The interface tension in the improved Blume-Capel model

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(Dated: March 30, 2018)

Abstract

We study interfaces with periodic boundary conditions in the low temperature phase of the improved Blume-Capel model on the simple cubic lattice. The interface free energy is defined by the difference of the free energy of a system with anti-periodic boundary conditions in one of the directions and that of a system with periodic boundary conditions in all directions. It is obtained by integration of differences of the corresponding internal energies over the inverse temperature. These differences can be computed efficiently by using a variance reduced estimator that is based on the exchange cluster algorithm. The interface tension is obtained from the interface free energy by using predictions based on effective interface models. By using our numerical results for the interface tension $\sigma$ and the correlation length $\xi$ obtained in previous work, we determine the universal amplitude ratios $R_{2nd,+} = \sigma_0 f_{2nd,+}^2 = 0.3863(6)$, $R_{2nd,-} = \sigma_0 f_{2nd,-}^2 = 0.1028(1)$ and $R_{exp,-} = \sigma_0 f_{exp,-}^2 = 0.1077(3)$. Our results are consistent with those obtained previously for the three-dimensional Ising model, confirming the universality hypothesis.

PACS numbers: 05.50.+q, 05.70.Jk, 05.10.Ln, 68.05.Cf

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I. INTRODUCTION

Interfaces appear in a large number of systems in soft condensed matter physics, in chemistry and in biology. These interfaces separate for example the components of a binary liquid mixture, or a liquid and its vapour. The behaviour of interfaces might be described by effective models such as the capillary wave model \cite{1}. Via duality interfaces are related with strings in gauge theories. In the last few years there has been fundamental progress in understanding the wide predictive power of effective models of strings. See for example \cite{2} and references therein. A key feature in this discussion is the Lorentz invariance of the gauge model, or in the case of the interface, the Galilean invariance of the underlying three-dimensional system. In the case of a spin model on a lattice, Galilean invariance is restored as the critical point is approached. In the present study we therefore focus on the neighbourhood of the critical point. Note however that for binary mixtures of fluids and off-lattice models of such systems, Galilean invariance is not limited to criticality.

If the phase transition of a binary system is continuous, it belongs to the universality class of the three-dimensional Ising model. In the neighbourhood of a continuous phase transition the behaviour of various quantities is given by power laws. For example the correlation length behaves as

$$\xi = f_\pm |t|^{-\nu} (1 + a_\pm |t|^\theta + bt + ...),$$

where $t = \beta_c - \beta$ is the reduced temperature, $\nu$ the critical exponent of the correlation length, and $f_\pm$ the amplitude in the low and high temperature phase. Note that mostly $t = (T - T_c)/T_c$ is used as definition of the reduced temperature. The present choice is more convenient for our purpose. Such power laws are affected by corrections. The leading confluent one comes with the exponent $\theta = \nu \omega \approx 0.5$ and the leading analytic correction is given by $bt$. For reviews on critical phenomena see for example \cite{3–6}.

Very recently the critical exponents of the three-dimensional Ising universality class have been computed very accurately by using the conformal bootstrap method \cite{7}. In particular $\nu = 1/y_t = 0.6299709(40)$, obtained from $3 - y_t = \Delta_\epsilon = 1.412625(10)$. And in table 2 of \cite{8} one finds $\omega = \Delta_\epsilon' - 3 = 0.82968(23)$ for the exponent of the leading correction. These estimates are consistent with, but more precise than $\nu = 0.63002(10)$ and $\omega = 0.832(6)$ obtained from a Monte Carlo study of the improved Blume-Capel model on the simple cubic lattice \cite{9}.
The interface tension $\sigma$ is the free energy per area of an interface in the thermodynamic limit. The interface free energy is, roughly speaking, the difference of the free energies of a system with an interface and a corresponding system without an interface. For a precise definition see section II A below. In the neighbourhood of the critical point, the interface tension behaves as

$$\sigma = \sigma_0 (-t)^\mu [1 + a_\sigma (-t) + \tilde{b} t + ...] ,$$

where $\mu = 2\nu$. Dimensionless combinations of amplitudes are, following Renormalization Group (RG)-theory, universal. Here we shall study

$$R_\pm = \sigma_0 f^2_\pm .$$

Both the amplitudes of the exponential and the second moment correlation length have been considered in the literature. $R_\pm$ has been determined for various experimental systems and has been computed by using for example field theoretic methods. Accurate estimates have been obtained by using Monte Carlo simulations of the Ising model.

Studying the improved Blume-Capel model, $a_\pm \approx 0$, eq. (1), and $a_\sigma \approx 0$, eq. (2), should simplify the analysis of the data obtained for the correlation length and the interface tension.

Recently we demonstrated that the exchange cluster algorithm [10, 11] can be employed to define variance reduced estimators of differences of observables measured in two slightly different systems [12, 13]. Here we apply this idea to the interface energy. In [14] we employed the exchange cluster algorithm to define a variance reduced estimator of the two-point function for systems with a spontaneously broken $Z_2$-symmetry. The numerical estimates obtained in [14] for the correlation length are used here to calculate $R_\pm$.

The outline of the paper is the following. In the next section we shall define the Blume-Capel model. We discuss the geometry of the systems that we simulate and define the interface free energy. Then we recall the exchange cluster algorithm and define the variance reduced estimator of the difference in the internal energy between the anti-periodic and the periodic system. Next we present our numerical results. We study the performance of the variance reduced estimator. We compute the interface tension for a large range of inverse temperatures. Finally we determine estimates for the universal amplitude combinations $R_\pm$. 

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II. THE MODEL

As in previous work, we study the Blume-Capel model on the simple cubic lattice. The bulk system, for a vanishing external field, is defined by the reduced Hamiltonian

\[ H = -\beta \sum_{<xy>} s_x s_y + D \sum_x s_x^2, \]  

(4)

where the spin might assume the values \( s_x \in \{-1, 0, 1\} \). \( x = (x_0, x_1, x_2) \) denotes a site on the simple cubic lattice, where \( x_i \in \{0, 1, \ldots, L_i - 1\} \) and \( <xy> \) denotes a pair of nearest neighbours on the lattice. The inverse temperature is denoted by \( \beta = 1/k_B T \). The partition function is given by \( Z = \sum_{\{s\}} \exp(-H) \), where the sum runs over all spin configurations. The parameter \( D \) controls the density of vacancies \( s_x = 0 \). In the limit \( D \to -\infty \) vacancies are completely suppressed and hence the spin-1/2 Ising model is recovered.

In \( d \geq 2 \) dimensions the model undergoes a continuous phase transition for \( -\infty \leq D < D_{\text{tri}} \) at a \( \beta_c \) that depends on \( D \), while for \( D > D_{\text{tri}} \) the model undergoes a first order phase transition, where \( D_{\text{tri}} = 2.0313(4) \) for \( d = 3 \), see ref. [15].

Numerically, using Monte Carlo simulations it has been shown that there is a point \((D^*, \beta_c(D^*))\) on the line of second order phase transitions, where the amplitude of leading corrections to scaling vanishes. We refer to the Blume-Capel model at values of \( D \) that are good numerical approximations of \( D^* \) as improved Blume-Capel model. For a more general discussion of improved models see for example section 3.5 of [16] or section 2.3.1 of [6]. In [9] we simulated the model at \( D = 0.655 \) close to \( \beta_c \) on lattices of a linear size up to \( L = 360 \). We obtained \( \beta_c(0.655) = 0.387721735(25) \) and \( D^* = 0.656(20) \). The amplitude of leading corrections to scaling at \( D = 0.655 \) is at least by a factor of 30 smaller than for the spin-1/2 Ising model. Following eq. (52) of ref. [14], the amplitude of the second moment correlation length in the high temperature phase at \( D = 0.655 \) is

\[ f_{2n,d,+} = 0.2284(1) - 2.1 \times (\nu - 0.629977) + 500 \times (\beta_c - 0.387721735) \]

using \( t = \beta_c - \beta \) as definition of the reduced temperature. \hspace{1cm} (5)

Note that \( \nu = 0.629977 \) is the estimate of the critical exponent of the correlation length given by ref. [17], which was the most accurate at the time. In the high temperature phase there is little difference between \( \xi_{2nd} \) and the exponential correlation length \( \xi_{\text{exp}} \) which is
defined by the asymptotic decay of the two-point correlation function. Following [18]:

$$\lim_{\xi \to 0} \frac{\xi_{exp}}{\xi_{2nd}} = 1.000200(3)$$ (6)

for the thermodynamic limit of the three-dimensional system.

