Monte Carlo Simulation of the Ferromagnetic Order-Disorder Transition in a Heisenberg Fluid

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(Received 20 March 1995)

We have performed Monte Carlo simulations of the ferromagnetic order-disorder transition in an off-lattice version of the Heisenberg model. Varying the temperature at a fixed density, we located the transition for three different densities by means of a finite-size scaling analysis. The obtained critical exponents differ from those for the lattice Heisenberg model. Although the limited size of our systems warrants caution, the results question whether the lattice and the off-lattice model are in the same universality class.

PACS numbers: 75.50.Mm, 61.20.Ja, 64.60.Fr

Off-lattice versions of the Heisenberg model have been introduced as a first step towards a model for ferrofluids [1,2]. Although the Heisenberg fluid model is too crude to be compared with real magnetic fluids, it embodies some of the complexities that can be anticipated in such fluids; e.g., the Heisenberg fluid displays a magnetic order-disorder transition besides phase transitions between a solid, a liquid, and a vapor phase. Its phase diagram has been studied by analytic methods [3,4] and by Monte Carlo (MC) simulations [1] which focused on the interplay between the magnetic and the liquid-vapor transition. The model also poses the question of whether the magnetic transition is in the same universality class as the corresponding transition in the lattice model. The Heisenberg fluid resembles the lattice model with an annealed site dilution, and the critical properties can be expected to be the same [5]. There is, however, to the best of our knowledge, little known about the fate of universality when diluting the sites in the lattice Heisenberg model [5]. According to the Fisher renormalization scheme [6], arguments predict that the dilution does not change the critical exponents. There seem to be no experimental results on critical exponents in a magnetic fluid.

Our study presents a first simulation of the magnetic critical properties in an off-lattice model. We use finite-size scaling (FSS) relations and other now relatively standard techniques, such as the use of the Binder parameter [7], to extract the critical behavior. Our results can be compared with accurate estimates of, e.g., the critical exponents for the lattice Heisenberg model obtained from previous MC simulations [8–10].

In the simulations we use the potential

$$\phi(\vec{r}_i,\vec{r}_j,\vec{s}_i,\vec{s}_j) = \begin{cases} \infty & r_{ij} < \sigma, \\ -J(r_{ij})\vec{s}_i \cdot \vec{s}_j & \sigma < r_{ij} < 2.5\sigma, \\ 0 & r_{ij} > 2.5\sigma, \end{cases}$$

where $\phi(\vec{r}_i,\vec{r}_j,\vec{s}_i,\vec{s}_j)$ denotes the potential between a particle i with position $\vec{r}_i$ and spin $\vec{s}_i$ and a particle j with position and spin $\vec{r}_j$ and $\vec{s}_j$. The position space is three dimensional and the spins are Heisenberg spins, i.e., each spin $\vec{s}_i$ is a three-dimensional vector of unit length. The hard-core repulsion at distances r_{ij} ($r_{ij} = |\vec{r}_i - \vec{r}_j|$) smaller than σ prohibits these interparticle distances, while two particles farther than 2.5σ away from each other do not interact. The Heisenberg-like interaction, at distances r_{ij} in between, has a ferromagnetic, Yukawa type coupling constant

$$J(r) = \epsilon \frac{\sigma}{r} \exp\left\{\frac{r-\sigma}{\sigma}\right\},$$

where ϵ sets the energy scale of the interaction. This potential is identical to the one used by Lomba *et al.*, except that they cut the potential at a much larger distance than 2.5σ.

We limit our study to the magnetic order-disorder transition away from the first-order liquid-vapor line. Following Lomba *et al.*, we vary the temperature T in our simulations while keeping the density fixed. We do this for three densities n: $n = 0.4$, $n = 0.6$, and $n = 0.7$ (all densities are expressed in units σ^{-3}). The use of systems with a number of particles N ranging from $N = 108$ to $N = 1372$ (for $n = 0.4$ and $n = 0.7$) or from $N = 108$ to $N = 2916$ (for $n = 0.6$) permitted us to investigate the critical behavior by a FSS analysis.

