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

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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 $h\rightarrow 0$, 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.

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

$$M(h)=M(+0)+c_1h^{\rho} \qquad \text{at} \quad h\rightarrow 0 \tag{1.1}$$

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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

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

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 $H=\beta h$.

Table 1: The MC simulated values of $\langle m_x \rangle$ of the 3D XY model for different lattice sizes L and external fields h at $\beta = 0.55$.

$10^4 h$	$\langle m_x \rangle$				
	L=512	L=384	L=256	L=192	L=128
3.125	0.6325486(84)	0.632530(13)	0.632525(18)		
8.75		0.633990(11)	0.634002(17)	0.633991(18)	
17.5			0.635550(14)	0.635551(14)	0.635560(16)
35				0.637904(10)	0.637903(17)

Table 2: The MC simulated values of $\langle m_x \rangle$ of the 3D XY model for different lattice sizes L and external fields h at $\beta = 0.5$.

$10^4 h$	$\langle m_x \rangle$				
	L=512	L=384	L=256	L=192	L=128
1.5625	0.521128(12)	0.521104(16)	0.521024(31)		
8.75			0.524326(13)	0.524323(21)	0.524277(22)
17.5				0.526867(16)	0.526897(21)
35				0.530807(12)	0.530776(19)

The simulation techniques based on a modification of the well known Wolff's single cluster algorithm [15] are described in our paper [1], where we provide also a comparison with the standard Metropolis algorithm, as well as with the results of other authors [13]. The new values of the magnetisation at $\beta = 0.55$ and $\beta = 0.5$ are given in Tables 1 and 2, respectively. In Tables 3 and 4, the corresponding values of the longitudinal susceptibility are listed. These new results are complementary to those in [1] in the sense that the set of h values is completed within the already considered range in order to allow statistically more reliable fits, and the results are extended to twice as small fields h as previously reported.

Note that the smaller fields are considered, the larger lattice sizes are necessary for a good estimation of the thermodynamic limit. The minimal acceptable lattice size increases roughly as $\propto h^{-1/2}$ [1]. Therefore here we have simulated lattices up to $L = 512$ to extract the thermodynamic limit for the smallest h values.

Remarkable computational resources are necessary for such simulations. They have been provided by the Shared Hierarchical Academic Research Computing Network (SHARCNET: `www.sharcnet.ca`). For the largest lattices (L=512), one job required nearly 1.25 GB operative memory and about 55 s CPU time per one modified Wolff's algorithm step. In this case jobs have been run on the clusters with Opteron 4×2.20 GHz nodes, and the total number of MC steps was 170000 and 110000 for β=0.5 and β=0.55, respectively. All results reported in this paper have been obtained within two months by running on average 8 jobs simultaneously.

Table 3: The MC simulated values of the longitudinal susceptibility $\chi_\parallel$ of the 3D XY model for different lattice sizes L and external fields h at $\beta=0.55$.

$10^4 h$	$\chi_\parallel$				
	L=512	L=384	L=256	L=192	L=128
3.125	5.61(18)	5.98(23)	6.34(25)		
8.75		3.76(13)	3.90(12)	3.793(97)	
17.5			2.881(71)	2.839(52)	2.820(38)
35				2.150(43)	2.119(33)

Table 4: The MC simulated values of the longitudinal susceptibility $\chi_\parallel$ of the 3D XY model for different lattice sizes L and external fields h at $\beta=0.5$.

$10^4 h$	$\chi_\parallel$				
	L=512	L=384	L=256	L=192	L=128
1.5625	14.31(51)	14.38(65)	16.64(81)		
8.75			6.57(11)	6.82(13)	7.00(12)
17.5				5.243(90)	5.208(64)
35				4.136(78)	4.040(57)

The conclusion that the actually simulated maximal sizes are large enough is based on an observation of a sufficiently fast convergence to the thermodynamic limit, as well as on a reasonably small influence of the finite size effects on the evaluated exponent ρ. At $\beta=0.55$, larger lattices have been simulated for the same values of h, as compared to the case $\beta=0.5$. It is motivated by the fact that the difference $M(h)-M(+0)$ is smaller for $\beta=0.55$ and, thus, it has to be determined with a smaller absolute error.

