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Are defects important for 3D phase transitions?

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We use single-cluster Monte Carlo simulations to study the role of topological defects in the three-dimensional classical Heisenberg model on simple cubic lattices of size up to 80^3. By applying reweighting techniques to time series generated in the vicinity of the approximate infinite volume transition point K_c, we obtain clear evidence that the temperature derivative of the average defect density $d\langle n\rangle/dT$ behaves qualitatively like the specific heat, i.e., both observables are finite in the infinite volume limit.

1. INTRODUCTION

It is well known that topological defects can play an important role in phase transitions [1,2]. Recently Lau and Dasgupta (LD) [3] have used Monte Carlo (MC) simulations to study the role of topological defects in the three-dimensional (3D) classical Heisenberg model, where the defects are point-like objects. Motivated by the importance of vortex points in the 2D XY model [4], LD tried to set up a similar pictorial description of the phase transition in the 3D Heisenberg model. Analyzing their simulations on simple cubic (sc) lattices of size $V = L^3$ with $L = 8, 12$ and 16, LD claimed that the temperature derivative of the average defect density, $\langle n\rangle$, diverges at the critical temperature T_c like $d\langle n\rangle/dT \sim t^{-\psi}$, $t = |T-T_c|/T_c$, with an exponent $\psi \approx 0.65$. They further speculated that $\psi = 1-\beta$, where $\beta \approx 0.36$ is the critical exponent of the magnetization, and then argued that $\langle n\rangle$ should behave like a "disorder" parameter.

The existence of such a strong divergence of $d\langle n\rangle/dT$ seems unlikely, because the definition of defects is quasi-local. It is therefore more likely [5] that $\langle n\rangle$ should qualitatively behave like the energy and $d\langle n\rangle/dT$ like the specific heat, which is a finite quantity for the 3D Heisenberg model.

Using standard finite-size scaling (FSS) arguments we hence expect to see on finite lattices either

$$d\langle n\rangle/dT = L^{\psi/\nu} f(x) \qquad (1)$$

or, if the second argument holds true,

$$d\langle n\rangle/dT = const + L^{\alpha/\nu} g(x), \qquad (2)$$

where $\nu \approx 0.7$ and $\alpha \approx -0.1$ are the correlation length and specific heat exponents for the 3D Heisenberg model [6,7], $x = tL^{1/\nu}$, and $f(x), g(x)$ are scaling functions.

2. SIMULATION

Using the single-cluster update algorithm [8] we ran simulations for sc lattices of size $V = L^3$ with L=8, 12, 16, 20, 24, 32, 40, 48, 56, 64, 72, 80 and periodic boundary conditions [9]. Our main emphasis was on the defect density $n = \sum q^2 n_{|q|}$, where $n_1, n_2, \ldots$ are defect densities of charge $q = \pm1, \pm2, \ldots$. To locate these charges we followed the definition of Berg and Lüscher [10] according to which the charge q_{i^*} at the dual lattice site i^* is given by

$$q_{i^*} = \frac{1}{4\pi} \sum_{i=1}^{12} A_i. \qquad (3)$$

The 12 A_i refer to the directed areas of the spherical triangles that can be formed from the spins located at the vertices of the cube enclosing q_{i^*}.

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All runs were performed at $K_0 = 0.6929$ with a statistics of approximately 20000 measurements taken every τ_n sweep, where τ_n is the (integrated) autocorrelation time of the charge density. For each run we recorded the time series of the energy density $e = E/V$, the magnetization density $m = |\sum_i \vec{s}_i|/V$, and the charge densities $n_{|q|}$. From this data we computed the specific heat

$$C = d\langle e\rangle/dT = VK^2(\langle e^2\rangle - \langle e\rangle^2), \tag{4}$$

the thermal expansion coefficient

$$C_q = Td\langle n\rangle/dT = VK(\langle en\rangle - \langle e\rangle\langle n\rangle), \tag{5}$$

and the topological susceptibility

$$\chi_q = d\langle n\rangle/d\mu = V(\langle n^2\rangle - \langle n\rangle^2), \tag{6}$$

where μ is the "field" in a fugacity term $\mu V n$, which one can imagine adding to the energy.

We also computed the eigenvalues of the 2×2 covariance matrix formed by e and n, which gives two uncorrelated quantities λ_1 and λ_2. To obtain results for the various observables $\mathcal{O}$ at K values in an interval around the simulation point K_0, we applied the reweighting method [11]. To obtain errors we devided each run into 20 blocks and used the standard Jackknife technique.

3. RESULTS

We focussed first on the scaling behavior of C_q at our previous estimate [7] of the critical coupling $K_c = 0.6930$, and checked a scaling Ansatz for C_q of the form

$$C_q = C_q^{\rm reg} - a_0 L^{\alpha'/\nu}. \tag{7}$$

Note that this Ansatz covers both scaling hypotheses (1) and (2). The resulting fit yields $\alpha'/\nu = -0.401(61)$, $C_q^{\rm reg} = 1.50(8)$, and $a_0 = 1.82(6)$, with a quality factor $Q = 0.30$. The good quality of the fit basically rules out the divergence predicted by the Ansatz (1) of LD, and strongly favours (2), which predicts a finite asymptotic value for C_q. We also tried to reproduce the exponent $\psi \approx 0.65$ of LD, by selecting only their lattice sizes, and fitting a straight line to our first 3 data points. But even then we obtain a much smaller value of $\psi/\nu \approx 0.36(3)$, leading to $\psi \approx 0.25(3)$.

