-dependent shift of a peak $T_{\text{peak}}(L)$, observed in some thermodynamic quantities (e.g., specific heat C_V, susceptibility χ, derivatives K_l). If corrections to scaling are neglected, the location of the peak $T_{\text{peak}}(L)$ has the general form $T_{\text{peak}}(L) = T_c + AL^{-1/\nu}$, where A is a quantity-dependent constant. Note that in order to
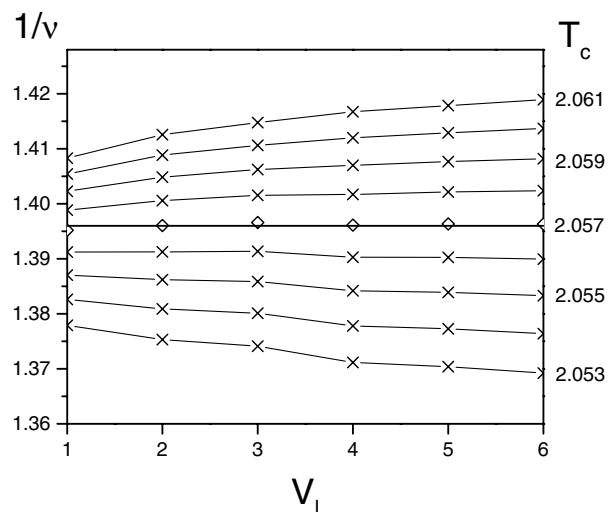

FIG. 1. Quantity dependence of scanning results for the functions V_l possessing the same scaling properties [17]. The horizontal line for $T_c = 2.057$ is drawn at $1/\nu = 1.396$.

determine T_c one has to estimate accurately the exponent ν as well as the values $T_{\text{peak}}(L)$. In the temperature range considered, well-defined peaks for all the sizes L_i have been observed for the functions $\partial M/\partial \beta$, $\bar{U}_3 = (M_3 - 3M_2M_1 + M_1^3)/[M_1(M_2 - M_1^2)]$, and $\chi_3 = N^2(M_3 - 3M_2M_1 + M_1^3)$ [17,18]. For all these cases, our estimate of $T_c \simeq 2.058 \pm 0.002$, found with $1/\nu = 1.396$ for the five largest sizes L, is in agreement with the scanning technique but not with the crossing technique. Moreover, the dependence $T_{\text{peak}}(L)$ versus $L^{-1/\nu}$ showed a pronounced curvature for smaller system sizes L. Hence, *the first puzzle uncovered in our study is the disparity in the estimates for T_c* found using two types of standard FSS techniques, namely, (i) the crossing technique for Binder parameter, as well as for the correlation length, and (ii) the scanning and shifting techniques. This disparity could not be entirely explained by the error bars and indicates strong crossover effects. Note that corrections to scaling were completely neglected in the methods of type (ii). In order to clarify the cause of the difference found for T_c, the scanning technique was used for the four largest systems only, giving $T_c = 2.054 \pm 0.001$ in agreement with the result of the crossing method. However, despite the *improvement* in T_c, the value $1/\nu = 1.312 \pm 0.007$ was a *deterioration*. This is *another puzzle* which needs explanation. Taking everything together these results support the presence of strong crossover effects in the system considered.

Knowing T_c, one can then estimate the critical exponents again using the FSS theory [1]. We have calculated the exponent ratios β/ν and γ/ν, the FSS behavior of $M(L, T_c)$, and the magnetic susceptibility $\chi(L, T_c)$. For $T_c = 2.057$, we found $\beta/\nu = 0.544 \pm 0.015$ and $\gamma/\nu = 1.90 \pm 0.03$, respectively. Nearly the same estimates were obtained using other FSS methods. Taking $T_c = 2.054$ for the four largest sizes L_i, we obtained $\beta/\nu = 0.520 \pm 0.008$ and $\gamma/\nu = 1.87 \pm 0.03$. The results for both

choices $T_c = 2.057$ and $T_c = 2.054$ are summarized in Table I in the first and second lines, respectively, beneath the "Fluid^2" heading. The estimates for $1/\nu$ were found by the scanning technique.