In the following our main estimation is based on the evaluation of the thermodynamic limit only from the largest-lattice data for each h, taken from [1] and completed with the recent values reported here. For testing purposes, we also have estimated the thermodynamic limit values as weighted averages (with the weights $\propto\sigma_i^{-2}$, where σ_i are the standard errors of the quantities involved) over the data for two largest lattices at each h.

3 Estimation of the exponent ρ

3.1 log-log fits of the susceptibility data

The exponent ρ most simply can be estimated from a slope of $\ln\chi_\parallel$ vs $\ln h$ plot, which tends asymptotically to $\rho-1$ in accordance with the singularity

$$\chi_\parallel \propto h^{\rho-1} \tag{3.1}$$

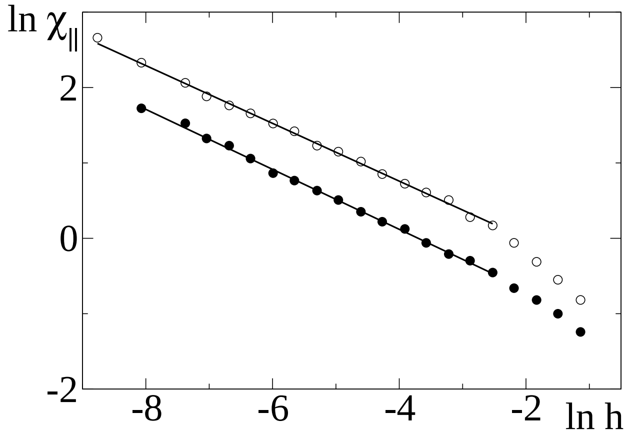

Figure 1: The $\ln\chi$ vs $\ln h$ plots for $\beta=0.55$ (solid circles) and for $\beta=0.5$ (empty circles).

of the longitudinal susceptibility at $h\to 0$, as given by (1.1) and (2.2). The linear log-log fits of the largest-lattice data for both values of β are shown in Fig. 1, giving $\rho=0.6021(48)$ at $\beta=0.55$ and $\rho=0.6166(34)$ at $\beta=0.5$. The corresponding values of $\chi^2/\text{d.o.f.}$ (the sum of weighted squared deviations per degree of freedom of the fit [16]) are 1.51 and 2.55. This method apparently provides rather stable results, as we can see it from comparison with the very similar estimates $\rho=0.6003(58)$ for $\beta=0.55$ and $\rho=0.6162(39)$ for $\beta=0.5$ obtained in [1] from the data with twice as large minimal values of h. The results also are insignificantly influenced by the finite size effects. Namely, such plots as in Fig. 1 yield $\rho=0.6014(29)$ for $\beta=0.55$ and $\rho=0.6143(21)$ for $\beta=0.5$ when the averaged over two largest lattices data are used, as explained at the end of Section 2. A refined analysis of the local gradients of these plots (Section 3.3), however, shows that the apparent accuracy and stability of such a method is somewhat misleading. Namely, due to the corrections to scaling neglected here, the differences between the actually measured and asymptotic slopes most probably are much larger than the indicated standard errors.

3.2 Fits of the magnetisation data

Here we consider the estimates of the exponent ρ obtained from many-parameter fits of the magnetisation data to the ansatz

$$M(h)=M(+0)+\sum_{n=0}^{m} c_n h^{\rho_n}, \tag{3.2}$$

where the exponents $\rho_n=(n+1)/2$ are provided by the standard theory [5], and m is the total number of correction terms included. We have tested how these estimates change if the fits are performed for twice as small fields as compared to the smallest h intervals considered in [1], including the recent simulation data. The comparison for $\beta=0.55$ is presented in Table 5. As we see, the fit results both for $m=1$ and $m=2$ change slightly

Table 5: The fit results for the exponent ρ and the χ^2/d.o.f. at $\beta=0.55$ depending on the number of correction terms m included in (3.2) and on the fitted range of the field h.

m	$h\times 10^3$	ρ	χ^2/d.o.f.
1	0.625 – 14	0.575(22)	0.88
	0.3125 – 7	0.565(28)	1.24
2	0.625 – 40	0.536(27)	1.16
	0.3125 – 20	0.569(38)	0.99