One can ask, if α' is equal to the specific-heat exponent α. Using our earlier MC result [7] of $\nu = 0.704(6)$, we get a value of $\alpha' = -0.282(46)$, which does, on the first glance, not strongly support this conjecture. The best field theoretical estimates are $\nu = 0.705(3)$, $\alpha = -0.115(9)$, and $\alpha/\nu = -0.163(12)$ (resummed perturbation series [12]), while our earlier MC study [7] yielded $\nu = 0.704(6)$, $\alpha = -0.112(18)$, and $\alpha/\nu = -0.159(24)$. However, the accuracy of the values of α is somewhat misleading, because they were obtained from hyperscaling, $\alpha = 2 - 3\nu$. The directly measured values have much larger error bars, for example $\alpha/\nu = -0.30(6)$ [6] and $\alpha/\nu = -0.33(22)$ [7].

To compare α' directly with the measured specific-heat exponent of the present MC simulation, we fitted C to

$$C = C^{\rm reg} - b_0 L^{\alpha/\nu}. \tag{8}$$

The resulting fit yields $\alpha/\nu = -0.225(80)$, $C^{\rm reg} = 4.8(7)$, and $b_0 = 4.1(5)$ with $Q = 0.55$, leading to $\alpha = -0.158(59)$. These values are in very good agreement with the hyperscaling prediction, but noteworthy is also the tendency for the values to come out too large.

Other estimates for α' and α can be obtained [9] by means of analogous fits of $\langle n\rangle$ and $\langle e\rangle$ at $K_c = 0.6930$, which yield $(\alpha' - 1)/\nu = -1.547(15)$, $\langle n\rangle^{\rm reg} = 0.1074(1)$, and $c_0 = 0.42(2)$, with $Q = 0.30$, and $(\alpha - 1)/\nu = -1.586(19)$, $\langle e\rangle^{\rm reg} = 2.0106(1)$, and $d_0 = 1.68(8)$, with $Q = 0.25$. This results in $\alpha'/\nu = -0.127(27)$, $\alpha' = -0.089(20)$, and $\alpha/\nu = -0.166(31)$, $\alpha = -0.117(23)$. The results for α and α/ν are in excellent agreement with the hyperscaling prediction, and have not been directly measured before with such a high precision. The results for α' and α'/ν are lower than those obtained from (7), but now they are almost consistent with the values for α and α/ν.

We further looked at the scaling behavior of χ_q, defined in eq.(6), which looked similar to C_q. Therefore we tried again a scaling Ansatz of the form

$$\chi_q = \chi_q^{\rm reg} - e_0 L^{\alpha''/\nu}. \tag{9}$$

A three-parameter fit yields $\alpha''/\nu = -0.554(57)$, $\chi_q^{\rm reg} = 0.67(2)$, and $e_0 = 0.95(6)$ with $Q = 0.41$, leading to $\alpha'' = -0.390(44)$. If one discards the two lowest L values from the fit, one observes a clear trend towards a lower α''-value, but with the drawback of increased error bars and no improvement in χ^2/dof (per degree of freedom).

We tested in all fits if there were corrections to FSS, and observed in all quantities a trend to the value of α/ν predicted by hyperscaling, but at the price of much larger error bars. Also the χ^2/dof did not improve. We also checked that our results did not depend strongly on the choice of K_c by repeating the fits of all quantities at $K_c \pm 0.0002$.

For λ_1 and λ_2 we used again the Ansatz

$$\lambda_i = \lambda_i^{\rm reg} - a_i L^{\alpha_i/\nu}, \qquad (10)$$

which results in $\alpha_1/\nu = -0.273(73)$, $\lambda_1^{\rm reg} = 5.1(5)$, and $a_1 = 4.7(2)$, with $Q = 0.49$, and $\alpha_2/\nu = -1.45(42)$, $\lambda_2^{\rm reg} = 0.1307(8)$, and $a_2 = 0.2(2)$, with $Q = 0.60$, leading to $\alpha_1 = -0.192(54)$ and $\alpha_2 = -1.02(31)$. This suggests $\alpha_1 \approx \alpha$ and $\alpha_2 \approx \alpha - 1$. Because $\lambda_1 + \lambda_2 = C + \chi_q$, this means that at least χ_q should see something of an exponent α_2. The existence of an uncorrelated observable which scales with an exponent different from α suggests that we see either corrections to FSS, a new scaling field, or that C_q and χ_q scale with some rationale multiple of α/ν. The problem is that there is no satisfactory theory of the scaling of topological quantities.

4. CONCLUSIONS

We have shown that in the 3D classical Heisenberg model the topological defect density $\langle n \rangle$ and its temperature derivative C_q behave qualitatively like the energy $\langle e \rangle$ and its temperature derivative C. We obtain evidence that asymptotically for large L the scaling of C_q is governed by the specific-heat critical exponent α. In particular, we can reject the conjecture of LD that C_q diverges with a new critical exponent ψ, and we find no evidence for an unusual behavior of the defects near the phase transition. For the topological susceptibility χ_q we find that it also remains finite, and that it can be fitted with an Ansatz of the form (2) as well, but that its scaling exponent deviates from α. In fact, our fits of the eigenvalues λ_i of the covariance matrix indicate that C_q and χ_q are a mixture of a part which scales with α, and a part which scales according to $\alpha - 1$.

Finally, the present fits of the specific heat at K_c yielded a value of α/ν of better accuracy and in better agreement with the hyperscaling value than fits of the specific-heat maxima as used in previous works [6,7]. Moreover, by fitting the *energy* at K_c, we obtained an estimate for α/ν with a precision unprecedented by direct numerical MC simulations.

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