

Theoretical estimates of the critical exponents of the superfluid transition in ^4He by lattice methods

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We improve the theoretical estimates of the critical exponents for the three-dimensional XY universality class that apply to the superfluid transition in ^4He along the λ line of its phase diagram. We obtain the estimates $\alpha = -0.0151(3)$, $\nu = 0.6717(1)$, $\eta = 0.0381(2)$, $\gamma = 1.3178(2)$, $\beta = 0.3486(1)$, and $\delta = 4.780(1)$. Our results are obtained by finite-size scaling analyses of high-statistics Monte Carlo simulations up to lattice size $L = 128$ and resummations of 22nd-order high-temperature expansions of two improved models with suppressed leading scaling corrections. We note that our result for the specific-heat exponent α disagrees with the most recent experimental estimate $\alpha = -0.0127(3)$ at the superfluid transition of ^4He in a microgravity environment.

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I. INTRODUCTION AND SUMMARY

The renormalization-group (RG) theory of critical phenomena classifies continuous phase transitions into universality classes, which are determined by only a few global properties of the system, such as the space dimensionality, the nature and the symmetry of the order parameter, the symmetry-breaking pattern, and the range of the interactions. Within a given universality class, the critical exponents and scaling functions describing the asymptotic critical behavior are identical for all systems. The three-dimensional XY universality class is characterized by a complex order parameter and symmetry breaking $O(2) \cong \mathbb{Z}_2 \otimes U(1) \rightarrow \mathbb{Z}_2$. An interesting representative of this universality class is the superfluid transition of ^4He along the λ line $T_\lambda(P)$, which provides an exceptional opportunity for a very accurate experimental test of the RG predictions, because of the weakness of the singularity in the compressibility of the fluid and of the purity of the samples. Exploiting also the possibility of performing experiments in a microgravity environment, the specific heat of liquid helium was measured up to a few nanokelvins from the λ transition.¹ The resulting estimate of the specific-heat exponent, obtained after some reanalyses of the experimental data,¹⁻³ is³

$$\alpha = -0.0127(3). \quad (1)$$

Other experimental results at the superfluid transition of ^4He , and for other physical systems in the XY universality class, are reported in Ref. 4.

On the theoretical side the XY universality class has been studied by various approaches, such as field-theoretical (FT) methods and lattice techniques based on Monte Carlo (MC) simulations or high-temperature (HT) expansions. A review of results can be found in Ref. 4. Accurate estimates of the critical exponents were obtained in Ref. 5 by combining MC simulations and HT expansions of improved Hamiltonians. This synergy of lattice techniques provided the estimate

$$\alpha = -0.0146(8), \quad (2)$$

which is substantially consistent with the experimental result (1), although slightly smaller. Other results obtained from FT

calculations,⁶⁻⁸ MC simulations,^{5,9} and HT expansions^{10,11} are less precise and in agreement with both estimates (1) and (2).

In this paper we significantly improve the theoretical estimates. This allows us to check whether the small difference between the theoretical and experimental estimates (1) and (2) disappears after a more accurate theoretical analysis, as recently suggested in Ref. 12. We again follow the strategy of Ref. 5, considering two classes of lattice Hamiltonians, the ϕ^4 lattice model and the dynamically diluted XY (ddXY) model. They depend on an irrelevant parameter, λ and D , respectively, which can be tuned to suppress the leading scaling corrections, giving rise to improved Hamiltonians. We improve the finite-size scaling (FSS) analysis of these models by significantly increasing the statistics (by approximately a factor of 10) and simulating larger lattices (up to lattice sizes $L = 128$). The precision of the data allows us to observe the expected next-to-leading scaling corrections, and therefore to have a much better control of the systematic errors. Moreover, we extend the HT expansion of the susceptibility and of the correlation length in the ϕ^4 and ddXY models to 22nd order, i.e., we add two terms to the HT series computed and analyzed in Refs. 5 and 11. Using this bulk of data and calculations, we perform several analyses, also combining information obtained from MC simulations and IHT analyses (IHT denotes the HT expansion specialized to improved models).

In Fig. 1 we show a summary of our results for the specific-heat critical exponent α , as obtained from the hyperscaling relation $\alpha = 2 - 3\nu$. We show three sets of estimates for the ϕ^4 and ddXY models, obtained by different methods. We first report the results of FSS analyses of MC data up to $L = 128$ (FSS). The three reported results for each model are obtained from the analysis (left) of a combination of two quantities (temperature derivatives of RG-invariant quantities) that does not have leading scaling corrections, (center) of the energy density, and (right) of the fourth-order (Binder) cumulant of the magnetization. Next, we report the results obtained from the analyses of the 22nd-order IHT series at the optimal values of the irrelevant parameters λ^* and D^* , biased using the MC estimates of β_c (MC+IHT). Finally, we