Table 6: The fit results for the exponent ρ and the χ^2/d.o.f. at $\beta=0.5$ depending on the number of correction terms m included in (3.2) and on the fitted range of the field h.

m	$h\times 10^3$	ρ	χ^2/d.o.f.
1	0.3125 – 10	0.630(15)	1.31
	0.15625 – 5	0.483(23)	1.28
2	0.3125 – 28	0.571(20)	1.72
	0.15625 – 14	0.484(33)	2.69

depending on the range of h values. Besides, the estimates $\rho=0.565(28)$ (at $m=1$) and ρ=0.569(38) (at m=2) for the smallest h intervals agree well with each other. These values are sufficiently stable with respect to the finite-size effects. The already mentioned test estimations, including the data for smaller lattices, yield $\rho=0.561(23)$ and $\rho=0.555(30)$, respectively. Hence, the small finite-size effects are such that ρ more probably will slightly increase for larger sizes, thus even more deviating from the standard theoretical value 0.5.

Contrary to the case $\beta=0.55$, the results are very unstable for $\beta=0.5$, as we can see it from Table 6. Due to the dramatic variations in their values, dependent on the fit interval, these estimations hardly can be considered as evidences for the asymptotic behaviour of the exponent ρ.

To find the reason for the instability, we have checked how the data points deviate from such fit curves. The deviations from the five-parameter fits with $m=2$ correction terms for the intervals $h\in[0.00015625;0.014]$ and $h\in[0.00015625;0.02]$ are shown in Fig. 2 (top). For comparison, we have shown here also the deviations for the interval $h\in[0.0003125;0.028]$ at $\beta=0.5$ (bottom left) and $\beta=0.55$ (bottom right). Apparently, there are some small deviations of oscillating type, which are not reasonably well described by the ansatz (3.2) even if some more correction terms are included. From this point of view, the observed oscillations are unexpected. A question can arise wether these are systematic deviations or only purely statistical fluctuations. Some systematic deviations, overlaping with statistical fluctuations, most probably are present, since the χ^2/d.o.f. values for the upper fits at $\beta=0.5$ (2.69 in one case and 2.9 in the other case) are remarkably larger than 1, whereas $\chi^2/\mathrm{d.o.f.}\sim 1$ is expected for moderately good fits [16]. In the lower pictures, the deviations are smaller. However, it is a striking fact that they look

