Two- and three-point functions at criticality:
Monte Carlo simulations of the three-dimensional
$(q + 1)$-state clock model

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Abstract

We simulate the improved $(q + 1)$-state clock model on the simple cubic lattice at the critical point on lattices of a linear size up to $L = 960$. We compute operator product expansion (OPE) coefficients for the three-dimensional XY universality class. These are compared with highly accurate estimates obtained by using the conformal bootstrap method. We find that the results are consistent.
I. INTRODUCTION

In recent years substantial progress in critical phenomena in three dimensions has been achieved by using the conformal bootstrap (CB) method. For reviews see for example [1, 2]. In particular in the case of the three-dimensional Ising universality class, the results for critical exponents are considerably more accurate than those obtained by other methods [3, 4]. Very recently also accurate results for the three-dimensional XY universality class were provided [5].

In addition to critical exponents, the CB provides accurate estimates for so called operator product expansion (OPE) coefficients $\lambda_{ijk}$. These are defined by the behaviour of three-point functions at the critical point. The OPE coefficients are difficult to access by other methods. In the case of the three-dimensional Ising universality class, only recently results have been obtained by using Monte Carlo simulations of lattice models [6–9]. These are far less precise than those obtained by using the CB. However the agreement of the results from the lattice and CB gives further support for the fact that both methods examine the same renormalization group (RG) fixed point.

The functional form of two-point functions of primary operators is fixed by conformal invariance

$$\langle O_1(x_1)O_2(x_2) \rangle = \frac{C_1 \delta_{\Delta_1 \Delta_2}}{|x_1 - x_2|^{2\Delta_1}} ,$$

where $O_i$ is the operator taken at the site $x_i$ and $\Delta_i$ is its scaling dimension.

Also the form of three-point functions is fixed by conformal invariance. Normalizing the operators such that $C_i = 1$, eq. (1), one gets [10]

$$\langle O_1(x_1)O_2(x_2)O_3(x_3) \rangle = \frac{\lambda_{123}}{|x_1 - x_2|^{\Delta_1 + \Delta_2 - \Delta_3}|x_2 - x_3|^{\Delta_2 + \Delta_3 - \Delta_1}|x_3 - x_1|^{\Delta_3 + \Delta_1 - \Delta_2}} ,$$

where the OPE coefficients $\lambda_{123}$ depend on the universality class.

In the present work, we apply the idea of ref. [9] to the XY universality class in three dimensions. To this end, we simulate the improved $O(2)$-symmetric $\phi^4$ model and the improved $(q + 1)$-state clock model on the simple cubic lattice at the critical temperature. In order to reduce the statistical error of the two and three-point functions, we use a variance reduction method [11, 12]. In order to reduce finite size effects, large linear lattice sizes $L$ are considered. In our simulations we go up to $L = 960$. On top of that still an extrapolation to $L \to \infty$ is needed. Our estimates for the OPE coefficients turn out to be consistent with
those obtained by using the CB.

In table I we summarize results for the scaling dimensions $\Delta_i$ and the OPE coefficients $\lambda_{ijk}$ obtained by using the CB. In the case of the scaling dimensions we give the most accurate results obtained from Monte Carlo simulations [13, 14] of lattice models for comparison. In the case of $\Delta_s$ we also give the estimate obtained by analysing specific heat data for $^4$He near the $\lambda$-transition [15–17]. Note that the scaling dimensions are related with the critical exponents that are usually discussed in critical phenomena [18]. In particular the critical exponent of the correlation length is given by $\nu = 1/(3 - \Delta_s)$ and the exponent of the correlation function at criticality $\eta = 2\Delta_\phi - 1$. The estimate of $\nu$ obtained by using high temperature (HT) series and Monte Carlo simulations of lattice models [19, 20] differs from that obtained from experiments [15–17] by several times the combined error. The recent Monte Carlo study [13] and the CB work [5] confirm the results of refs. [19, 20].

The outline of the paper is the following. In section II we define the models that are simulated and we summarize numerical results, for example for the critical temperature, which are used in our simulations. Next in section III we define the observables and briefly recall the variance reduction method. In section IV we discuss the simulations and analyse our numerical results. Finally we conclude and give an outlook.

II. THE LATTICE MODELS

We performed preliminary simulations by using the $O(2)$-symmetric $\phi^4$ model on the lattice. The final results were obtained from simulations of the $(q + 1)$-state clock model with $q = 32$. Note that in the limit $q \to \infty$ the dynamically diluted XY model studied in refs. [19, 20] is reached. Both models have a parameter that can be tuned such that leading corrections to scaling vanish. Models taken at a good approximation of this value are denoted as improved. In the following we define the models and summarize estimates of the improved models and the inverse critical temperature given in the literature.
TABLE I. Scaling dimensions and OPE coefficients for the three-dimensional XY universality class.
Comparison of conformal bootstrap (CB) results with estimates from Monte Carlo (MC) or experiment (EXP). The leading charge 0, 1, and 2 scalars are denoted by s, φ, t, respectively. For a discussion of the meaning of the errors that are quoted see the references.

