COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **4**, No. 1, pp. 124-134

Commun. Comput. Phys.
July 2008

Advanced Monte Carlo Study of the Goldstone Mode Singularity in the 3D XY Model

J. Kaupužs[1,*], R. V. N. Melnik[2] and J. Rimšāns[1]

[1] *Institute of Mathematics and Computer Science, University of Latvia, 29 Raiņa Boulevard, LV1459, Riga, Latvia.*
[2] *Wilfrid Laurier University, Waterloo, Ontario, N2L 3C5, Canada.*

Received 3 September 2007; Accepted (in revised version) 5 November 2007

Communicated by Joan Adler

Available online 27 February 2008

Abstract. Advanced Monte Carlo simulations of magnetisation and susceptibility in 3D XY model are performed at two different coupling constants $\beta = 0.55$ and $\beta = 0.5$, completing our previous simulation results with additional data points and extending the range of the external field to twice as small values as previously reported ($h \geq 0.00015625$). The simulated maximal lattices sizes are also increased from $L = 384$ to L=512. Our aim is an improved estimation of the exponent ρ, describing the Goldstone mode singularity $M(h) = M(+0) + ch^{\rho}$ at $h \to 0$, where M is the magnetisation. The data reveal some unexpected small oscillations. It makes the estimation by many-parameter fits of the magnetisation data unstable, and we are looking for an alternative method. Our best estimate $\rho = 0.555(17)$ is extracted from the analysis of effective exponents determined from local fits of the susceptibility data. This method gives stable and consistent results for both values of β, taking into account the leading as well as the subleading correction to scaling. We report also the values of spontaneous magnetisation.

AMS subject classifications: 65C05, 82B20, 82B80
Key words: Monte Carlo simulation, XY model, magnetisation and susceptibility, high performance computing, coupling constants, singularities, lattices.

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1 Introduction

Our previous Monte Carlo (MC) study of the three-dimensional (3D) XY [1] model has revealed some interesting features indicating that the magnetisation $M(h)$, dependent on the external field h below the phase transition temperature, very likely behaves as

$$M(h) = M(+0) + c_1 h^{\rho} \qquad \text{at} \quad h \to 0 \tag{1.1}$$

*Corresponding author. *Email addresses:* `kaupuzs@latnet.lv` (J. Kaupužs), `rmelnik@wlu.ca` (R. V. N. Melnik), `rimshans@mii.lu.lv` (J. Rimšāns)

with the exponent ρ somewhat larger than $1/2$. This is a challenging result, since the standard theory (see, e.g., [2–6] and references therein) predicts the Goldstone mode singularity (1.1) with $\rho=1/2$. The result $1/2<\rho<1$, however, is expected from an alternative theoretical treatment [7–9].

In this paper we report the results of an advanced MC study, including new simulation data for smaller fields h and larger linear lattice sizes L. Our aim is to make a refined estimation of the exponent ρ. It could help to clarify the fundamental question whether the asymptotics (1.1) is exactly what is provided by the Gaussian spin wave theory (to which the standard theory reduces asymptotically at $h\to 0$), yielding $\rho=1/2$ in three dimensions ($d=3$), or there are deviations from the Gaussian behaviour like at the critical point. We recall [1] that the Gaussian theory predicts $\sim k^{-2}$ singularity (at $k\to 0$) for the transverse Fourier-transformed two-point correlation function depending on the wave vector $\mathbf{k}$, whereas $\sim k^{-2+\eta^*}$ singularity with positive

$$\eta^* = 2 - d/(\rho+1) \tag{1.2}$$

corresponds to $\rho>1/2$ and $d=3$, which is comparable with the known $\sim k^{-2+\eta}$ behaviour of the two-point function at the critical point [10].

2 Simulation results

We consider the 3D XY model on a simple cubic lattice with the Hamiltonian $\mathcal{H}$ given by

$$\frac{\mathcal{H}}{T} = -\beta \left(\sum_{\langle ij \rangle} \mathbf{s}_i \mathbf{s}_j + \sum_i \mathbf{h} \mathbf{s_i} \right), \tag{2.1}$$

where T is temperature, $\mathbf{s}_i$ is the spin variable (two-component vector of unit length in the xy-plane) of the i-th lattice site, β is the coupling constant, and $\mathbf{h}$ is the external field. We consider the field which is oriented along the x axis with positive x-component $h_x \equiv h = |\mathbf{h}|$.

Recently a remarkable progress in Monte Carlo simulations of this model have been achieved by extending the simulation results to substantially larger lattice sizes $L\leq 384$ [1] as compared to $L\leq 160$ in earlier MC studies [11–13]. Here we report the results of extended MC simulations for even larger lattice sizes $L\leq 512$.

Like in our previous work [1], the simulations have been carried out in the ordered phase at $\beta = 0.5, 0.55 > \beta_c$, where $\beta_c \simeq 0.4542$ [14] is the critical point. The x-projection of magnetisation per spin $\langle m_x \rangle$, as well as the longitudinal susceptibility

$$\chi_\parallel = \frac{\partial \langle m_x \rangle}{\partial H} = V\left(\langle m_x^2 \rangle - \langle m_x \rangle^2\right) \tag{2.2}$$

have been evaluated for different L, where $V = L^3$ is the volume and $H = \beta h$.