Comparing our results with the previous ones [8], we conclude that (i) the ratios of critical exponents β/ν and γ/ν found in our study are closer to the values known for the lattice model [17,19]; (ii) the critical exponent ν is extremely sensitive to the estimate of critical temperature T_c used; (iii) even for larger systems, which this study considers, a systematic deviation from the lattice exponents is seen that cannot entirely be justified by the error bars; and (iv) the disparity in estimates found for the critical temperature T_c, using the crossing and shifting techniques, has no explanation within the standard FSS approach. Hence, our data have to be considered as results for *effective exponents* and one can expect that the true asymptotic behavior would be visible only for much larger systems. If nonasymptotic crossover effects are considered, one may think of the presence of the Wegner correction term. However, this is expected to be negligible for our largest system sizes. One has to ask, therefore, what the reason is for such a strong crossover in the system we considered, compared to the lattice model.

In order to investigate this problem in more detail let us recall an idea encountered in the Fisher renormalization [7] for a system under thermodynamic constraint. According to this idea, the critical singularities in the grand canonical ensemble, with fixed chemical potential μ, may be different from those describing the system in the canonical ensemble with fixed density n. One has to perform the corresponding Legendre transformation carefully, taking into account the properties of singular functions in the grand canonical ensemble. In particular, this gives the well-known relation [see, e.g., Eq. (2.38a) in [7]]

$$\tau = a_0 t^{x_\alpha}(1 + a_1 t^{\Delta_\alpha}), \qquad (2)$$

which connects the reduced temperature scales t and τ in the two different ensembles with fixed n and μ, respectively. The values of x_α and Δ_α in (2) depend on the sign of the specific heat critical exponent α and are equal to

$(1 - \alpha)^{-1}$ or 1 and $\alpha(1 - \alpha)^{-1}$ or $-\alpha$ for α positive or negative, respectively. It is seen already from (2) that *independent of whether Fisher renormalization changes the critical exponents in the ensemble with fixed n, a new type of corrections to scaling appears in the canonical ensemble*. These corrections, being proportional to α, must not be confused with Wegner corrections to scaling; and because of the smallness of α in the Heisenberg universality class, they have to be taken into account within the FSS analysis. We note also that Eq. (2) is not the only source [20] for the appearance of new corrections (as was assumed, e.g., in [21]) in the canonical ensemble. There is another reason, which also follows from thermodynamics. For example, using hyperscaling relations for the critical exponents, it can be easily proved [20] that the second term in the known expression $\chi_{T,n} = (\partial M/\partial h)_{T,n} = (\partial M/\partial h)_\mu - (\partial M/\partial \mu)_T (\partial N/\partial \mu)_T^{-1}(\partial N/\partial h)_\mu$ produces an additional correction to the magnetic susceptibility $\chi_{T,n}$ with an exponent proportional to α. Hence, these new corrections to scaling cannot be included in the standard FSS by means of simple rescaling of t, which follows from (2) and as was proposed in [21].

In order to prove our predictions and to estimate the range of asymptotic behavior in which the new correction can be neglected, we have performed additional calculations. In Fig. 2 the results, obtained for the temperatures $T_{\text{peak}}(L)$, where the maximums of the functions $\partial M/\partial \beta$ and $\chi(T, L)$ are located, are shown for different sizes of L. These results have been fitted (dashed lines) for the *four largest* system sizes by using the expression

$$T_{\text{peak}}(L) = T_c + AN^{-1/3\nu}(1 + BN^{-|\alpha|/3\nu}), \qquad (3)$$

with the values of $1/\nu$ and α known for the lattice model [17,19]. The quantity-dependent constants A and B were then estimated. It is seen in Fig. 2 that (i) the fitting curves are in rather good agreement with the MC data obtained

TABLE I. Summary of results with n being the reduced density. In the first three rows (denoted as Fluid^1) the results from [8] are given. In the last row the universal quantities known for the lattice Heisenberg model [17,19] are presented. Our results are shown in the rows denoted as Fluid^2.