| Quantity method | value         | ref.         |
|-----------------|---------------|--------------|
| Δs              | EXP 1.50946(22) [15–17] |              |
|                 | MC 1.51122(15) [13]     |              |
|                 | CB 1.51136(22) [5]      |              |
|                 | CB 1.5117(25) [3]       |              |
| Δφ              | MC 0.519050(40) [13]    |              |
|                 | CB 0.519088(22) [5]     |              |
|                 | CB 0.51926(32) [3]      |              |
| Δt              | MC 1.2361(11) [14]      |              |
|                 | CB 1.23629(11) [5]      |              |
| λφφs            | CB 0.687126(27) [5]     |              |
|                 | CB 0.68726(65) [3]      |              |
| λsss            | CB 0.830914(32) [5]     |              |
|                 | CB 0.8286(60) [3]       |              |
| λttt            | CB 1.25213(14) [5]      |              |
| λφφt            | CB 1.213408(65) [5]     |              |

A. The O(2)-symmetric φ^4 model

The O(2)-symmetric φ^4 model on the simple cubic lattice is defined by the reduced Hamiltonian

$$\mathcal{H}_{\phi^4} = -\beta \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x \left[ \vec{\phi}_x^2 + \lambda (\vec{\phi}_x^2 - 1)^2 \right],$$

(3)

where \(\vec{\phi}_x \in \mathbb{R}^N\) with \(N = 2\) is the field at the site \(x = (x^{(0)}, x^{(1)}, x^{(2)})\), where \(x^{(i)} \in 0, 1, 2, ..., L_i - 1\). Here we are labeling the components of \(x\) by an upper index. A lower index is used to discriminate different sites on the lattice. \(\langle xy \rangle\) denotes a pair of nearest neighbour sites on the simple cubic lattice. In our simulations \(L_0 = L_1 = L_2 = L\) throughout.
For the $O(2)$-symmetric $\phi^4$ model on the simple cubic lattice the authors of ref. [20] find for the improved model $\lambda^* = 2.15(5)$ and $\beta_c = 0.5091503(3)$ [3] and $0.5083355(3)$ [4] for for $\lambda = 2.1$ and 2.2, respectively. These estimates are obtained by requiring that $(Z_a/Z_p)^* = 0.3203(1)$ [3], where $Z_p$ and $Z_a$ are the partition functions for a system with periodic boundary conditions in all directions and anti-periodic in one direction and periodic in the remaining ones, respectively. The superscript $*$ refers to the fixed point value for the given lattice geometry. In the case of $\beta_c$, the number given in [] is the error due to the uncertainty of $(Z_a/Z_p)^*$. Here we have reanalysed unpublished data generated in 2013 for $\lambda = 2.1$ using the estimates of $(Z_a/Z_p)^*$ and $(\zeta_{2nd}/L)^*$ given in ref. [13] as input. We arrive at

$$\beta_c(\lambda = 2.1) = 0.5091504(1),$$

where the number quoted in () includes both the statistical as well as the systematical error. We simulate the $O(2)$-symmetric $\phi^4$ model by using a hybrid of local Metropolis, local overrelaxation and single cluster [21] updates. For a discussion of this algorithm see for example Appendix A of ref. [14].

B. The $(q+1)$-state clock model

The model can be viewed as a generalization of the $q$-state clock model. The field $\vec{s}_x$ at the site $x = (x^{(0)}, x^{(1)}, x^{(2)})$, where $x^{(i)} \in 0, 1, 2, ..., L_i - 1$, might assume one of the following values

$$\vec{s}_x \in \{(0, 0), (\cos(2\pi m/q), \sin(2\pi m/q))\},$$

where $m \in \{1, ..., q\}$. In our simulations we take $L_0 = L_1 = L_2 = L$ throughout. Compared with the $q$-state clock model, $(0, 0)$ is added as possible value of the field variable. In our simulation program, we store the field variables by using labels $m = 0, 1, 2, ..., q$. We assign

$$\vec{s}(0) = (0, 0)$$

and for $m > 0$

$$\vec{s}(m) = (\cos(2\pi m/q), \sin(2\pi m/q)) .$$

The reduced Hamiltonian is given by

$$\mathcal{H} = -\beta \sum_{xy} \vec{s}_x \cdot \vec{s}_y - D \sum_x \vec{s}_x^2 - \vec{H} \sum_x \vec{s}_x .$$
In our simulations, we consider a vanishing external field $\vec{H} = \vec{0}$ throughout. We introduce the weight factor

$$w(\vec{s}_x) = \delta_{0,s_x^2} + \frac{1}{q} \delta_{1,s_x^2} = \delta_{0,m_x} + \frac{1}{q} \sum_{n=1}^{q} \delta_{n,m_x}$$  \hspace{1cm} (9)

that gives equal weight to $(0,0)$ and the collection of all values $|\vec{s}_x| = 1$. Now the partition function can be written as

$$Z = \sum_{\{\vec{s}\}} \prod_x w(\vec{s}_x) \exp(-\mathcal{H}) ,$$  \hspace{1cm} (10)

where $\{\vec{s}\}$ denotes a configuration of the field.