A. Definition of the interface free energy

Here we briefly recall a few basic definitions at the example of the Blume-Capel model. For a more detailed discussion see for example [1, 19, 20] or section 6 of ref. [16] and references therein. Our starting point is the difference of the free energies of a system with an interface and one without. In order to force an interface into the system, we consider so called anti-periodic boundary conditions. These are implemented by replacing in the reduced Hamiltonian, eq. (4), the terms $\beta s_x s_y$ by $-\beta s_x s_y$ for nearest neighbour pairs with $x_0 = L_0 - 1$ and $y_0 = 0$ or vice versa. For the following discussion it is useful to introduce a reduced Hamiltonian with a coupling $J_{<xy>,b}$ that depends on the link $<xy>$ and the type of the boundary conditions $b \in \{a, p\}$:

$$H_b = -\beta \sum_{<xy>} J_{b,<xy>} s_x s_y + D \sum_x s_x^2 .$$ (7)

In the case of periodic boundary conditions,

$$J_{p,<xy>} = 1 \quad \text{for all } <xy> .$$ (8)

For anti-periodic boundary conditions

$$J_{a,<xy>} = -1 \quad \text{if } x_0 = 0 \text{ and } y_0 = L_0 - 1 \text{ or vice versa.}$$

$$J_{a,<xy>} = 1 \quad \text{else.}$$ (9)

Our first definition of the interface free energy is

$$F_{s}^{(1)} = -\ln(Z_a/Z_p) + \ln L_0 ,$$ (10)

where $\ln L_0$ takes into account the translational invariance. The partition function for the boundary condition $b$ is given by

$$Z_b = \sum_{\{s\}} \exp(-H_b) .$$ (11)
The definition \((\ref{10})\) is motivated by the idea that for anti-periodic boundary conditions there is exactly one interface and no interface for periodic boundary conditions. A better approximation is given by

\[
F_s^{(2)} = \ln L_0 - \ln \left( \frac{1}{2} \ln \frac{1 + Z_a/Z_p}{1 - Z_a/Z_p} \right),
\]

where it is assumed that for anti-periodic boundary conditions there is an odd number of interfaces, while for periodic ones there is an even number. It is assumed that these interfaces do not interact. Note that \(F_s^{(2)}\) in contrast to \(F_s^{(1)}\) has a finite \(L_0 \to \infty\) limit.

### B. Finite \(L_0\) effects

In this section we briefly review results obtained in the literature. For a more detailed discussion see section 6 of ref. \([16]\) and references therein. The ratio of partition functions can be expressed in terms of eigenvalues \(\lambda\) of the transfer matrix \(T\) in 0-direction

\[
\frac{Z_a}{Z_p} = \frac{\text{Tr} \ T^{L_0} P}{\text{Tr} \ T^{L_0}} = \frac{\sum_i \left[ \lambda_{i,s}^{L_0} - \lambda_{i,a}^{L_0} \right]}{\sum_i \left[ \lambda_{i,s}^{L_0} + \lambda_{i,a}^{L_0} \right]},
\]

where the matrix \(P\) represents anti-periodic boundary conditions. Note that in the literature also the transfer matrix set up in a direction parallel to the interface has been considered, see for example \([21]\). The subscripts \(s\) and \(a\) stands for symmetric and anti-symmetric with respect to the spinflip \(s_x \to -s_x\) for all \(x\) on a slice of the lattice. Let us assume that \(i = 0, 1, 2, \ldots\) and \(\lambda_{i,s}\) and \(\lambda_{i,a}\) are decreasing with increasing \(i\). The symmetric eigenstates of the transfer matrix are eigenstates of \(P\) with eigenvalue 1 and the anti-symmetric ones are eigenstates of \(P\) with eigenvalue \(-1\). The tunneling correlation length is given by \(\xi_t = -1/\ln(\lambda_{0,a}/\lambda_{0,s})\). Here we consider the case that the tunneling correlation length \(\xi_t\) is large compared with the bulk correlation length \(\xi\). Hence

\[
\lambda_{0,s} > \lambda_{0,a} \gg \lambda_{1,s} > \lambda_{1,a}, \ldots.
\]

In the limit \(L_1, L_2 \to \infty\), \(\lambda_{is}\) and \(\lambda_{ia}\) become degenerate. The splitting decreases exponentially fast in \(L_1, L_2\). Taking into account only the largest two eigenvalues one finds

\[
\left( \frac{\lambda_{0,a}}{\lambda_{0,s}} \right)^{L_0} = \frac{Z_p - Z_a}{Z_p + Z_a}.
\]

Comparing with eq. \((\ref{12})\) we get

\[
F_s^{(2)} = \ln(2\xi_t),
\]
where for $L_1, L_2 \gg \xi_{\text{exp}}$ leading corrections are $O(\exp(-L_0/\xi_{\text{exp}}))$. Note that the bulk correlation length is given by

$$
\xi_{\text{exp}} = - \lim_{L_1, L_2 \to \infty} \frac{1}{\ln(\lambda_{1s}/\lambda_{0s})} = - \lim_{L_1, L_2 \to \infty} \frac{1}{\ln(\lambda_{1a}/\lambda_{0a})}.
$$

A more accurate expression for the corrections would require precise knowledge of the splitting between $\lambda_{1s}$ and $\lambda_{1a}$ as a function of $L_1$ and $L_2$.

The fact that the corrections vanish exponentially fast in $L_0$ enables us to choose $L_0$ such that finite $L_0$ corrections can be completely ignored in the analysis of the data. Numerical experiments show that $L_0$ taken to be a few times $L_1, L_2$ is sufficient to this end. For details see section V below.

III. PREDICTIONS BY THE EFFECTIVE FIELD THEORY

Interfaces can be described by effective $d-1$-dimensional models, where $d$ is the dimension of the bulk system. In the context of statistical physics such models are called capillary wave models. For a review see e.g. ref. [1]. In its simplest form it is a massless Gaussian theory, where the field corresponds to the transversal fluctuations of the interface. Note that in three dimensions, by duality, interfaces correspond to strings in gauge theories. Therefore effective theories describing such strings are in fact directly related to interfaces. In recent years there has been great progress in the understanding of the predictive power of such effective models; see e.g. [2, 22] and refs. therein. It turns out that the Lorenz symmetry of the underlying gauge model, or in our case the Galilean symmetry of the three-dimensional system, imposes constraints on the possible corrections to the free field theory.

In our study we are concerned with interfaces living on a torus with a cross section of the size $L_1 L_2$. For the analysis of our data we need the functional form of the free energy of the interfaces as a function of $L_1$ and $L_2$.