In the simulations, the positions were sampled with a regular Metropolis scheme, and the spin degrees of freedom with the Wolff algorithm [11]. Two sweeps, in each of which we attempt to move each particle once, are followed by the construction of one Wolff cluster after which the Monte Carlo proceeds with the next two sweeps. The acceptance ratio of the trial moves was around 50%. The size of the Wolff cluster around T_c varied between 15% of the total number of particles N for $N = 108$ and 5% for $N = 2916$. A system is typically followed for 10^6 sweeps with the corresponding 0.5×10^6 Wolff updates (except the $N = 2916$ system, which we simulated for 0.48×10^6 sweeps with 0.24×10^6 Wolff updates).

After each Wolff update we measure the magnetization $\vec{m}$, $\vec{m} = (\sum_{i=1}^{N} \vec{s}_i)/N$, and the energy U of the system. For each N, n, and T we calculate the average magnetization moments $\langle m^k \rangle_{\mathrm{mc}}$ ($m = |\vec{m}|$, $k = 1, 2, 3, 4$, and the subscript mc stands for microcanonical) as a function of the energy per particle u of the system, and sample the

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energy distribution $P(u)$. With the multihistogram technique we can then, for a given N and n, reconstruct the canonical averages $\langle m^k \rangle$ for all temperatures T around the temperatures $\{T_i\}$ at which we performed the simulations [9,12]. The microcanonical magnetization moments and the energy distribution are averaged over and stored after blocks of 10^4 consecutive Wolff updates for error analysis. Simulations of systems smaller than 1372 particles ran on a Cray YMP-EL. The largest systems ran on a Cray C-98.

For the density $n = 0.6$ we simulated systems of $N = 108$, 256, 500, 1372, and 2916 particles. The system with $N = 108$ was simulated at $T = 3.1$, 3.15, and 3.2; the systems with $N = 256$ and $N = 500$ at $T = 3.05$, 3.1, 3.15, 3.2, and 3.25; the system with $N = 1372$ at $T = 3.13$, 3.16, and 3.19; and the system with $N = 2916$ at $T = 3.12$, 3.15, and 3.18 (all temperatures are given in units ϵ/k_B with k_B Boltzmann's constant). Figure 1 shows the Binder parameter $u_4 = 1 - \langle m^4 \rangle / 3\langle m^2 \rangle^2$ [7] as a function of T for the five system sizes. We estimate T_c from the intersection temperatures T_i of the $N = 108$ curve with the other curves. A fit of $T_i(b) = T_c + c/\ln b$ with $b = (N/108)^{1/3}$ yields $T_c = 3.153(3)$, $c = (-1 \pm 2) \times 10^{-3}$ with a goodness of fit $Q = 0.84$ [8,9]. The same procedure for the intersections of the $N = 256$ curve with the curves for larger N yields $T_c = 3.151(3)$, $c = (5 \pm 19) \times 10^{-4}$ with $Q = 0.69$. The same fit to the values of the Binder parameters at the intersection point yields $u_{4c} = 0.6081(8)$, $c = (2 \pm 5) \times 10^{-4}$, $Q = 0.96$ for intersections with the $N = 108$ curve. The $N = 256$ curve yields $u_{4c} = 0.608(1)$, $c = (-1 \pm 6) \times 10^{-4}$, $Q = 0.08$. The critical Binder parameter for the lattice Heisenberg model is $u_{4c} = 0.6217(8)$ [8,9].

FSS predicts the magnetization at T_c, m_c to vary with the linear system size L as $m_c \propto L^{-\beta/\nu}$, with β and ν the magnetization and correlation length exponents, respectively [7]. A straight line fit of $\log m_c$ vs $\log L$ is best ($Q = 0.88$) for an estimate of $T_c = 3.145$ and gives $\beta/\nu = 0.5546(17)$, see Fig. 2. For an estimate of $T_c = 3.14$ we find $\beta/\nu = 0.5402(16)$, $Q = 0.14$, while the estimate $T_c = 3.15$ yields $\beta/\nu = 0.5690(17)$ with $Q = 0.32$. Straight line fits of the higher moments $\langle m^k \rangle$ at T_c vs $\log L$ ($k = 2, 3, 4$) all yield best fits for $T_c = 3.145$ and identical values for β/ν. One finds $\beta/\nu = 0.514(1)$ for the lattice Heisenberg model [8–10].