Note that in the limit $q \to \infty$, we recover the dynamically diluted XY (ddXY) model studied in refs. [19, 20]. The reduced Hamiltonian of the ddXY model has the same form as eq. (8):

$$\mathcal{H}_{ddXY} = -\beta \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y - D \sum_x \vec{\phi}_x^2 - \vec{H} \sum_x \vec{\phi}_x ,$$  \hspace{1cm} (11)

where $\vec{\phi}_x$ is a vector with two real components. The partition function is given by

$$Z = \prod_x \left[ \int d\mu(\phi_x) \right] \exp(-\mathcal{H}_{ddXY}) ,$$  \hspace{1cm} (12)

with the local measure

$$d\mu(\phi_x) = d\phi_x^{(1)} d\phi_x^{(2)} \left[ \delta(\phi_x^{(1)}) \delta(\phi_x^{(2)}) + \frac{1}{2\pi} \delta(1 - |\vec{\phi}_x|) \right] .$$  \hspace{1cm} (13)

In ref. [13] we simulated the model $q = 8$. We find $D^* = 1.058(13)$, see eq. (63) of [13]. For nearby values of $D$ we obtain

$$\beta_c(D = 1.05) = 0.56082390(10) ,$$  \hspace{1cm} (14)
$$\beta_c(D = 1.07) = 0.55888340(10) .$$  \hspace{1cm} (15)

In the appendix B 2 of ref. [13] we study the $q$-dependence of non-universal quantities such as the critical temperature. We find that already for $q = 8$ the estimates differ only by little from those for the limit $q \to \infty$. At the level of our statistical accuracy, estimates for $q \geq 10$ can not be distinguished from those for the limit $q \to \infty$. Taking the results of the appendix B 2 of ref. [13] we arrive at

$$\beta_c(D = 1.05) = 0.56082418(10)[10] ,$$  \hspace{1cm} (16)
$$\beta_c(D = 1.07) = 0.55888368(10)[10] .$$  \hspace{1cm} (17)
for $q \geq 10$. The number in $[]$ gives the uncertainty of the extrapolation. The major part of
the simulations here is performed for $q = 32$. In this case 6 bits are needed to store the field
variable at one site. Also the arrays needed to store possible changes in the weight that are
used to speed up the Metropolis and cluster updates are still small enough to fit into the
cache of the CPU. We use a hybrid of local Metropolis and single cluster updates \cite{21} to
simulate the model. For a detailed discussion see section IV of ref. \cite{13}.

III. THE OBSERVABLES

Let us define the observables measured on the finite lattice. Here we use the notation of
the $O(2)$-invariant $\phi^4$ model. Note that in our measurements, following ref. \cite{9} we replace
the field at the site $x$ by the sum of its six nearest neighbours. The idea is that statistical
noise is reduced and furthermore in the case of the $(q + 1)$-state clock model the rotational
invariance is better approximated.

Let us define the correlation functions that are measured in the simulations. In the
following we use the notation

$$\vec{\phi}_x = \begin{pmatrix}
\phi_{x,0} \\
\phi_{x,1} \\
. \\
. \\
. \\
\phi_{x,N-1}
\end{pmatrix},$$

\hspace{1cm} (18)

for the field variable. We study correlation functions of $\phi$ and the two derived quantities $s$
and $t$. The scalar $s$ with charge 0 is given by

$$s_x = \sum_i \phi_{x,i} \phi_{x,i} - \bar{s},$$

\hspace{1cm} (19)

where $\bar{s} = \langle \sum_i \phi_{x,i} \phi_{x,i} \rangle$ for the given lattice size. The scalar with charge 2 is given by the
traceless compound

$$t_{x,ij} = \phi_{x,i} \phi_{x,j} - \delta_{ij} \frac{\phi_x^2}{N}$$

\hspace{1cm} (20)

with $N = 2$. Note that these lattice quantities also contain scaling fields with the same
symmetry properties but larger scaling dimensions than the lowest. Therefore the correlation
functions show corrections at small distances.
The two-point functions, without any normalization are

\[ g_{\phi\phi}(x_1, x_2) = \sum_i \langle \phi_{x_1,i} \phi_{x_2,i} \rangle, \]  
\[ g_{ss}(x_1, x_2) = \langle s_{x_1} s_{x_2} \rangle, \]  
\[ g_{tt}(x_1, x_2) = \sum_{ik} \langle t_{x_1,i,k} t_{x_2,i,k} \rangle. \]

We consider the following three-point correlation functions:

\[ G_{\phi\phi s}(x_1, x_2, x_3) = \sum_i \langle \phi_{x_1,i} \phi_{x_2,i} s_{x_3} \rangle, \]  
\[ G_{sss}(x_1, x_2, x_3) = \langle s_{x_1} s_{x_2} s_{x_3} \rangle, \]  
\[ G_{ttt}(x_1, x_2, x_3) = \sum_{ik} \langle t_{x_1,i,k} t_{x_2,i,k} s_{x_3} \rangle, \]  
\[ G_{\phi\phi t}(x_1, x_2, x_3) = \sum_{ik} \langle \phi_{x_1,i} \phi_{x_2,i} t_{x_3,i,k} \rangle. \]

Note that our normalizations of the two- and three-point functions are not the same as those of refs. \[3, 5\]. This leads to a factor of \( \sqrt{2} \) in the result for \( \lambda_{\phi\phi t} \), while it cancels in the other three cases \[22\].