In the literature, the so called Nambu-Goto model is frequently discussed as effective string model. Its action is proportional to the area of the interface. The partition function of the Nambu-Goto model with periodic boundary conditions in both directions has been worked out in ref. [23]. In the appendix of ref. [23] the partition function is expanded in terms of powers of $1/(\sigma L_1 L_2)$. For the free energy of the interface with periodic boundary
conditions in a three-dimensional system follows

$$ F_s = \sigma L_1 L_2 + c_0 - \frac{1}{2} \ln \sigma - 2 \ln \eta(i\nu)/\eta(i) - f_1(u) \frac{1}{\sigma L_1 L_2} - \tilde{f}_2(u) \frac{1}{(\sigma L_1 L_2)^2} + \ldots, \quad (18) $$

where $\tilde{f}_2(u) = f_2(u) - 0.5f_1(u)^2$ and $u = L_1/L_2$ and $\eta$ is Dedekind’s function

$$ \eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad q = \exp(2\pi i \tau). \quad (19) $$

Explicit expressions for $f_1(u)$ and $f_2(u)$ are given in eq. (A.10) and (A.11) of ref. [23], respectively. In our numerical study we consider the case $L_1 = L_2$ throughout. One gets

$$ f_1(1) = 1/4, \quad \tilde{f}_2(1) = -0.014107\ldots. \quad (20) $$

Note that $F_s = \sigma L_1 L_2 + \tilde{c}_0 - 2 \ln \eta(i\nu)/\eta(i)$ is already predicted by the Gaussian interface model and does not rely on the Galilean symmetry of the underlying system. The action of an effective interface model could contained additional terms, such as a curvature term, that are not present in the Nambu-Goto model, altering the coefficients in eq. (18). It turns out that Galilean symmetry of the three-dimensional system ensures that terms up to $O(1/(\sigma L_1 L_2)^2)$ obtained from the Nambu-Goto model should be valid.

For the model studied here, the Galilean symmetry is broken by the lattice and only restored in the critical limit. We expect that the correction exponent that is related to this restoration of symmetry is close to 2 [24]. Furthermore, from the numerical results obtained in [25] we conclude that for $\xi \approx 2$, the deviation of $f_1(1)$ from its continuum value is of the order of 10%. We expect that the deviation in the case of the improved Blume-Capel model has a similar amplitude as in the case of the Ising model. Note that for real binary mixtures, Galilean symmetry should be present at any temperature.

The constant $c_0$ in eq. (18) is not fixed by the effective model. However Renormalization Group (RG)-theory predicts that

$$ C_0 = \lim_{\beta \to 0} c_0(\beta) - \frac{1}{2} \ln[\sigma(\beta)] \quad (21) $$

assumes a universal value. In ref. [25] we obtained $C_0 = 0.3895(8)$ analysing our data obtained for the three-dimensional Ising model. A semiclassical calculation [26] gives $C_0 \approx 0.29$. See eqs. (14,15) of ref. [27],
IV. THE MONTE CARLO ALGORITHM

Here we essentially follow ref. [25], where the analogous problem was studied for the three-dimensional Ising model on the simple cubic lattice. The main difference is that the interface energy \( E_s \) is computed by using the variance reduced estimator discussed below.

We compute the interface free energy by

\[
F_1^s(\beta) = F_1^s(\beta_0) - \int_{\beta_0}^{\beta} d\beta E_s(\beta),
\]

(22)

where the integration is performed numerically, using the trapezoidal rule. The starting point of the integration, \( F_1^s(\beta_0) \) is determined by using a variant of the boundary flip algorithm [28].

The interface energy is defined as

\[
E_s = E_a - E_p,
\]

(23)

where

\[
E_b = \langle \hat{E}_b \rangle, \quad \hat{E}_b = \sum_{<xy>} J_{b,<xy>} s_x s_y.
\]

(24)

Note the unconventional sign that we take to be consistent with our previous work. In [25], where we simulated the Ising model on the simple cubic lattice, we performed independent simulations of systems with periodic and anti-periodic boundary conditions in order to determine \( E_p \) and \( E_a \).

By using the exchange cluster algorithm [10, 11] we simulate the systems with periodic and anti-periodic boundary conditions jointly. The exchange cluster algorithm enables us to define a variance reduced estimator of the difference \( E_a - E_p \). In the following, we recall the steps of the exchange cluster algorithm [10–13]. Then we discuss the alignment of the configurations that is needed to get a considerable reduction of the variance. To get an ergodic update, the exchange cluster algorithm has to be supplemented by standard updates of the individual configurations. Finally we summarize the complete update and measurement cycle.

A. The exchange cluster update

Let us briefly recall the basic properties of the exchange cluster update [10, 11] at the example of our problem. We simulate a system with periodic and a system with anti-periodic
boundary conditions jointly. The type of the boundary conditions is indicated by the first
index of the field variable. Hence \( s_{p,x} \) and \( s_{a,x} \) denote the spin at the site \( x \) of the system
with periodic and anti-periodic boundary conditions, respectively. The elementary step of
the exchange cluster update is to swap the value of the spin between the two systems:

\[
s'_{a,x} = s_{p,x} \quad , \quad s'_{p,x} = s_{a,x} .
\]

This operation is performed for all sites within a cluster or for none. In ref. \[29\] the cluster
algorithm had been applied to the one component \( \phi^4 \) model on the lattice. To this end
embedded Ising variables were introduced. The exchange cluster algorithm can be derived
in a similar fashion. The swap of the spins can be written in terms of embedded Ising
variables \( \sigma_x \in \{-1, 1\} \):

\[

\begin{align*}
    s'_{a,x} &= \frac{1 + \sigma_x}{2} s_{a,x} + \frac{1 - \sigma_x}{2} s_{p,x} , \\
    s'_{p,x} &= \frac{1 + \sigma_x}{2} s_{p,x} + \frac{1 - \sigma_x}{2} s_{a,x} .
\end{align*}
\]

(25)

For \( \sigma_x = -1 \) the exchange is performed, while for \( \sigma_x = 1 \) the old values are kept. Plugging
eq. (25) into the reduced Hamiltonian \( H(\{s'_a\}, \{s'_p\}) = H_a(\{s'_a\}) + H_p(\{s'_p\}) \), eq. (7), one
reads off the coupling constants \( \beta_{\text{embed},<xy>} \) for the embedded Ising variables. The clusters
are defined by frozen links. Frozen links are those links that are not deleted. The probability
to delete a link \( <x,y> \) is given by \[29\]:

\[
p_{d,<xy>} = \min[1, \exp(-2\beta_{\text{embed},<xy>})] ,
\]

(26)

where following eq. (24) of \[13\]

\[

\beta_{\text{embed},<xy>} = \beta \frac{J_{p,<xy>} + J_{a,<xy>}}{4} (s_{p,x} - s_{a,x})(s_{p,y} - s_{a,y}) .
\]

(27)

Hence

\[

\beta_{\text{embed},<xy> \in B} = 0 \quad \text{and} \quad \beta_{\text{embed},<xy> \notin B} = \frac{\beta}{2} (s_{p,x} - s_{a,x})(s_{p,y} - s_{a,y}) ,
\]

(28)

where \( B \) denotes the set of all pairs of nearest neighbours \( <xy> \) with \( x_0 = 0 \) and \( y_0 = L_0 - 1 \),
or vice versa. As discussed in section IV of \[13\], for \( J_{p,<xy>} \neq J_{a,<xy>} \), an external field arises,
eq. (25) of \[13\]:

\[

h_{\text{embed},x,<xy>} = \beta \frac{J_{p,<xy>} - J_{a,<xy>}}{4} (s_{p,x} - s_{a,x})(s_{p,y} + s_{a,y}) ,
\]

(29)
where the indices $x, <xy>$ refer to the fact that the field at the site $x$ arises from the interactions on the link $<xy>$. This means in our case

$$h_{x,<xy>,\text{embed}} = \frac{\beta}{2}(s_{p,x} - s_{a,x})(s_{p,y} + s_{a,y})$$