The susceptibility χ, $\chi = L^3(\langle m^2 \rangle - \langle m \rangle^2)/k_B T$, has, as a function of T, a maximum χ_m. According to FSS, $\chi_m \propto L^{\gamma/\nu}$ with $\gamma/\nu = 3 - 2(\beta/\nu)$ and γ the susceptibility exponent. A straight line fit of $\log \chi_m$ vs $\log L$ yields $\gamma/\nu = 1.856(9)$ with $Q = 0.38$. The ratio γ/ν can also be estimated from $\chi_c = \chi(T_c)$ for which the same scaling as for χ_m is predicted. Straight line fits of $\log \chi_c$ vs $\log L$ are good fits (with $Q > 0.6$) for a wide range of temperatures although with a systematic variation in the resulting γ/ν. If we take T_c in the range $3.145 < T_c < 3.155$, we estimate $\gamma/\nu = 1.84(2)$. The Heisenberg lattice value is $\gamma/\nu = 1.973(2)$ [8–10]. The ratio χ_c/χ_m is according to FSS independent of L for large sufficiently L [7]. Fitting this ratio for the five system sizes to a constant c, we obtain a best fit $c = 0.953(1)$ ($Q = 0.38$) for the estimate $T_c = 3.155$. For the estimate $T_c = 3.15$ the fit worsens to $Q = 0.03$ [$c = 0.946(1)$], while for $T_c = 3.16$ we have $Q = 0.11$ [$c = 0.958(1)$].

The ratio $1/\nu$ can, e.g., be obtained from the minima in $\partial m/\partial T$ as a function of T. They should scale as $(\partial m/\partial T)_{\min} \propto L^{(1-\beta)/\nu}$. However, the curve of $\log(\partial m/\partial T)_{\min}$ vs $\log L$ shows a pronounced curvature

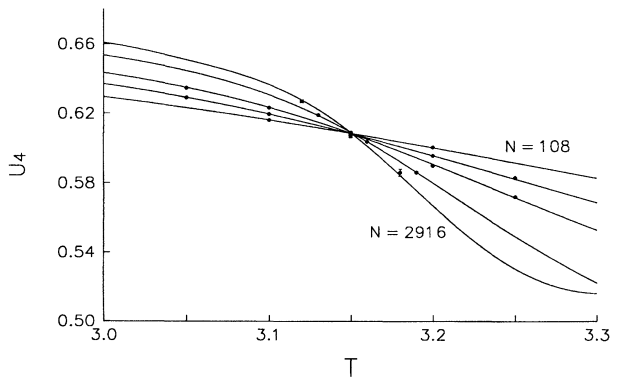

FIG. 1. Binder parameter u_4 versus the temperature T for systems ranging from $N = 108$ to $N = 2916$ at the density $n = 0.6$. The dots are averages over single simulations and the lines result from interpolation by histogram reweighting.

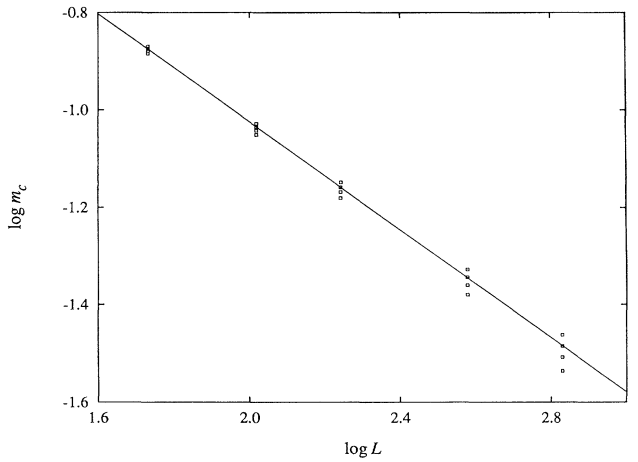

FIG. 2. Log-log plot of the magnetization at T_c, m_c versus the linear system size L. The squares are the results for the five system sizes at the density $n = 0.6$ and four estimates of T_c: $T_c = 3.14$, 3.145, 3.15, 3.156. At any L, m_c decreases for a higher estimate of T_c. Error bars on the squares do not exceed the symbol size. The line is the straight line fit to the points for $T_c = 3.145$. The points for the other estimates of T_c show an increased curvature.