A. Our choices for \( x_1, x_2, \) and \( x_3 \)

The variance reduction method requires that the lattice is subdivided into blocks. For technical reasons we compute correlation functions only for the sites at the centre of these blocks. These sites are given by \( x^{(i)} = n_s k_i \). In our simulations we have used the three different choices \( n_s = 2, 4, \) and 6. Throughout the linear lattice size \( L \) is a multiple of \( n_s \) and \( k_i \in \{0, 1, ..., L/n_s - 1\} \). In the following we refer to \( n_s \) as stride. In order to keep the study tractable, we have to single out a few directions for the displacements between the points. In the case of the two-point functions we consider displacements along the axes, the face diagonals, and the space diagonals. In the following, these are indicated by \( (a) \), \( (f) \), and \( (d) \), respectively. In our simulation program we summed over all choices that are related by symmetry to reduce the statistical error. In the following we shall denote the two-point function by \( g_{r,\mathcal{O}_1,\mathcal{O}_2}(x) \), where \( r \in \{a, f, d\} \) gives the direction and \( x = |x_1 - x_2| \) is the distance between the two points. In the case of the three-point functions

\[ G_{r,\mathcal{O}_1,\mathcal{O}_2,\mathcal{O}_3}(x) = \langle \mathcal{O}_1(x_1)\mathcal{O}_2(x_2)\mathcal{O}_3(x_3) \rangle \]  

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we consider two different geometries that are indicated by \( r \). For \( r = f \) the largest displacement is along a face diagonal. For example

\[
x_3 - x_1 = (j, 0, 0) , \quad x_3 - x_2 = (0, j, 0) .
\]  

(29)

Our second choice is indicated by \( r = d \) and the largest displacement is along a space diagonal. For example

\[
x_3 - x_1 = (j, 0, 0) , \quad x_3 - x_2 = (0, j, j) ,
\]  

(30)

where \( j = n_s k \), where \( k \) is integer. Also here we sum in our simulation over all choices that are related by symmetry to reduce the statistical error. The argument \( x \) of \( G \) gives the smallest distance between two points \( x = j \).

In order to eliminate the constants \( C_i \), eq. (1), and the power law behaviour from the three-point functions, we directly normalized our estimates of the three-point functions by the corresponding ones of two-point functions. For the direction \( r = f \) we get for example

\[
\lambda_{\phi\phi t} \simeq 2^{-\Delta_t/2} \frac{G_{f,\phi\phi t}(x)}{g_{a,\phi\phi}(x) g_{f,tt}^{1/2} (\sqrt{2}x)}. 
\]  

(31)

Based on the numbers given in table II we used as numerical values \( \Delta_t = 1.23629 \), \( \Delta_s = 1.5113 \), and \( \Delta_\phi = 0.51908 \) for the scaling dimensions. Note the systematical error of the estimate of \( \lambda_{ijk} \) due to the uncertainty of the scaling dimensions is negligible.

B. Variance reduced measurement

The variance reduction method used here is based on the ideas of refs. [11, 12]. The method is discussed in detail in section V of ref. [9]. Here we summarize the basics for completeness.

In the case of an \( N \)-point correlation function, the lattice is partitioned into \( N \) areas \( B_i \), where each of these areas contains one of the sites \( x_1, x_2, \ldots, x_N \). These areas are chosen such that for each pair \( i \neq j \) none of the sites in \( B_i \) is a nearest neighbour of a site in \( B_j \). Let us denote the collection of the remaining sites as \( R \). Now the sampling of the correlation function can be reorganized in the following way.

In a straight forward approach one would estimate the expectation value of the \( N \)-point correlation function by averaging over \( M \) configurations

\[
\overline{O_1(x_1)O_2(x_2)\ldots O_N(x_N)} = \frac{1}{M} \sum_{\alpha} O_{1,\alpha}(x_1)O_{2,\alpha}(x_2)\ldots O_{N,\alpha}(x_N) ,
\]  

(32)
where \( \alpha \) labels configurations that have been generated by using a Markov chain. We assume that the process is equilibrated and the configurations are generated with a probability density proportional to the Boltzmann factor. \( O_{i,\alpha}(x_i) \) denotes the value of \( O_i(x_i) \) assumed for configuration \( \alpha \).

In the case of the variance reduced measurement, we first average \( O_i(x_i) \) over configurations on \( B_i \) that have been generated, while keeping the field on \( R \) fixed:

\[
\overline{O_1(x_1)O_2(x_2)\ldots O_N(x_N)} = \frac{1}{M} \sum_\alpha \overline{O_{1,\alpha}(x_1)O_{2,\alpha}(x_2)\ldots O_{N,\alpha}(x_N)},
\]

where

\[
\overline{O_{i,\alpha}(x_i)} = \frac{1}{m} \sum_\gamma O_{i,\alpha,\gamma}(x_i).
\]

Here we have generated \( m \) configurations labeled by \( \gamma \) on \( B_i \), keeping the field on \( R \) fixed. The configurations on \( R \) are labeled by \( \alpha \). The effect of this averaging for each site separately is that we consider \( m^N \) configurations for the \( N \)-point function. For small \( m \) this translates into

\[
\epsilon^2 \propto \frac{1}{m^N}
\]

for the statistical error \( \epsilon \) of the estimate of the \( N \)-point correlation function. As \( m \) increases, the effect of fixing the configuration on \( R \) becomes visible and \( \epsilon^2 \) converges to a finite limit as \( m \to \infty \) and can be reduced only by increasing \( M \). There is in general an optimal value of \( m \). This value of \( m \) depends on the choice of \( O_i \) and the distances. Finding a good choice of \( m \) requires some numerical experimentation. Below we shall specify our implementation of this general idea.

We only used the sites \( (j_0n_s, j_1n_s, j_2n_s) \), with \( j_i \in \{0, n_s, 2n_s, \ldots, L_i/n_s - 1\} \) for the measurements of the two- and three-point functions. As areas we consider blocks of the size \( l_b^3 \), where \( l_b = 2n_s - 1 \). The sites used for the measurement are at the centre of the blocks.