(30)

for $x_0 = L_0 - 1$ and $y_0 = 0$ or vice versa. In total the embedded external field is $h_{x,\text{embed}} = \sum_{y,nn,x} h_{x,<xy>,\text{embed}}$, where $y,nn,x$ means that $y$ is a nearest neighbour of $x$. Hence there might be a non-vanishing external field at $x_0 = 0$ and $x_0 = L_0 - 1$, while it vanishes at all other sites. For a given decomposition into clusters there is huge freedom in the selection of clusters, where the exchange of spins is performed. As long as for a given decomposition into clusters, the probability to undo the exchange is the same as the exchange itself, detailed balance is satisfied. Similar to refs. [12, 13] it seems optimal to exchange as many spins as possible between the two systems. The exchange of spins is only hindered by the effective external field $h_{x,\text{embed}}$. Hence we only compute those clusters, which are frozen by the external field. To this end, we first run through the planes given by $x_0 = 0$ and $x_0 = L_0 - 1$. A site is frozen with the probability $p_{f,h} = 1 - p_{d,h}$, where

$$p_{d,h} = \min[1, \exp(-2h_{x,\text{embed}})] .$$

(31)

After running through these two planes, freezing sites, we construct all clusters that contain sites that are frozen due to the external field. To this end, the probability (26) is used. Then the spins in these clusters remain unchanged, while the spins at all other sites are exchanged between the two systems.

B. The variance reduced estimator of the difference of the internal energies

Following eq. (30) of [13] the variance reduced estimator of the difference is given by

$$\hat{E}_{s,\text{imp}} = \frac{1}{2} \left[ (\hat{E}_a - \hat{E}_p') + (\hat{E}_a' - \hat{E}_p) \right] ,$$

(32)

where $\hat{E}_a$ and $\hat{E}_p$ are the standard estimators evaluated before and $\hat{E}_a'$ and $\hat{E}_p'$ after the exchange cluster update. Since the spin is exchanged for all sites that do not belong to the frozen clusters, we get an exact cancellation for all nearest neighbour pairs $<xy> \notin B$, where both $x$ and $y$ do not belong to the frozen exchange clusters.
In our program, we evaluate the contributions from pairs of nearest neighbour sites \(<xy>\in B\), by implementing eq. (32) directly:

\[
\Delta \hat{E}_{imp,1} = -\frac{1}{2} \sum_{<xy>\in B} s_{a,x}s_{a,y} + s_{p,x}s_{p,y} + s'_{a,x}s'_{a,y} + s'_{p,x}s'_{p,y}.
\] (33)

The contribution from nearest neighbour pairs where both sites belong to the frozen clusters and \(<xy>\) is not in the boundary:

\[
\Delta \hat{E}_{imp,2} = \sum_{<xy>\not\in B, x\in C, y\in C} s_{a,x}s_{a,y} - s_{p,x}s_{p,y}.
\] (34)

And finally the contribution, where \(<xy>\) is not in the boundary, the site \(x\) is in the frozen clusters, but \(y\) is not

\[
\Delta \hat{E}_{imp,3} = \frac{1}{2} \sum_{<xy>\not\in B, x\in C, y\not\in C} s_{a,x}(s_{a,y} + s_{p,y}) - s_{p,x}(s_{a,y} + s_{p,y}).
\] (35)

In total

\[
\hat{E}_{s,imp} = \Delta \hat{E}_{imp,1} + \Delta \hat{E}_{imp,2} + \Delta \hat{E}_{imp,3}.
\] (36)

We note that the effort to compute \(\hat{E}_{s,imp}\) is essentially proportional to the total volume of the frozen exchange clusters. In the following we shall denote the collection of frozen exchange clusters simply by exchange cluster.

C. Aligning the configurations

In refs. \[13, 14\] we learnt that in the case of spontaneous symmetry breaking, it is important to align the magnetisation of the two systems that are simulated. This way, the frozen exchange clusters remain small compared with the volume of the system and the variance reduction is effective. In the case of the problem studied here, two steps are needed to this end. First we exploit the translational symmetry of the system with anti-periodic boundary conditions in 0-direction to shift the interface between the phases to the boundary. This way, typical configurations show a unique magnetisation.

A backward shift by \(i_s \in \{0,1,2,...,L_0-1\}\) is performed in the following way: For anti-periodic boundary conditions, if \(x_0 + i_s < L_0\)

\[
s'_{a,x_0,x_1,x_2} = s_{a,x_0+i_s,x_1,x_2}.
\] (37)
and else
\[ s'_{a,x_0,x_1,x_2} = -s_{a,x_0+i_s-L_0,x_1,x_2} \quad \text{(38)} \]

For periodic boundary conditions, if \( x_0 + i_s < L_0 \)
\[ s'_{p,x_0,x_1,x_2} = s_{p,x_0+i_s,x_1,x_2} \quad \text{(39)} \]
and else
\[ s'_{p,x_0,x_1,x_2} = s_{p,x_0+i_s-L_0,x_1,x_2} \quad \text{(40)} \]

To get a correct algorithm, we need a characterization of the position of the interface that is not altered by the exchange cluster update. To this end, we compute
\[ P(x_0) = \sum_{x_1,x_2} s_{a,x} s_{p,x}, \quad \text{(41)} \]
which remains unchanged by the exchange of spins between the two systems. For a similar construction see eq. (8) of ref. [14].

At the centre of the interface, we expect that the number of spins with \( s_{a,x} = -1 \) and with \( s_{a,x} = 1 \) is roughly the same. Therefore the position of the interface should be given by the position \( x_{0,\text{min}} \) of the minimum of \(|P(x_0)|\). If the minimum of \(|P(x_0)|\) is degenerate, we pick one randomly. In order to shift the interface to \( x_0 = 0 \), we choose \( i_s = x_{0,\text{min}} \). Furthermore, we like to have the same sign of the overall magnetisation for both systems. Therefore, after shifting, with newly computed \( P(x_0) \), if \( \sum_{x_0} P(x_0) < 0 \) we multiply \( s_{p,x} \) by \(-1\) for all \( x \). In case \( \sum_{x_0} P(x_0) = 0 \) we perform the operation with probability 1/2. After this alignment is done, the exchange cluster update as discussed above is performed along with the measurement of the variance reduced estimator of the energy difference. Next we undo the alignment: With probability 1/2 all spins of the system with periodic boundary conditions are multiplied by \(-1\). Then random shifts, eq. (37,38,39,40), by \( i_{s,a} \) and \( i_{s,p} \) for anti-periodic and periodic boundary conditions, respectively, are performed. The values of \( i_{s,a} \) and \( i_{s,p} \) are selected in \( \{0,1,2,\ldots,L_0-1\} \) with equal probability.

D. The complete update cycle

Since the exchange cluster update is not ergodic, it is supplemented by standard updates of the individual systems. To this end we use the local heat-bath algorithm, the local
Todo-Suwa \cite{30,31} algorithm and standard single cluster updates \cite{32}, where ergodicity is provided by the local heat-bath algorithm. An update cycle is composed by one sweep with the local heat bath algorithm for both systems, \(N_{clu}\) single cluster updates of the system with periodic boundary conditions only and one sweep with the local Todo-Suwa algorithm for both systems. Finally \(N_{ex}\) exchange cluster updates are performed along with the alignment and the shifts discussed above.

We chose \(N_{clu}\) such that \(N_{clu}\) times the average cluster size is roughly equal to the volume of the lattice. We update only the system with periodic boundary conditions by using the single cluster algorithm, since here in contrast to the anti-periodic boundary conditions, the introduction of an auxiliary array that indicates whether a site belongs to the cluster is not required. The number \(N_{ex}\) is chosen as odd number. This way configurations of the systems with periodic and anti-periodic boundary conditions are effectively swapped, avoiding large autocorrelation times for the system with anti-periodic boundary conditions, where no single cluster updates are performed. Note that it turns out that the clusters that have to be constructed for the exchange cluster update take on average only a small fraction of the volume of the system. Therefore, similar to \(N_{clu}\) we choose \(N_{ex}\) such that \(N_{ex}\) times the average total cluster size equals roughly the volume of the lattice.