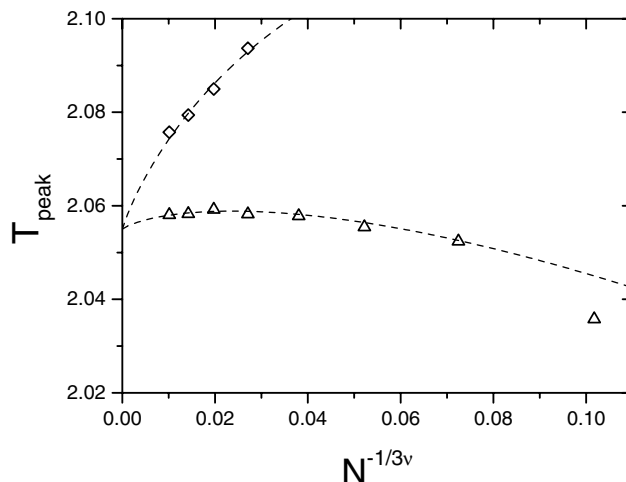|	U_4	$1/\nu$	β/ν	γ/ν
Fluid^1				
$n = 0.4$	0.613	1.35(5)	0.55(2)	1.86(3)
$n = 0.6$	0.608	1.41(3)	0.56(2)	1.85(1)
$n = 0.7$	0.605	1.42(3)	0.55(2)	1.84(3)
Fluid^2				
$n = 0.6$	0.619	1.40(1)	0.54(2)	1.90(3)
		1.31(1)	0.52(1)	1.87(3)
Lattice	0.622	1.421(5)	0.514(1)	1.973(2)

FIG. 2. Size dependence of the maximum locations in the derivative $\partial M/\partial \beta$ (triangles) and susceptibility $\chi(T, L)$ (diamonds). The results of fitting to MC data (dashed curves) are found using (3) with $1/\nu$ and α known for the lattice model.

even for smaller values of L, (ii) such a simple procedure allows one to understand the strong deviation from the linear dependence $T_{\text{peak}}(L) = T_c + AN^{-1/3\nu}$ that follows from (3) when the correction to scaling is neglected, and (iii) the disparity in estimates found for T_c within the crossing and shifting techniques can be explained. Using the fitting procedure, described above, we have found that the estimate $T_c = 2.055 \pm 0.001$ gives a rather good fit for all the data $T_{\text{peak}}(L)$, obtained from the maximum positions of $\partial M/\partial\beta$, $\chi(T,L)$, $\bar{U}_3(T,L)$, and $\chi_3(T,L)$. Another finding was that in contrast to the strong quantity dependence of A, the parameter B in (3) is almost independent of the quantity considered [22]. Note that if the rescaling relation (2) is considered as the unique reason for the appearance of the new correction, then the parameter B is quantity independent. From the fitting procedure it has been found that $B \simeq 1.3 \pm 0.2$ for all five sets of $T_{\text{peak}}(L)$ studied. Having the value of B, we can then estimate the minimal number of particles N_{min} such that the correction term in (3) can be neglected if $N > N_{\text{min}}$. This gives $N_{\text{min}} \simeq 10^8$ [then the relative contribution of the second term in the bracket of (3) is less than 0.5], and, therefore, it is clear why the true asymptotic behavior could not be observed earlier [8] or in our MC study. Finite systems with $N > N_{\text{min}}$ have not been considered so far in MC simulations. Hence, only the effective exponents could be studied for smaller size systems.

In conclusion, we note that if the absolute specific heat exponent α is small enough, Fisher corrections to scaling discussed are very important in models *with constraints*. At $d = 3$ α is very small for the Ising, the XY, and the Heisenberg classes of universality, as well as for other systems. In particular, we are convinced that the problems found in the Ising fluid [9,10] have the same origin. In this respect it is also worth referring the reader to Ref. [23], where, within the ϵ-expansion scheme, it was proven analytically that the leading correction to scaling in a compressible Heisenberg magnet as well as in a randomly diluted, weakly inhomogeneous Heisenberg model is equal to $-\alpha$, and this supports our conclusions. More detailed results including the determination of the values of the asymptotic exponents will be given elsewhere.

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