Computing the block averages we used local updates only. In particular in the case of the \( (q+1) \)-clock model, we used the first version of the Metropolis update discussed in section IV. A. of ref. [13]. Computing averages for the blocks, keeping the remainder \( R \) fixed, we update more frequently towards the centre of the blocks. To this end we perform a cycle of updates, similar to the cycle used in a multigrid updating scheme. In particular, we sweep over subblocks of the size \( 3^3, 5^3, \ldots, l_b^3 \). In addition, as smallest subset, we consider the central site and its 6 nearest neighbours. For each of these sweeps we perform a measurement. The
frequency $n_x$ of the sweeps is chosen such that the number of sites times $n_x$ is roughly the same for all sizes. For example in the case $n_s = 6$, where $l_b = 11$, in one such cycle 268 measurements are performed. In our production runs for $n_s = 6$, we performed 160 update cycles for a given configuration on the remainder $R$. Hence in total $160 \times 268 = 42880$ measurements are performed for a given configuration on $R$.

Note that for our setup two blocks with the central sites $x_1$ and $x_2$ are separated if $|x_1^{(i)} - x_2^{(i)}| \geq 2n_s$ for at least one direction $i$. Computing the two- and three-point functions, one therefore has to note that only results for $|x_k^{(i)} - x_l^{(i)}| \geq 2n_s$ for at least one direction $i$ are valid.

The simulation is build up in the following way: First we equilibrate the system without measuring by performing 2000 times the following sequence of updates: One sweep with the Metropolis update type two, one sweep with the Metropolis update type one, and $L$ times a single cluster update. These updates are discussed in section IV of ref. [13].

For each measurement, we performed ten times the following sequence of updates: two Metropolis sweeps followed by $L$ single cluster updates. In the first and the sixth sequence, the first Metropolis is of type two, while all others are of type one. Note that here the measurements, including the updates of the blocks for variance reduction, are far more expensive than the updates of the system as a whole. Therefore between the measurements, a relatively large number of updates is performed, in order to measure on essentially uncorrelated configurations. In principle the final configurations of separated blocks could be used as update of the main Markov chain. In our case a $1/2^3$ of the blocks could be used to this end. For simplicity we abstained from doing so.

C. Finite size effects

Compared with the linear size $L$ of the lattice, the distances that we consider for our two- and three-point functions are small. In that respect they can be viewed as local scalar operators with charge 0 such as the energy density. The energy density on a finite lattice of the linear size $L$, for a vanishing external field, behaves as

$$E(\beta_c, L) = cL^{-\Delta s} + E_{ns}(0) \ .$$

For a discussion see section IV of ref. [9].

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In the analysis of our data, we assume that the finite size scaling behaviour of the two- and three-point functions is given by eq. (36), where, of course, the values of the constants depend on the quantity that is considered. Given the huge amount of data, we abstain from sophisticated fitting with Ansätze motivated by eq. (36). Instead we consider pairs of linear lattice sizes \( L_1 = L, \ L_2 = 2L \) and compute

\[
G_{\text{ext}}(2L) := G(2L) + \frac{G(2L) - G(L)}{2^{\Delta_s} - 1},
\]

(37)

where \( G \) is the quantity under consideration. Eq. (37) is derived by inserting \( L_1 \) and \( L_2 \) into eq. (36) and solving the system of two equations with respect to the non-singular (ns) part. As in the case of eq. (31), we use \( \Delta_s = 1.5113 \) as numerical value for the scaling dimension. Note that in the analysis of the numerical data, for simplicity, we apply eq. (37) to our estimates of the scaling dimension and the OPE coefficients \( \lambda_{ijk} \) computed for finite lattice sizes \( L \).

IV. NUMERICAL RESULTS

A. Preliminary simulations

In order to check the \( q \)-dependence of our results for the \( (q + 1) \)-state clock model we have simulated the linear lattice size \( L = 120 \) with stride \( n_s = 2 \) for \( q = 8, 16, \) and 32. In all three cases \( D = 1.05 \). In the case of \( q = 8 \) we simulated at \( \beta = 0.56082390, \) eq. (14) and for \( q = 16 \) and 32 at \( \beta = 0.56082418, \) eq. (16). The statistics is 139100, 139640, and 259820 measurements, respectively. For each measurement, we performed \( m = 40 \) measurements on the blocks. For each block measurement we performed one sweep over the \( 3^3 \) blocks. We compared the results for the four different OPE coefficients for all distances studied. At the level of our statistical accuracy, we find no dependence on \( q \). Therefore we are confident that the results obtained below for \( q = 32 \) are essentially unaffected by the breaking of the \( O(2) \)-symmetry.

Furthermore we simulated the \( O(2) \)-symmetric \( \phi^4 \)-model at \( \lambda = 2.1 \) and \( \beta = 0.5091504, \) eq. (11). We simulated the linear lattice size \( L = 120 \) and used the stride \( n_s = 2 \). We performed 81970 measurements with \( m = 60 \) updates of the blocks for each measurement. We compared our results for the OPE coefficients with those for the \( (q + 1) \)-state clock model discussed above. In particular comparing with the \( q = 32 \) case, we only find a difference that
is clearly out of the error bars for $\lambda_{sss}$ at the distance $x = 4$. In the case of the $\phi^4$ model we get 0.87927(40) and 0.84335(64) for the directions $f$ and $d$, respectively. These numbers can be compared with 0.87698(30) and 0.84026(49) for the $(32 + 1)$-state clock model. We also simulated the $\phi^4$-model for the stride $n_s = 4$ and the linear lattice size $L = 240$. Here we find no difference compared with the corresponding simulations of the $(32 + 1)$-state clock model discussed below. Hence the small distance effects in the correlation functions are mainly caused by the lattice and the nearest neighbour interaction. The local potential of an improved model plays virtually no role.