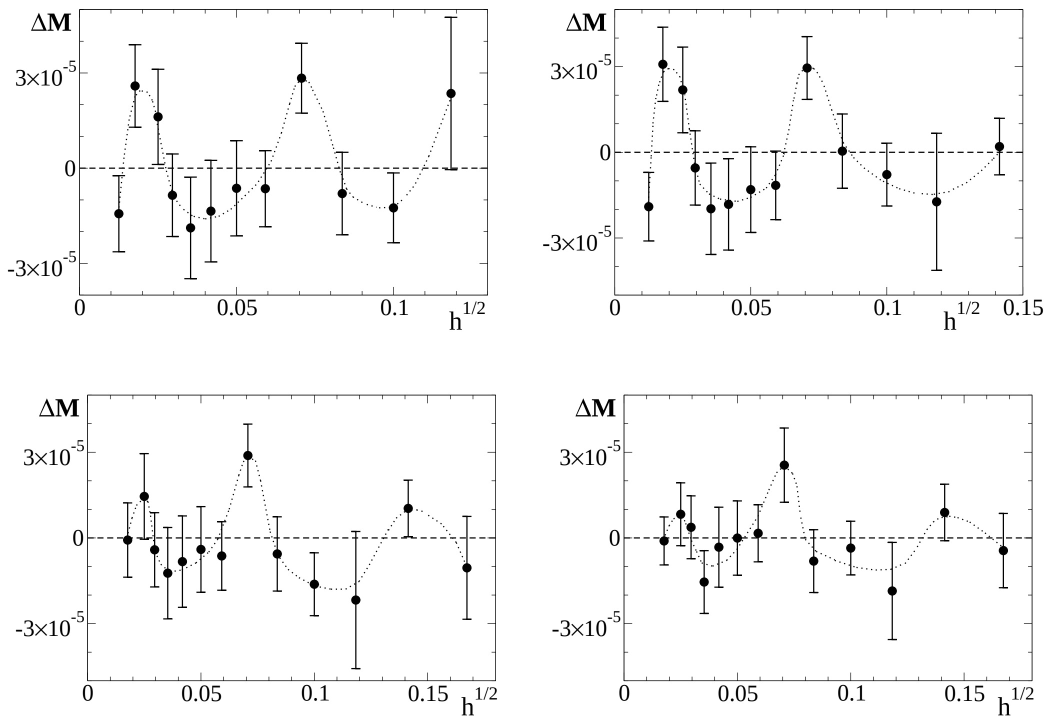

Figure 2: Deviations of the magnetisation data from the five-parameter fit curves for $\beta = 0.5$, $h \in [0.00015625;0.014]$ (top left); $\beta = 0.5$, $h \in [0.00015625;0.02]$ (top right); $\beta = 0.5$, $h \in [0.0003125;0.028]$ (bottom left); and $\beta = 0.55$, $h \in [0.0003125;0.028]$ (bottom right). The dotted lines are guides to eye.

very similar for $\beta = 0.5$ (left) and $\beta = 0.55$ (right), only the deviation amplitude is somewhat smaller at $\beta = 0.55$. Since these are two statistically independent simulations, such a similarity could not be caused by random fluctuations. Hence, the systematic oscillations are present. The above oscillations can be interpreted as a transient nonasymptotic behaviour, since a power-like behaviour of $M(h) - M(+0)$, accompanied by power-like corrections, is expected at $h \to 0$.

The systematic oscillations explain the instability in the estimation of ρ, since many-parameter fits are very sensitive to any small systematic deviations. Besides, according to the lower plots in Fig. 2, similar oscillations take place at $\beta = 0.5$ and at $\beta = 0.55$. Although in the latter case their amplitude is smaller, one has to take into account that the values of $M(h) - M(+0)$ also are smaller in this case. Hence, one may expect that at $\beta = 0.55$ the results will become as unstable as in the case of $\beta = 0.5$ if the h interval will be extended from $h \geq 0.0003125$ to $h \geq 0.00015625$, like for $\beta = 0.5$.

These fits can be stabilised by widening the fit intervals. The number of fit parameters also should be chosen not too large. For example, the four-parameter fits with $m = 1$, including only the leading correction to scaling, yield $\rho = 0.5869(81)$ for $h \in [0.00015625;0.014]$ and $\rho = 0.580(10)$ for $h \in [0.00015625;0.01]$ at $\beta = 0.5$. These two estimates agree well with each other and also with similar ($m = 1$) ones for $\beta = 0.55$ in Table 5, indicating that the true asymptotic ρ value very likely is near 0.58 or somewhat smaller. However, the fit quality becomes worse for such wider, as compared to those in Table 6, intervals. Namely, we have $\chi^2/\text{d.o.f.}{=}3.72$ for $h{\in}[0.00015625;0.014]$ and $\chi^2/\text{d.o.f.}{=}4.04$ for $h{\in}[0.00015625;0.01]$.

3.3 Analysis of the effective exponents

As discussed in Section 3.2, the many-parameter magnetisation fits do not provide sufficiently stable and reliable results in general, therefore we are looking here for an alternative method by fitting the susceptibility data for the largest lattices simulated here and in [1]. Although the susceptibility data seem to be relatively inaccurate, one should take into account that the relative errors of $M(h)-M(+0)$ also are not so small for the smallest h values. An advantage of the susceptibility data is that one needs not to subtract a constant background term. Hence, there are less fit parameters. It can ensure a sufficient stability and accuracy of the evaluated exponent ρ even if the data are less accurate than those for $M(h)$.

Basically, we refine the estimation in Section 3.1 by evaluating locally the slope of the $\ln\chi_\parallel$ vs $\ln h'$ plot within $h' \in [h/4;4h]$, which gives an effective exponent $\rho_{\text{eff}}(h)$, with the following idea to fit (extrapolate) the $\rho_{\text{eff}}(h)$ vs $h^{1/2}$ plot using the ansatz

$$\rho_{\text{eff}}(h) = \rho + a_1 h^{1/2} + a_2 h. \tag{3.3}$$

In such a way we evaluate the asymptotic exponent ρ, taking into account the leading as well as the subleading correction to scaling, represented by the expansion in powers of $h^{1/2}$. Even if the correction-to-scaling exponents in reality are slightly different from these ones suggested by the standard theory, such a method makes sense as a reasonable extrapolation, which can be well controlled visually.