Note that in the actual program, to save CPU-time, the spin values are exchanged only for the frozen clusters, while at the same time the type of the boundary conditions is swapped.

Let us summarize the steps of one update cycle by using a piece of pseudo-C code:

```c
sweep with the local heat bath algorithm for both systems;
for(iclu=0;iclu<nclu;iclu++)
{
    single cluster update of the system with periodic boundary conditions;
}
sweep with the local Todo-Suwa algorithm for both systems;
for(iex=0;iex<nex;iex++)
{
    align configurations;
    exchange cluster update with measurement of variance reduced energy
```
difference;
unalign configurations;
}

For a more formal discussion of the algorithm it is useful to write the updates as matrices $P_{AL}$ that act on probability distributions. The subscript $AL$ indicates the algorithm that is used. The indices of the matrix are given by the configurations. One update cycle is represented by the matrix

$$P_{cycle} = P_{NEX, A}^{Nex} P_{TS} P_{SC}^{NEx} P_{HB},$$

where $HB$ denotes a sweep over both systems using the heat-bath algorithm, $SC$ a single cluster update of the system with periodic boundary conditions, $TS$ a sweep over both systems using the Todo-Suwa algorithm, and $U, EX, A$ the exchange cluster update along with the alignment and unalignment of the configurations for periodic and anti-periodic boundary conditions. Here we follow the convention that the matrices act on vectors on the right. A correct algorithm should be ergodic and should satisfy stability

$$w = P_{cycle} w,$$

where $w$ denotes the distribution that we intend to generate, which is in our case the Boltzmann distribution $w = \exp(-H_a - H_p)/Z$. Eq. (43) is satisfied if stability is satisfied for each of the factors of $P_{cycle}$. For the Todo-Suwa algorithm, the single cluster algorithm and the heat-bath algorithm this has been shown in the literature. The alignment of the configurations modifies the Boltzmann distribution by introducing a constraint. Let us denote this distribution by $\tilde{w}$. We constructed the constraint such that it is kept by the exchange cluster update. Furthermore, the exchange cluster update inherits detailed balance from the cluster update of the embedded Ising model $[29]$. Hence $\tilde{w} = P_{EX} \tilde{w}$. Finally, the unalignment restores the Boltzmann distribution $w$ from the Boltzmann distribution with constraint $\tilde{w}$. Hence $w = P_{U, EX, A} w$.

V. NUMERICAL RESULTS

We performed simulations with the boundary flip algorithm $[28]$ to get the starting value for the integration $[22]$. The results for $F_s^{(1)}(\beta_0)$, eq. $[10]$, are summarized in table $[1]$. Here
TABLE I. Numerical results for $F^{(1)}(\beta_0)$ obtained for lattices with $L_1 = L_2 = L$ by using the boundary flip algorithm. 

| $\beta_0$ | $L$ | $L_0$ | $F^{(1)}$       |
|----------|-----|-------|----------------|
| 0.391    | 32  | 32    | 8.49222(39)    |
| 0.391    | 32  | 64    | 8.54138(39)    |
| 0.391    | 32  | 128   | 8.54183(55)    |
| 0.3885   | 64  | 64    | 7.44256(60)    |
| 0.3885   | 64  | 128   | 7.50640(40)    |
| 0.3885   | 64  | 256   | 7.5101(13)     |
| 0.388    | 128 | 128   | 8.4422(25)     |
| 0.388    | 128 | 256   | 8.50764(88)    |
| 0.388    | 128 | 512   | 8.5109(15)     |
| 0.38776  | 256 | 256   | 6.9731(19)     |
| 0.38776  | 256 | 512   | 7.0493(18)     |

we do not go further into the details of the simulations, since they are very similar to those of ref. We just note that the boundary flip algorithm becomes inefficient in the limit $Z_a/Z_p \rightarrow \infty$. Practically one is limited to $\sqrt{\sigma L} \lesssim 4$ for $L = L_1 = L_2$. To reach larger values of $\sqrt{\sigma L}$, we perform the numerical integration of $E_s$ over $\beta$, eq. (22).

A. Computing $E_s$ by using the exchange cluster algorithm

We implemented the code in standard C and used the SIMD-oriented Fast Mersenne Twister algorithm as random number generator. As check of the code, we performed high statistics simulations for $L = L_1 = L_2 = 2$ and $L_0 = 3$ and 4. For comparison we computed the observables exactly, up to rounding errors, by performing the sum over all configurations. Our simulation program passed this benchmark.

We performed a large number of simulations with the exchange cluster algorithm for lattices of the size $L = L_1 = L_2$ and $L_0 = L$, $2L$, or $4L$. In particular we considered $L = 32$, 64, 128, and 256 in the range $0.391 \leq \beta \leq 0.44$, $0.3885 \leq \beta \leq 0.44$, $0.388 \leq \beta \leq 0.4$, and
$0.38776 \leq \beta \leq 0.394$, respectively. Details are summarized in table III. In certain intervals $[\beta_a, \beta_f]$ we simulated at sampling points $\beta_i$ that are separated by $\Delta \beta = \beta_{i+1} - \beta_i$. For example for $L = L_0 = 256$ we simulated at 581 different values of $\beta$. Note that the intervals and the step size $\Delta \beta$ are chosen such that the systematic error of the numerical integration is about one order of magnitude smaller than the statistical error. The systematic error of the numerical integration was estimated by thinning out the sampling points. For $L = 32$ we performed $10^6$ update cycles after equilibration for each value of $\beta$. For larger $L$ we performed fewer updates. For example for $L = L_0 = 256$ for $\beta \leq 0.391$ we performed $10^5$ update cycles after equilibration. For $0.391 < \beta \leq 0.393$ we performed $4 \times 10^4$ update cycles and for $0.393 < \beta \leq 0.394$ we performed $2 \times 10^4$ update cycles. The simulations for $L = L_0 = 256$ and $10^5$ update cycles took about 6 days on a single core of a Xeon(R) E5-2660 CPU each.

First we investigated the performance of the exchange cluster update and the variance reduced estimator associated with it. Then we analysed our numerical results obtained for the interface energy and free energy.

1. Average size of the exchange cluster per area

In figure I we plot the average size of the exchange cluster per area $C_{ex}$ for $L = 64$ and the two lengths $L_0 = 64$ and 128. Here area is $L_1L_2$ and the size of the cluster is the number of sites contained in it. For $\beta \gtrapprox 0.3905$ the sizes for $L_0 = 64$ and 128 can not be discriminated at the level of our statistical accuracy. For smaller values of $\beta$, the cluster size for $L_0 = 128$ is larger than that for $L_0 = 64$. For $L = 32$ and the lengths $L_0 = 32$ and 64 we find that for $\beta \gtrapprox 0.396$, the cluster sizes for $L_0 = 32$ and 64 can not be discriminated. Also here, for smaller values of $\beta$, the cluster size is larger for the larger $L_0$. In the case of $L = 128$ and $L_0 = 128$ we generated only data for $\beta \geq 0.389$. For these values of $\beta$ we find that the cluster sizes agree at the level of our accuracy for $L_0 = 128$ and 256. For $L = 256$ we find that for $\beta \gtrapprox 0.38805$ the sizes for $L_0 = 256$ and 512 can not be discriminated at the level of our statistical accuracy. Again, for smaller values of $\beta$, the cluster size is larger for the larger $L_0$. These threshold values of $\beta$ correspond to $L/\xi_{exp} \approx 12.8, 13.0$, and 13.6 for $L = 32, 64$, and 256, respectively.