Since the simulation of the $\phi^4$ model takes about three times as much CPU as that of the $(q + 1)$-state clock model [13] and 16 times as much memory is needed to store the configurations, we simulated the $(q + 1)$-state clock model with $q = 32$ in the major part of our study.

**B. Production runs using the $(32 + 1)$-state clock model**

In the major part of our study we simulated the $(32 + 1)$-state clock model with the linear lattice sizes $L = 240$, 480, and 960. We performed measurements by using the strides $n_s = 2$, 4, and 6. In principle one could do the measurements for these three different strides in the same set of simulations. However, for simplicity, for a given simulation we performed measurements for one value of $n_s$ only.

Our final results are mainly based on the simulations with $n_s = 6$. For $n_s = 6$ we performed 70587, 11196, and 1272 update and measurement cycles for $L = 240$, 480, and 960, respectively. On one core of an AMD EPYC 7351P 16-Core Processor the simulations using $n_s = 6$ took about 10 years in total.

**C. Scaling dimensions from the two-point correlation functions**

As a check we extract the scaling dimensions $\Delta_\phi$, $\Delta_s$, and $\Delta_t$ from the behaviour of the two-point functions $g(x)$. In the first step we compute

$$\Delta_{eff}(x, \Delta x) = -\frac{1}{2} \frac{\ln((g(x + \Delta_x)/g(x)))}{\ln((x + \Delta x)/x)},$$

where $\Delta x = n_s$, $\Delta x = \sqrt{2}n_s$, and $\Delta x = \sqrt{3}n_s$ for $r = a$, $f$ and $d$, respectively.
FIG. 1. We plot our numerical estimates of $\Delta t$ as a function of the distance $x$ between the lattice sites. Here we plot results for the direction $f$ only. The stride is $n_s = 6$ throughout. We give estimates computed for the linear lattice sizes $L = 240$, $480$, and $960$ and the extrapolations using the pairs $(240, 480)$ and $(480, 960)$ of linear lattice sizes. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

These results are extrapolated to the infinite volume by using eq. (37).

In Fig. 1 we demonstrate the effectiveness of the extrapolation. We give the results for $\Delta t$ obtained for the linear lattice sizes $L = 240$, $480$, and $960$. The measurements are performed with the stride $n_s = 6$. Here we give results for the direction $f$ only. We see a clear dependence of the results on $L$ that increases with increasing distance. In contrast, the extrapolated results for $(L_1, L_2) = (240, 480)$ and $(L_1, L_2) = (480, 960)$ differ only by little.

Next we check for the effect of operators with higher dimension in the same channel. The effect should decay with increasing distance between the two sites. In Fig. 2 we plot extrapolated results for $(L_1, L_2) = (480, 960)$ of $\Delta t$. Data are taken from our runs for the strides $n_s = 2$ and $6$. We give results for all three directions that we consider. Similar to
FIG. 2. We plot $\Delta_t$ obtained by extrapolating our results for $(L_1, L_2) = (480, 960)$ as a function of the distance $x$ between the lattice sites. These results are obtained by using the strides $n_s = 2$ and $n_6$. We omit the results for $n_s = 4$ to keep the figure readable. $a$, $f$, and $d$ denote the three different directions that we consider. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

The observations are similar for $\Delta_s$ and $\Delta_\phi$ that we do not discuss in detail here.

Our numerical result for $\Delta_t$ is consistent with that obtained by using the CB method [5] and previous Monte Carlo simulations. However we do not reach the accuracy of [5] and the lattice result [14]. As our final estimate we might quote $\Delta_t = 1.2352(23)$ from the extrapolation of $(L_1, L_2) = (480, 960)$ for the direction $f$ and the pair of distances $(12, 18) \times \sqrt{2}$. Looking at Figs. 1 and 2 it seems plausible that for this choice, systematical errors due to the finite value of $x$ and due to the imperfection of the extrapolation to the
infinite volume are not larger than the statistical error.

In a similar way we get $\Delta_\phi = 0.51953(32)$ from the extrapolation of $(L_1, L_2) = (480, 960)$, the stride $n_s = 2$, the direction $f$ and the pair of distances $(12, 14) \times \sqrt{2}$, or $\Delta_\phi = 0.51864(52)$ for the stride $n_s = 6$ and the pair of distances $(12, 18) \times \sqrt{2}$. Finally we obtain from the measurements with the stride $n_s = 6$, the direction $f$, and the pair of distances $(12, 18) \times \sqrt{2}$ the estimate $\Delta_\phi = 1.5098(21)$.

D. The OPE coefficients and the three-point functions

Here we follow a similar procedure as for the scaling dimensions. In the first step we compute estimates of $\lambda_{ijk}$ for given linear lattice sizes $L$ by using eq. (31) and analogous equations. Then we extrapolate to the infinite volume by using eq. (37). Similar to ref. [9] we have measured the three-point function for two different geometries that we denote by $f$ and $d$. It turns out that small distance corrections are smaller for $f$. Final results are however fully consistent. Therefore in the following we restrict the detailed discussion on geometry $f$.