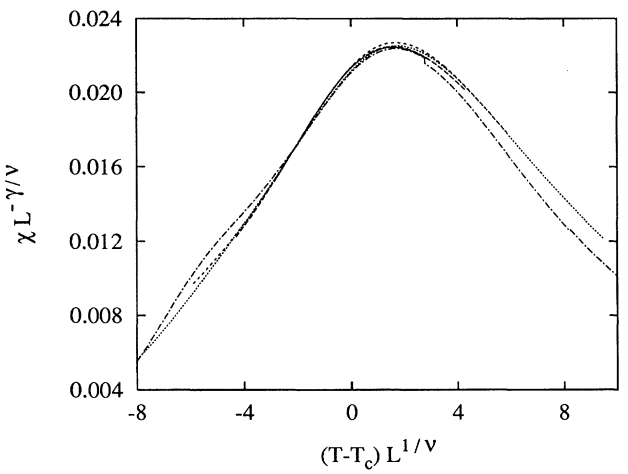

FIG. 3. Data-collapse plot for the susceptibility with $T_c = 3.15$, $\gamma/\nu = 1.85$, and $1/\nu = 1.41$. The plot shows the five system sizes at $n = 0.6$.

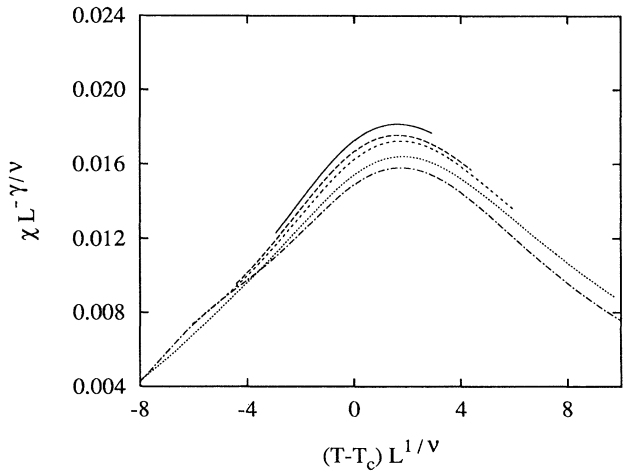

FIG. 4. Same as Fig. 2 with $T_c = 3.15$ and the lattice Heisenberg exponents $\gamma/\nu = 1.973$ and $1/\nu = 1.421$. The curves are shifted downward with increasing system size: The top curve is for the $N = 108$ system and the bottom curve for $N = 2916$.

leading to the poor value $Q = 0.01$ for a straight line fit. Limiting the fit to the $N = 500$, 1372, and 2916 systems yields $Q = 0.58$ and $(1 - \beta)/\nu = 0.86(3)$. With $\beta/\nu = 0.56(2)$ we obtain $1/\nu = 1.42(3)$. The magnetization derivative $\partial m/\partial T$ at T_c should scale in the same fashion but yields once more curved lines on a log-log plot for all reasonable estimates of T_c. Even if we limit the fit to the three largest systems, we retain rather poor fits: $Q = 0.21$–0.24 with $(1 - \beta)/\nu = 0.86(2)$ for all estimates of T_c between 3.13 and 3.16. If we inspect the slope $\partial u_4/\partial T$ at T_c, which FSS predicts to scale as $(\partial u_4/\partial T)_{T_c} \propto L^{1/\nu}$, we find good straight line fits of $\log(\partial u_4/\partial T)_{T_c}$ vs $\log L$ for a large range of choices for T_c. If we take $T_c = 3.15$, we estimate $1/\nu = 1.40(3)$. The Heisenberg lattice value is $1/\nu = 1.421(5)$ [8–10].

Our final estimates are $T_c = 3.150(5)$, $u_{4c} = 0.6081(8)$, $\beta/\nu = 0.56(2)$, $\gamma/\nu = 1.85(1)$, and $1/\nu = 1.41(3)$ for the density $n = 0.6$. The data-collapse plots in Figs. 3 and 4 show again that the simulations favor this estimate of γ/ν above the value for the lattice model.