We interpret these findings as follows: For sufficiently low values of $\beta$, the probability
TABLE II. List of the simulations with the exchange cluster algorithm. In the first column we give \( L = L_1 = L_2 \), in the second column the values of \( L_0 \) that have been simulated. In the third and fourth column we give the start \( \beta_a \) and end point \( \beta_f \) of the interval in the inverse temperature that is considered. Finally in the last column, we give the step size \( \Delta \beta \) that is used in the interval.

| \( L \) | \( L_0 \) | \( \beta_a \) | \( \beta_f \) | \( \Delta \beta \) |
|------|-----|------|------|-------|
| 32   | 32,64,128 | 0.391 | 0.394 | 0.00002 |
| 32   | 32,64,128 | 0.394 | 0.396 | 0.00005 |
| 32   | 32,64,128 | 0.396 | 0.4   | 0.0001  |
| 32   | 32,64   | 0.4   | 0.42  | 0.0005  |
| 32   | 32      | 0.42  | 0.44  | 0.001   |
| 64   | 64,128,256 | 0.3885 | 0.391 | 0.00001 |
| 64   | 64,256   | 0.391 | 0.394 | 0.00002 |
| 64   | 128     | 0.391 | 0.392 | 0.00002 |
| 64   | 64      | 0.394 | 0.397 | 0.00005 |
| 64   | 64      | 0.397 | 0.4   | 0.0001  |
| 64   | 64      | 0.4   | 0.42  | 0.0005  |
| 64   | 64      | 0.42  | 0.44  | 0.001   |
| 128  | 128     | 0.388 | 0.391 | 0.00001 |
| 128  | 256     | 0.388 | 0.3885| 0.000005|
| 128  | 256     | 0.3885| 0.39  | 0.00001 |
| 128  | 512     | 0.388 | 0.38955| 0.00001|
| 128  | 128     | 0.391 | 0.394 | 0.00002 |
| 128  | 128     | 0.394 | 0.3975| 0.00005|
| 128  | 128     | 0.3975| 0.4   | 0.0001  |
| 256  | 256     | 0.38776| 0.38780| 0.000001|
| 256  | 256     | 0.38780| 0.38790| 0.000002|
| 256  | 256     | 0.38790| 0.38820| 0.000005|
| 256  | 256     | 0.38820| 0.39100| 0.00001 |
| 256  | 256     | 0.39100| 0.39400| 0.00002 |
| 256  | 512     | 0.38776| 0.38820| 0.00001 |
to have more than one interface is negligible. If there is only one interface, the exchange cluster contains only sites in the neighbourhood of the boundary. The size of the exchange cluster is governed by the interface. Hence as soon as \( L_0 \) is large compared with the width of the interface, there is no dependence of the size of the exchange cluster on \( L_0 \).

Next let us study the dependence of the cluster size per area on \( L \). For example at \( \beta = 0.396 \), where we see virtually no dependence on \( L_0 \), we find 2.6751(14), 2.9827(16), 3.2523(36), and 3.4935(46) for \( L = 32, 64, 128, \) and 256 respectively. Note that the simulation for \( L = 256 \) at \( \beta = 0.396 \) was performed mainly to get cluster size. The behaviour of the cluster size is roughly consistent with a logarithmic growth in \( L \). Using the Ansatz

\[
C_{ex}^2 = c + a \ln L
\]

we get \( c = -1.37(4) \), \( a = 2.463(11) \) and \( \chi^2/\text{d.o.f.} = 7.18 \) taking all four values of \( L \) into account. Skipping \( L = 32 \) we get \( c = -1.07(9) \), \( a = 2.397(21) \), and \( \chi^2/\text{d.o.f.} = 0.88 \). A similar fit for \( C_{ex} \) itself produces much larger values of \( \chi^2/\text{d.o.f.} \).
2. Reduction of the statistical error

We computed the naive statistical error of the difference of the internal energies as

$$\epsilon^2(E_s) = \epsilon^2(E_a) + \epsilon^2(E_p) ,$$

(45)

where we ignore correlations between the two systems, which are caused by the exchange cluster update. This should resemble quite well the situation of independent simulations for periodic and anti-periodic boundary conditions. The improvement that we get by using the cluster exchange algorithm and the variance reduced estimator associated with it is characterized by

$$r_{\text{gain}} = \epsilon^2(E_s)/\epsilon^2(E_{s,\text{imp}}) .$$

(46)

In figure 2 we plot $r_{\text{gain}}^{1/2}$ for $L = 64$ and $L_0 = 64$ and 128. For other lattice sizes $L, L_0$ we get similar results. We find that for fixed parameters of the algorithm, the gain increases with increasing $\beta$ and $L_0$. The steps in $r_{\text{gain}}^{1/2}$, plotted as a function of $\beta$, are due to a change of $N_{\text{ex}}$. For $L_0 = 64$ we use $N_{\text{ex}} = 3$ up to $\beta = 0.38943$, $N_{\text{ex}} = 5$ from $\beta = 0.38944$ up to

FIG. 2. We plot $r_{\text{gain}}^{1/2}$, eq. (46), for $L = 64$ and $L_0 = 64$ and 128 as a function of $\beta$. 

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0.39015, \( N_{ex} = 7 \) from \( \beta = 0.39016 \) up to \( \beta = 0.391 \) and \( N_{ex} = 15 \) from \( \beta = 0.39102 \) up to 0.44. For \( L_0 = 128 \), we use \( N_{ex} = 3 \) up to \( \beta = 0.38903, N_{ex} = 5 \) from \( \beta = 0.38904 \) up to 0.3893, \( N_{ex} = 7 \) from \( \beta = 0.38931 \) up to 0.391, \( N_{ex} = 9 \) for \( \beta = 0.39102 \) and \( N_{ex} = 15 \) for \( \beta = 0.39104 \) up to 0.392. Note that we made no effort to fine tune the parameter \( N_{ex} \) of the algorithm. It is chosen such that \( N_{ex} \) times the average size of the exchange cluster is roughly equal to the lattice size. In our simulations we find a gain \( r_{gain} \), depending on \( \beta \), \( L \), and \( L_0 \) that ranges from a factor of \( \approx 4 \) up to \( \approx 70 \).

In a preliminary stage of our study, we had implemented the exchange cluster algorithm without the alignment of the configurations discussed in section IV A. In this case we see a much larger size of the exchange cluster. Furthermore the reduction of the variance is moderate.

B. Finite \( L_0 \) effects

Next we investigated finite \( L_0 \) effects in \( E_s \) and \( F_s \). In figure 3 we plot minus the difference \( \Delta E_s = E_s(L = 64, L_0 = 64) - E_s(L = 64, L_0 = 128) \). We find that \( \Delta E_s \) vanishes within the statistical errors for \( \beta \gtrapprox 0.3907 \). In the following, to be on the safe side, we shall assume that for \( L_0 = L = 64 \) finite \( L_0 \) effects can be ignored for \( \beta \gtrapprox 0.3915 \).