In Fig. 3 we plot results for $\lambda_{\phi\phi\phi}$ obtained from simulations with the stride $n_s = 6$ and the linear lattice sizes $L = 240, 480,$ and $960$. In addition we give the results of the extrapolation using eq. (37) and the pairs of lattice sizes $(L_1, L_2) = (240, 480)$ and $(L_1, L_2) = (480, 960)$. We see a clear dependence of the results on $L$ that increases with increasing distance $x$. In contrast, the extrapolated results for $(L_1, L_2) = (240, 480)$ and $(L_1, L_2) = (480, 960)$ differ only by little. Only for distances $x \geq 48$ the estimate obtained from the pair $(L_1, L_2) = (240, 480)$ decreases.

Next in Fig. 4 we plot the extrapolated results for $(L_1, L_2) = (480, 960)$ obtained for the strides $n_s = 2, 4$ and $6$. Fig. 4 suggests that for the distance $x = 24$ finite $x$ effects are at most of the same size as our statistical error. Fig. 3 suggests that the same holds for systematic effects of the extrapolation $L \to \infty$ for the pair of lattice sizes $(480, 960)$. For the stride $n_s = 6$ we read off $\lambda_{\phi\phi\phi} = 0.6881(10)$ at $x = 24$.

Next let us discuss the numerical results for $\lambda_{sss}$. First we convinced ourself that also here the extrapolation by using eq. (37) is effective. In Fig. 5 we give results of the extrapolation using the linear lattice sizes $L = 480$ and $960$ for the strides $n_s = 2, 4,$ and $6$. The relative statistical error is larger than for $\lambda_{\phi\phi\phi}$. The effect of the variance reduction is more important
FIG. 3. We plot our numerical results for $\lambda_{\phi \phi s}$ as a function of the distance $x$. Here we consider simulations with stride $n_s = 6$ and three-point functions for the geometry $f$. We give results for the linear lattice sizes $L = 240, 480$ and 960. These results are extrapolated by using eq. (37) for the pairs $(240, 480)$ and $(480, 960)$ of linear lattice sizes. The distance $x$ for the pair $(240, 480)$ is slightly shifted to make the figure more readable. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

than for $\lambda_{\phi \phi s}$. Going to larger distances, it is mandatory to use larger block sizes.

Looking at the figure, it seems plausible that for the stride $n_s = 6$ at the distance $x = 18$, the small distance error is at most of similar size as the statistical one. We read off $\lambda_{sss} = 0.8303(41)$.

Next, in Fig. 6 we plot our extrapolated results for $\lambda_{tts}$ obtained from the simulations with the strides $n_s = 2, 4, 6$. As our final result we regard the estimate $\lambda_{tts} = 1.2530(16)$ obtained by using the stride $n_s = 6$ at the distance $x = 18$.

Finally, in Fig. 7 we plot our numerical results for $\lambda_{\phi \phi t}$. We read off $\lambda_{\phi \phi t} = 1.214(7)$ for $x = 18$ and the stride $n_s = 6$. For the distance $x = 24$ we get $\lambda_{\phi \phi t} = 1.213(10)$ instead.
FIG. 4. We plot our numerical results for $\lambda_{\phi\phi_s}$ as a function of the distance between the lattice sites. Here we consider simulations with stride $n_s = 2, 4, 6$ and three-point functions for the geometry $f$. We give results for the extrapolation of the lattice sizes $(L_1, L_2) = (480, 960)$. The values of $x$ for $n_s = 2$ and 6 are slightly shifted to reduce the overlap of the symbols. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

Note that we have multiplied our numbers, which are based on eqs. (21, 23, 27), by a factor of $\sqrt{2}$ to match with the conventions of ref. [3].

We have demonstrated that OPE coefficients for the three-dimensional XY universality class can be determined by using Monte Carlo simulations of a lattice model with a relative error of about 1% or less. Our results are fully consistent with those recently obtained by using the CB method. One has to note however that the estimates obtained by using the CB method are by about two orders of magnitude more precise than those obtained here.
FIG. 5. We plot our numerical results for $\lambda_{sss}$ as a function of the distance between the lattice sites. Here we consider simulations with stride $n_s = 2, 4, 6$ and three-point functions for the geometry $f$. We give results for the extrapolation of the lattice sizes $L = 480$ and 960. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

V. SUMMARY AND DISCUSSION

We have determined OPE coefficients for the three-dimensional XY universality class by using Monte Carlo simulations of lattice models. In particular we have studied the improved $O(2)$-symmetric $\phi^4$ model and the improved $(q + 1)$-state clock model on the simple cubic lattice at the critical temperature. We simulated the improved $(q + 1)$-state clock model using linear lattice sizes up to $L = 960$. We extrapolate the results to the limit $L \to \infty$. We find results that are fully consistent with those of the conformal bootstrap method, further confirming that the conformal bootstrap (CB) method and the lattice model examine the same RG fixed point.

The measurement, which takes considerably more CPU time than the generation of the configurations, could be easily parallelized and could hence be speeded up for example by
FIG. 6. We plot our numerical results for $\lambda_{tts}$ as a function of the distance $x$ between the lattice sites. Here we consider simulations with stride $n_s = 2, 4, 6$ and three-point functions for the geometry $f$. We give results for the extrapolation of the lattice sizes $L = 480$ and $960$. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line.

running it on graphics processing units (GPUs). Even if we could speed up the measurement by a factor of 100 this way, the accuracy of the CB seems to be out of reach.

Still our approach is somewhat cumbersome and it would be desirable to relate the OPE coefficients with quantities that can be accessed more easily on finite lattices.