The choice of sufficiently wide fit intervals $h' \in [h/4;4h]$ ensures that the evaluated effective exponents are not sensitive to small local oscillations like those in Fig. 2. They show only the general trend with decreasing the field h. Thus, the fit of ρ_{eff} plot provides a reasonable estimate of the asymptotic exponent ρ.

A great advantage of this method is that we can directly (visually) control the quantity of interest – the estimate of ρ depending on the h interval. In particular, we can see how well the evaluated effective exponents lie on a smooth curve and how large is the extrapolation gap. Thus we can judge how plausible is the extrapolated value. To the contrary, the many-parameter fits discussed in Section 3.2 can be controlled only indirectly by looking on small deviations from the fit curves. From such plots of deviations we cannot see directly how they influence the final result.

The plot of effective exponent for $\beta = 0.55$ is shown in Fig. 3. Within a wide range of fields h, it is well approximated by a parabola in the scale of $h^{1/2}$ in accordance with (3.3). Such a fit, shown by solid line, gives $\rho = 0.558(21)$. Taking into account that the data sets used in the determination of ρ_{eff} are overlapping, the resulting statistical error is calculated as $\sigma = (\sum_i \sigma_i^2)^{1/2}$, where σ_i are statistically independent contributions provided by the raw susceptibility data. We observe that the last five (smallest h) data points of ρ_{eff}

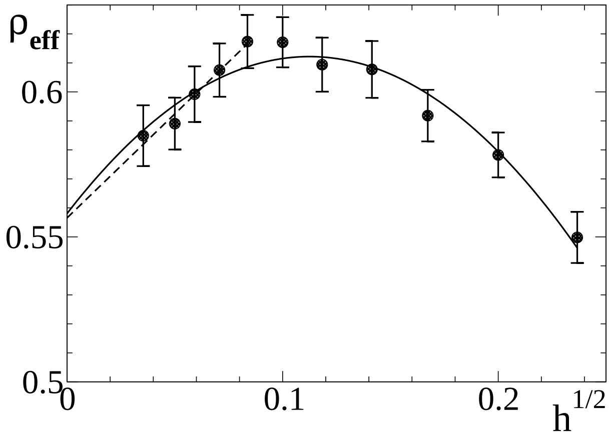

Figure 3: The effective exponent ρ_{eff} depending on $h^{1/2}$ for $\beta = 0.55$. The fit to (3.3) is shown by solid line. The dashed line represents the linear fit without the second-order correction.

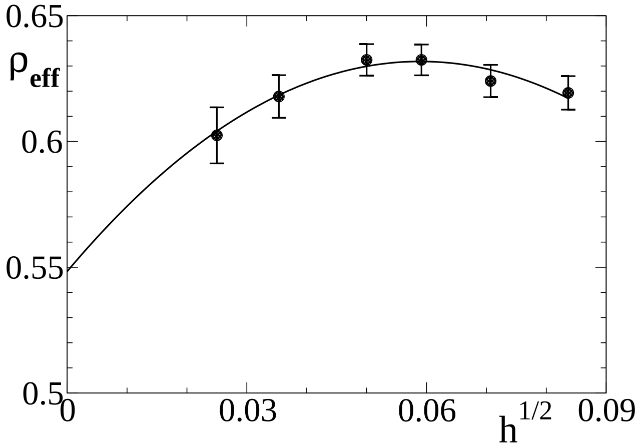

Figure 4: The effective exponent ρ_{eff} depending on $h^{1/2}$ for $\beta = 0.5$. The fit to (3.3) is shown by solid line.

very well lie on a straight line. It corresponds to (3.3) with only the leading correction term included ($a_2 = 0$). The linear fit gives $\rho = 0.557(19)$. In the other case of $\beta = 0.5$, we also observe that the effective exponent data fit well on a parabola, but only in a remarkably narrower range of h, as shown in Fig. 4. As a result, we obtain a less accurate value $\rho = 0.548(29)$. In this case the linear fit is omitted, since we do not observe a good linearity within a sufficiently wide interval of $h^{1/2}$. Evidently, all these estimates are well consistent thus supporting the theoretically expected universality of the exponent ρ. Hence, the weighted averaging over the results of quadratic fits, including two corrections to scaling, provides our best estimate $\rho = 0.555(17)$.