In figure 4 we show the corresponding difference \( \Delta F_s = F_s(L = 64, L_0 = 64) - F_s(L = 64, L_0 = 128) \). Similar to the finding above, we find that \( \Delta F_s \) vanishes within the statistical errors for \( \beta \gtrapprox 0.3907 \). Here we should note that results for different values of \( \beta \) are statistically correlated due to the fact that \( F_s \) is obtained by integrating \( E_s \). In the following we assume that at our level of statistical accuracy, for \( L_0 = L = 64 \) finite \( L_0 \) effects in \( F_s \) can be safely ignored for \( \beta \gtrapprox 0.3915 \). Translating this into a dimensionless ratio, we get that for \( L_0 = L \) finite \( L_0 \) effects in \( F_s \) can be safely ignored if \( L/\xi_{exp} \gtrapprox 16 \). Checking our numerical results for \( L = 32, 128, \) and 256, we confirm this finding. Performing a similar analysis, we conclude that for \( L_0 = 2L \) finite \( L_0 \) effects in \( F_s^{(2)} \) can be ignored if \( L/\xi_{exp} \gtrapprox 6 \). Note that all data used below satisfy these requirements. For our final estimates of \( F_s \) obtained by integrating \( E_s \), eq. [22], we lowered the value of \( L_0 \) by a factor of two at certain values of \( \beta \), where the difference between \( E_s(L, L_0, \beta) \) and \( E_s(L, 2L_0, \beta) \) is negligible. For example for \( L = 32 \), we started the integration at \( \beta = 0.391 \) with \( L_0 = 128 \). For 0.393 < \( \beta \) < 0.44 we used \( E_s(32, 64) \) and then for 0.4 < \( \beta \) < 0.44 we used instead \( E_s(32, 32) \). On the other
FIG. 3. We plot minus the difference of the interface energy for $L = 64$ between $L_0 = 64$ and 128. The solid red line simply indicates zero. For a discussion see the text.

hand for $L = 256$ we used $L_0 = 256$ throughout. The particular choice for each value of $L$ is related to the accuracy of data that we had generated.

C. Critical behaviour of the interface energy $E_s$

The interface free energies that are obtained from integrating the interface energies are, by construction, statistically correlated. In order to avoid this complication we analyse directly the interface energies.

We start from the Ansatz

$$F_s = \sigma(\beta) L^2 + c_0(\beta) - \frac{1}{4 \sigma(\beta) L^2}$$

for the interface free energy, where

$$\sigma(\beta) = \sigma_0 t_m^{2\nu} \left[ 1 + at_m^\theta + bt_m + \ldots \right] ,$$

(47)

(48)
FIG. 4. We plot the difference of the interface free energy for $L = 64$ between $L_0 = 64$ and 128. The solid red line simply indicates zero. For a discussion see the text.

where we expect that $|a|$ is small, since we study an improved model. For convenience we have introduced $t_m = -t = \beta - \beta_c$ here. Following RG-theory the constant behaves as

$$c_0(\beta) = c + \ln \xi + ... = \tilde{c} - \nu \ln t_m + \tilde{c}t_m^\theta + \tilde{d}t_m + ... \quad (49)$$

where again $|\tilde{c}|$ is expected to be small.

Taking the derivative of eq. (47) with respect to $\beta$, we arrive at

$$E_s = 2\nu \sigma_0 t_m^{2\nu-1} [1 + \tilde{a}t_m^\theta + \tilde{b}t_m] L^2 - \nu t_m^{-1} + \tilde{d} + \frac{1}{4L^2} \frac{2\nu}{\sigma_0 t_m^{2\nu-1}} \frac{1 + \tilde{a}t_m^\theta + \tilde{b}t_m}{(1 + \tilde{a}t_m^\theta + \tilde{b}t_m)^2}, \quad (50)$$

where we ignored corrections that are represented by ... in eqs. (48,49). Furthermore, we skipped the term $\tilde{c}t_m^\theta - 1$ which should be negligible for the improved model. We define

$$\tilde{a} = a \left(1 + \frac{\theta}{2\nu}\right), \quad \tilde{b} = b \left(1 + \frac{1}{2\nu}\right) \quad (51)$$

to keep eq. (50) readable.
1. Numerical results

We have fitted our numerical data for $L = 32, 64, 128, \text{ and } 256$ using the Ansatz (50). We fixed $\nu = 0.6299709, \omega = 0.82968$ and $\beta_c = 0.387721735$. In order to keep finite $L$ effects small, we took only data with $\sqrt{\sigma L} \gtrsim 6$ into account. In order to estimate systematic errors due to subleading corrections that are not included in the Ansatz and due to deviations of the coefficient of $1/(\sigma(\beta)L^2)$ from $-1/4$, we varied the range of parameters that are included into the fit. For example for $\sqrt{\sigma L} \gtrsim 6$ and $\beta \leq 0.392$ we get $\sigma_0 = 7.4039(19), \sigma_0 \tilde{a} = -0.04(10), \sigma_0 \tilde{b} = -19.8(9), \tilde{d} = 2.0(1.2)$, and $\chi^2/\text{d.o.f.} = 1.099$. For $\sqrt{\sigma L} \gtrsim 6, 0.392 < \beta \leq 0.4$ we get $\sigma_0 = 7.4054(34), \sigma_0 \tilde{a} = -0.12(9), \sigma_0 \tilde{b} = -19.05(50), \tilde{d} = 0.7(3)$, and $\chi^2/\text{d.o.f.} = 1.048$. We observe that the results obtained from these two disjoint data sets are consistent. The amplitude $\sigma_0 \tilde{a}$ is consistent with zero at the level of our statistical accuracy, as expected for the improved model.

As central value of $\sigma_0$ we have taken the result of the fit with $\sqrt{\sigma L} \gtrsim 6$ and $\beta \leq 0.392$:

$$\sigma_0 = 7.404(5) + 6700 \times (\beta_c - 0.387721735) \quad (52)$$

The error is taken such that also the results of other fits, in particular the one with $0.392 < \beta \leq 0.4$, are covered. The dependence on the value of $\beta_c$ is estimated by redoing the fit for $\beta \leq 0.392$ with a slightly shifted value of $\beta_c$. Note that the dependence on the value of $\beta_c$ becomes weaker, when data for larger values of $\beta$ are fitted. The dependence on $\nu$ and $\omega$ is small, and can be ignored at our level of accuracy. Combining the estimate of $\sigma_0$ and that of the amplitude of the second moment correlation length in the high temperature phase, eq. (5), we arrive at

$$R_{2nd,+} = \sigma_0 f_{2nd,+}^2 = 0.3863(6) \quad (53)$$

Fitting all our data for $\sqrt{\sigma L} \gtrsim 6$ and $\beta \leq 0.4$ we arrive at

$$\sigma(t) = 7.40535(-t)^{1.2599418} \left[ 1 - 0.011 (-t)^{0.52267} + 1.4352 t \right] \quad (54)$$

where $t = 0.387721735 - \beta$. Below we shall see that this parametrizes the interface tension in the interval $0.389 \leq \beta \leq 0.4$ quite well. Throughout, the deviation from the true value should be less than or equal to $3 \times 10^{-7}$ as shown in table [111]
TABLE III. In the first column we give the inverse temperature $\beta$. In the second column our estimates of $\sigma$ obtained from the analysis of the interface tension. In () we give the statistical error, while the numbers in [] give the value of $\sigma$ minus the estimate obtained from eq. (54). In column 3 we give $c_0 + \frac{1}{4} \ln \sigma$ and in columns 4 and 5 the products $\sigma \xi_{2nd}^2$ and $\sigma \xi_{exp}^2$, respectively. The numbers for $\xi_{2nd}$ and $\xi_{exp}$ are taken from table II of ref. [14].