The analysis for $n = 0.4$ and $n = 0.7$ is similar although somewhat less convincing because of the absence of a $N = 2916$ system. Moreover, the data for $N = 0.7$ show in general more scatter than at the lower densities. For $N = 0.4$ we obtain $T_c = 1.940(5)$, $u_{4c} = 0.6130(8)$, $\beta/\nu = 0.55(2)$, $\gamma/\nu = 1.86(3)$, and $1/\nu = 1.35(5)$. For $n = 0.7$ we obtain $T_c = 3.79(1)$, $u_{4c} = 0.605(2)$, $\beta/\nu = 0.55(2)$, $\gamma/\nu = 1.84(3)$, and $1/\nu = 1.42(3)$. The results are summarized in Table I.

We tried to ascertain whether our data are compatible with the lattice Heisenberg exponents and the inclusion of corrections to FSS. We fitted χ_m for $n = 0.6$ by $\chi_m(L) = c_1 L^{\gamma/\nu} + c_2 L^{-y+\gamma/\nu}$ with γ/ν fixed at the lattice Heisenberg value 1.975 [8–10]. If we fix y at values $0 < y \leq 0.1$, the fit routine gives values $c_1 < 0$, which is unphysical. For $y = 0.2$ we obtain $c_1 = 0.0066(9)$, $c_2 = 0.016(1)$, $Q = 0.35$. The goodness of fit decreases with increasing y with, e.g., $Q = 0.21$ for $y = 0.4$. Hence the assumption of lattice Heisenberg critical behavior with corrections to scaling does not fit the data better.

Monte Carlo simulations of an off-lattice Heisenberg fluid are in agreement with a FSS description, but with exponents and a critical Binder parameter that are slightly, but significantly, different from those for the lattice. The limited system sizes and the limited range of sizes require this observation to be taken cautiously. Nevertheless, the discrepancies are serious enough to challenge the view that the ferromagnetic transition is the same for the lattice and the off-lattice model.

We thank D. Levesque, H. J. Hilhorst, H. W. J. Blöte, J. R. Heringa, and G. Stell for their interest and their suggestions. Computing time on the C-98 was granted

TABLE I. Summary of results. n is the density; T_c the critical temperature; u_{4c} the critical value of the Binder parameter; and β/ν, γ/ν, and $1/\nu$ are exponent ratios. The last row gives the results for the lattice Heisenberg model from Refs. [8–10]. The critical temperature in this row is for the simple cubic lattice [$T_c = 2.0542(2)$ for the bcc lattice [10]].

n	T_c	u_{4c}	β/ν	γ/ν	$1/\nu$
0.4	1.940(5)	0.6130(8)	0.55(2)	1.86(3)	1.35(5)
0.6	3.150(5)	0.6081(8)	0.56(2)	1.85(1)	1.41(3)
0.7	3.79(1)	0.605(2)	0.55(2)	1.84(3)	1.42(3)
Lattice	1.44293(8)	0.6217(8)	0.514(1)	1.973(2)	1.421(5)

by the Institut de Développement et des Ressources en Informatique Scientifique (IDRIS). M.J.P.N. benefited from a grant from the French government.

[1] E. Lomba, J. J. Weiss, N. G. Almarza, F. Bresme, and G. Stell, Phys. Rev. E **49**, 5169 (1994).
[2] J. S. Høye and G. Stell, Phys. Rev. Lett. **36**, 1569 (1976).
[3] P. C. Hemmer and D. Imbro, Phys. Rev. A **16**, 380 (1977).
[4] J. M. Tavares, M. M. Telo da Gama, P. I. C. Teixeira, J. J. Weis, and M. J. P. Nijmeijer (to be published).
[5] R. B. Stinchcombe, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 7.
[6] M. E. Fisher, Phys. Rev. **176**, 257 (1968).
[7] K. Binder, Z. Phys. B **43**, 119 (1981).
[8] P. Peczak, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **43**, 6087 (1991).
[9] C. Holm and W. Janke, Phys. Rev. B **48**, 936 (1993).
[10] K. Chen, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **48**, 3249 (1993).
[11] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[12] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989).