The above estimates change only slightly if the averaged data for two largest lattices (at each h) are used instead of the largest-lattice data. In this case the quadratic fit gives

$\rho=0.548(13)$, and the linear one provides $\rho=0.550(13)$ at $\beta=0.55$. The quadratic fit then gives $\rho=0.566(19)$ at $\beta=0.5$. The averaged over both couplings ($\beta=0.55$,0.5) result remains almost unchanged, i. e., $\rho=0.554(11)$, indicating that the finite-size effects are insignificant here.

Our current best value $\rho=0.555(17)$ agrees well with the estimates extracted from the magnetisation data within $h\geq 0.0003125$, where the many-parameter fits discussed in Section 3.2 provide relatively stable results. In particular, it closely agrees with the ρ values for $\beta=0.55$, obtained in Section 3.2, as well as with our previous estimate $\rho=0.552(18)$ reported in [1]. It agrees within error bars also with the four-parameter fit results for $h\geq 0.00015625$ at $\beta=0.5$, if the fit intervals are chosen appropriate, as discussed at the end of Section 3.2.

According to (1.2), our estimate $\rho=0.555(17)$ corresponds to the value $0.071(21)$ of the exponent η^* describing the singularity $\sim k^{-2+\eta^*}$ of the transverse two-point correlation function.

4 Spontaneous magnetisation

Apart from the exponent ρ, the fits of the magnetisation data to (3.2) provide estimates of the spontaneous magnetisation $M(+0)$. In the remaining part of the paper we will discuss the fits with $m=1$ and $m=2$ correction terms for the smallest h intervals considered in Section 3.2. For $\beta=0.55$, it gives $M(+0)=0.630771(95)$ at $m=1$ and $M(+0)=0.63077(11)$ at $m=2$. Since such fits do not provide stable and reliable values of ρ at $\beta=0.5$, in this case we have evaluated $M(+0)$ using the exponent $\rho=0.555(17)$ as a given parameter, estimated independently in Section 3.3. The fit with $m=1$ then yields $M(+0)=0.519301(73)$ at $\beta=0.5$, taking into account the uncertainty in the above value of ρ. This method gives $M(+0)=0.630736(64)$ at $\beta=0.55$ in close agreement with the two other estimates reported above. Generally, the actually obtained values of the spontaneous magnetisation agree well with those ones extracted only from the data of [1] at consistent with our current results choice of the exponent ρ about 0.55.

5 Conclusions

Advanced Monte Carlo simulations of the magnetisation and longitudinal susceptibility in the 3D XY model have been performed (Section 2) for two values of the coupling constant $\beta=0.55$ and $\beta=0.5$ below the critical temperature, extending the range of the external field h to twice as small values as compared to those in our previous work [1]. The maximal simulated linear lattice sizes have been increased from $L=384$ to $L=512$.

Based on the extended data, an improved estimation of the exponent ρ, describing the singularity $M(h)-M(+0)\propto h^\rho$ of the magnetisation at $h\to 0$, has been performed. We have found that the method of fitting the effective exponent $\rho_{\text{eff}}(h)$ (Section 3.3), extracted from the susceptibility data, provides more stable results as compared to the many parameter fits of the magnetisation data (Section 3.2). The method of effective exponent gives well consistent results for both values of β. Our best combined estimate is $\rho=0.555(17)$, which agrees also with the values extracted from the magnetisation data for appropriately chosen fit intervals. Apart from the exponent ρ, the spontaneous magnetisation $M(+0)$ also has been evaluated (Section 4).

Acknowledgments

This work was made possible by the facilities of the Shared Hierarchical Academic Research Computing Network (SHARCNET: `www.sharcnet.ca`). The actual MC simulations have been performed within two months by running on average 8 one-processor jobs simultaneously.

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