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FIG. 7. We plot our numerical results for $\lambda_{\phi\phi t}$ as a function of the distance between the lattice sites. Here we consider simulations with stride $n_s = 2, 4, 6$ and three-point functions for the geometry $f$. We give results for the extrapolation of the lattice sizes $L = 480$ and $960$. For comparison we give the estimate obtained by using the conformal bootstrap method [5] as solid black line. Note that we have multiplied our numbers, which are based on eqs. (21, 23, 27), by a factor of $\sqrt{2}$ to match with the conventions of ref. [5].

[1] D. Simmons-Duffin, *The Conformal Bootstrap* [arXiv: 1602.07982], Proceedings, Theoretical Advanced Study Institute in Elementary Particle Physics: New Frontiers in Fields and Strings (TASI 2015): Boulder, CO, USA, June 1-26, 2015.

[2] D. Poland, S. Rychkov, and A. Vichi, *The Conformal Bootstrap: Theory, Numerical Techniques, and Applications*, [arXiv:1805.04405], Rev. Mod. Phys. 91, 15002 (2019).

[3] F. Kos, D. Poland, D. Simmons-Duffin, and A. Vichi, *Precision Islands in the Ising and O(N) Models*, [arXiv:1603.04436], JHEP 08 (2016) 036.
[4] D. Simmons-Duffin, *The Lightcone Bootstrap and the Spectrum of the 3d Ising CFT*, [arXiv:1612.08471], JHEP 03 (2017) 086.

[5] S. M. Chester, W. Landry, J. Liu, D. Poland, D. Simmons-Duffin, N. Su, and A. Vichi, *Carving out OPE space and precise O(2) model critical exponents*, [arXiv:1912.03324], JHEP 06 (2020) 142.

[6] M. Caselle, G. Costagliola, and N. Magnoli, *Numerical determination of the operator-product-expansion coefficients in the 3D Ising model from off-critical correlators*, [arXiv:1501.04065], Phys. Rev. D 91, 061901 (2015).

[7] G. Costagliola, *Operator product expansion coefficients of the 3D Ising model with a trapping potential*, [arXiv:1511.02921], Phys. Rev. D 93, 066008 (2016).

[8] V. Herdeiro, *Numerical estimation of structure constants in the three-dimensional Ising conformal field theory through Markov chain uv sampler*, [arXiv:1705.11045], Phys. Rev. E 96, 033301 (2017).

[9] M. Hasenbusch, *Two- and three-point functions at criticality: Monte Carlo simulations of the improved three-dimensional Blume-Capel model*, [arXiv:1711.10946], Phys. Rev. E 97 (2018) 012119.

[10] A. M. Polyakov, *Conformal symmetry of critical fluctuations*, JETP Lett. 12, 381 (1970); [Pisma Zh. Eksp. Teor.Fiz. 12, 538 (1970)].

[11] G. Parisi, R. Petronzio, and F. Rapuano, *A measurement of the string tension near the continuum limit*, Phys. Lett. B 128, 418 (1983).

[12] M. Lüscher and P. Weisz, *Locality and exponential error reduction in numerical lattice gauge theory*, [arXiv:hep-lat/0108014] JHEP 09, 010 (2001).

[13] M. Hasenbusch, *Monte Carlo study of an improved clock model in three dimensions*, [arXiv:1910.05916], Phys. Rev. B 100, 224517 (2019).

[14] M. Hasenbusch and E. Vicari, *Anisotropic perturbations in three-dimensional O(N)-symmetric vector models*, [arXiv:1108.0491], Phys. Rev. B 84, 125136 (2011).

[15] J. A. Lipa, D. R. Swanson, J. A. Nissen, T. C. P. Chui, and U. E. Israelsson, *Heat Capacity and Thermal Relaxation of Bulk Helium very near the Lambda Point*, Phys. Rev. Lett. 76, 944 (1996).

[16] J. A. Lipa, D. R. Swanson, J. A. Nissen, Z. K. Geng, P. R. Williamson, D. A. Stricker, T. C. P. Chui, U. E. Israelsson, and M. Larson, *Specific Heat of Helium Confined to a 57- µm
Planar Geometry, Phys. Rev. Lett. **84**, 4894 (2000).

[17] J. A. Lipa, J. A. Nissen, D. A. Stricker, D. R. Swanson and T. C. P. Chui, Specific heat of liquid helium in zero gravity very near the λ-point, [arXiv:cond-mat/0310163](https://arxiv.org/abs/cond-mat/0310163), Phys. Rev. B **68**, 174518 (2003).

[18] A. Pelissetto and E. Vicari, Critical Phenomena and Renormalization-Group Theory, [cond-mat/0012164](https://arxiv.org/abs/cond-mat/0012164), Phys. Rept. **368**, 549 (2002).

[19] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Critical behavior of the three-dimensional XY universality class, [cond-mat/0010360](https://arxiv.org/abs/cond-mat/0010360), Phys. Rev. B **63** (2001) 214503.

[20] M. Campostrini, M. Hasenbusch, A. Pelissetto, and E. Vicari, The critical exponents of the superfluid transition in He4, [cond-mat/0605083](https://arxiv.org/abs/cond-mat/0605083), published as Theoretical estimates of the critical exponents of the superfluid transition in He4 by lattice methods, Phys. Rev. B **74** (2006) 144506.

[21] U. Wolff, Collective Monte Carlo Updating for Spin Systems, Phys. Rev. Lett. **62**, 361 (1989).

[22] D. Simmons-Duffin, private communication (2020).