| $\beta$ | $\sigma$ | $c_0 + 0.5 \ln \sigma$ | $\sigma \xi_{2nd}^2$ | $\sigma \xi_{exp}^2$ |
|----------|--------|------------------------|-----------------------|-------------------------|
| 0.4      | 0.02842920(50)[+29] | 0.3893(28) | 0.101796(6) | 0.108488(37) |
| 0.396    | 0.01740643(34)[±0] | 0.3908(19) | 0.102230(6) | 0.108280(36) |
| 0.394    | 0.01232175(15)[-22] | 0.3923(11) | 0.102418(6) | 0.108112(37) |
| 0.393    | 0.00991738(13)[-16] | 0.3916(10) | 0.102497(6) | 0.108091(36) |
| 0.392    | 0.00762273(17)[-31] | 0.3955(44) | 0.102570(7) | 0.107921(36) |
| 0.391    | 0.00545890(14)[-9] | 0.3900(36) | 0.102664(7) | 0.107885(37) |
| 0.39     | 0.00345657(13)[-11] | 0.3909(32) | 0.102734(7) | 0.107876(37) |
| 0.389    | 0.00167139(11)[-13] | 0.3910(25) | 0.102784(11) | 0.107786(54) |

D. Analysing the interface free energy

Finally we computed $R_{2nd,-}$, $R_{exp,-}$ and the constant $C_0$, eq. (21). To this end, we take the interface tension $\sigma$ computed at the values of $\beta$ that we had simulated at in ref. [14]. As Ansatz we used $F_s = \sigma L^2 + c_0 - \frac{1}{4\sigma L^2}$ with $\sigma$ and $c_0$ as free parameters of the fit. We took data obtained for $\sqrt{\sigma L} \gtrsim 6$ into account. Only in the case of $\beta = 0.389$, our smallest linear size $L = 128$ does not satisfy this criterion. We checked possible effects at $\beta = 0.39158$, where we get a similar value of $\sqrt{\sigma L}$ for $L = 64$ as for $L = 128$ at $\beta = 0.389$. Comparing the results for the pair of lattice sizes $L = 64$ and 128 with that for $L = 128$ and 256, we conclude that the possible systematical error is smaller than our statistical error at $\beta = 0.389$. Our results are summarized in table III. For $\beta = 0.389$, 0.39, and 0.392 the pair $L = 128$ and 256 of lattice sizes is used, for $\beta = 0.393$ and 0.394 the lattice sizes $L = 64$, 128 and 256 enter the fit and for $\beta = 0.396$ and 0.4, the sizes $L = 64$ and 128 are used.

The estimates of $c_0 + 0.5 \ln \sigma$ are constant within the range of $\beta$-values that we have
We plot $\sigma \xi_{2nd}^2$ as a function of $\xi_{2nd}^{-\omega}$. The data for the Ising model are taken from ref. [25]. The filled circle on the $y$-axis gives our estimate of $R_{2nd,-}$. As our final result we quote

$$C_0 = 0.391(2)$$

which is the average of the estimates for $\beta = 0.389, 0.39, 0.391$ and 0.392. Our result is fully consistent with $C_0 = 0.3895(8)$ obtained in ref. [25] studying the Ising model. The result of [25] is more accurate, since interface free energies for smaller values of $\sqrt{\sigma}L$ were included in the analysis.

In figure 5 we plot $\sigma \xi_{2nd}^2$ as a function of $\xi_{2nd}^{-\omega}$. For comparison we plot the corresponding results for the three-dimensional Ising model given in table 11 of ref. [25].

We analysed our numerical results by using the Ansatz

$$\sigma \xi^2 = R_- + a \xi^{-\omega} + b \xi^{-2}$$

Fitting with different ranges of the data and also skipping the term $a \xi^{-\omega}$ we arrive at the estimates

$$R_{2nd,-} = 0.1028(1)$$
VI. COMPARISON WITH RESULTS GIVEN IN THE LITERATURE

In experiments on binary mixtures the correlation length can be determined accurately only in the high temperature phase. Therefore only estimates of $R_{2nd,+}$ are available. Reviews of experimental results are given in [34, 35]. In their table I, the authors of [35] summarize results for various binary liquid mixtures. As mean value they quote $R_+ = 0.386$ without error bar. This is also the favoured value of ref. [34]. Given the scattering of the data, the error might be a 2 or 3 on the second digit. A bit more recently $R_+ = 0.41(4)$ was obtained from the study of a cyclohexane-aniline mixture in [36]. Previous experimental results are summarized in [36] as $R_+ = 0.37(3)$. Our result is nicely consistent with the experimental ones, confirming that the phase transition of the binary liquid mixtures belongs to the Ising universality class.

Theoretical estimates of $R_\pm$ have been computed by using various methods. Brézin and Feng [37] computed $R_{2nd,-}$ to order $\epsilon^2$ in the $\epsilon$-expansion. The numerical evaluation of their result for $\epsilon = 1$ gives results in the range from $\approx 0.051$ up to $\approx 0.057$. Compared with our results, this is too small by a factor of about 2. Münster [26] performed a semiclassical calculation at one-loop level, which was extended to two-loop in ref. [38]. Their central result is given in eq. (36) of [38]

$$ R_{2nd,-} = \frac{2}{u_R} \left\{ 1 + \sigma u \frac{u_R^3}{4\pi} + \sigma_2 \left( \frac{u_R^3}{4\pi} \right)^2 + O \left( u_R^3 \right) \right\} , $$

where the error bar is chosen such that the results of various fits are covered.
where $\sigma_{1l} = -0.2002602...$ and $\sigma_{2l} = -0.0076(8)$. Plugging in $u^*_R = 14.08(1)$ [14], we arrive at $R_{2nd.-} = 0.1088(2)$, where the number in brackets gives the error due to the errors of $\sigma_{2l}$ and $u^*_R$. The error due to the truncation of the series is hard to estimate. The result given in table 1 of [38] for various resummation schemes might suggest that the error is in the third digit.

In the literature one can find a number of Monte Carlo studies of the Ising model on the simple cubic lattice. In table [IV] we give results obtained in the last two decades. Our present results are consistent with those obtained from simulations of the Ising model, but are more accurate. For a summary of Monte Carlo studies performed before 1997 see table 8 of ref. [27].

VII. SUMMARY AND CONCLUSIONS

We have studied the behaviour of the interface free energy in the improved three-dimensional Blume-Capel model. The interface free energy is determined by the difference of the free energy of a system with anti-periodic and a system with periodic boundary conditions. For the precise definition see eqs. (10,12). We computed the interface free energy by integrating the interface energy $E_s$ over the inverse temperature $\beta$ numerically. The interface free energy $F_s$ at the starting point of the integration was determined by using the boundary flip algorithm [28]. The interface energy $E_s$ was computed by using a variance reduced estimator based on the exchange cluster update [10, 11]. Compared with the standard estimator, the square of the statistical error is reduced by a factor of up to 70. This finding is in line with refs. [12, 13], where we demonstrated that the exchange cluster update allows to define variance reduced estimators of quantities related to the critical Casimir effect. It seems likely that the exchange cluster update allows to define variance reduced estimators for a wide range of quantities related to defects in $\mathbb{Z}_2$-invariant systems.

The dependence of the interface free energy on the transversal extensions is well described by effective interface models. Recently there had been progress in the understanding of the predictive power of these models. See for example refs. [2, 22] and refs. therein. For a more detailed discussion see sec. [III] Here we only used these results to extract the interface tension $\sigma$ and the constant $c_0$, eq. (18), from our data for the interface free energy. In order to probe the predictions of effective interface models very accurate data for a range of
interface areas would be needed.

Using our estimates for the interface tension and the results for the correlation length obtained in ref. [14], we computed the universal amplitude ratios $R_{2\text{nd},+}$, $R_{2\text{nd},-}$, and $R_{2\text{nd},+}$ with high accuracy. Our estimate of $R_{2\text{nd},+}$ coincides with estimates obtained from experiments on binary liquid mixtures [34–36]. There is also good agreement for all three quantities with estimates obtained for the Ising model on the simple cubic lattice [25, 27, 39]. These findings confirm the universality hypothesis.

VIII. ACKNOWLEDGEMENT

This work was supported by the Deutsche Forschungsgemeinschaft under the grants No HA 3150/3-1 and HA 3150/4-1.

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