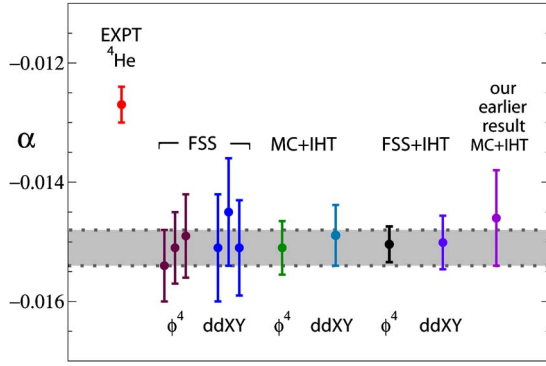


FIG. 1. (Color online) Summary of our results for the specific-heat exponent α . Abbreviations are explained in the text. The colored region corresponds to our final estimate $\alpha = -0.0151(3)$.

show results obtained by requiring the FSS and IHT analyses to give consistent results for the exponent ν (FSS+IHT). These results come from different analyses of the available MC data and HT calculations. Although they are not completely independent, their comparison represents a highly nontrivial cross-check of the results and of their errors. In Fig. 1 we also show our earlier MC+IHT result obtained in Ref. 5.

The results shown in Fig. 1 provide a rather accurate estimate of α , which we summarize by taking

$$\alpha = -0.0151(3) \quad (3)$$

as our final estimate. This result significantly improves our earlier estimate (2), but it does not reduce the difference from the experimental result (1). Moreover, now the errors are so small that their difference appears significant. According to our analyses, values of the specific-heat exponent $\alpha > -0.014$ should be highly unlikely. We think that this discrepancy calls for further investigations. We mention that a proposal of a space experiment has been presented in Ref. 13.

We also anticipate our best estimates of the other critical exponents:

$$\nu = 0.6717(1), \quad (4)$$

$$\eta = 0.0381(2), \quad (5)$$

$$\gamma = 1.3178(2), \quad (6)$$

$$\delta = 4.780(1), \quad (7)$$

$$\beta = 0.3486(1). \quad (8)$$

Moreover, we obtain an accurate estimate of the exponent ω associated with the leading scaling corrections, i.e., $\omega = 0.785(20)$, and of the exponent ω_2 associated with the next-to-leading scaling corrections, i.e., $\omega_2 = 1.8(2)$.

Our results improve earlier theoretical estimates; we mention the field-theoretical results $\nu = 0.6703(15)$ (from six-loop fixed-dimension perturbative series) and $\nu = 0.6680(35)$ [from $O(\epsilon^5)$ series], the MC estimates $\nu = 0.6723(11)$, $0.6716(5)$, and $0.6717(3)$, respectively, from Refs. 9, 5, and

12, and the HT results $\nu = 0.674(2)$ and $0.67166(55)$ from Refs. 10 and 11, respectively. Other results can be found in Ref. 4.

The paper is organized as follows. In Sec. II we define the ϕ^4 and ddXY lattice models. Section III is dedicated to a summary of the basic RG ideas concerning FSS in critical phenomena. In Sec. IV we present our MC simulations and the FSS analyses of the data. The computation and analysis of the HT expansion are presented in Sec. V. We report an analysis of the IHT expansions of improved ϕ^4 and ddXY models biased using the MC estimates of β_c (MC+IHT), and a combined analysis requiring the consistency of the IHT and FSS results (FSS+IHT). In Ref. 14 we report the HT expansion (up to 22nd order for the susceptibility and the correlation length) of several quantities for the most general model defined on a simple cubic lattice with two-component site variables and nearest-neighbor couplings.

II. LATTICE MODELS

As in Ref. 5, we consider two classes of models defined on a simple cubic lattice and depending on an irrelevant parameter. They are the ϕ^4 lattice model and the dynamically diluted XY model. The Hamiltonian of the ϕ^4 lattice model is given by

$$\mathcal{H}_{\phi^4} = -\beta \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x [\vec{\phi}_x^2 + \lambda(\vec{\phi}_x^2 - 1)^2], \quad (9)$$

where $\vec{\phi}_x = (\phi_x^{(1)}, \phi_x^{(2)})$ is a two-component real variable. The ddXY model is defined by the Hamiltonian

$$\mathcal{H}_{\text{dd}} = -\beta \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y - D \sum_x \vec{\phi}_x^2 \quad (10)$$

with the local measure

$$d\mu(\phi_x) = d\phi_x^{(1)} d\phi_x^{(2)} \left(\delta(\phi_x^{(1)}) \delta(\phi_x^{(2)}) + \frac{1}{2\pi} \delta(1 - |\vec{\phi}_x|) \right), \quad (11)$$

and the partition function

$$\int \prod_x d\mu(\phi_x) e^{-\mathcal{H}_{\text{dd}}}. \quad (12)$$

The parameters λ in \mathcal{H}_{ϕ^4} and D in \mathcal{H}_{dd} can be tuned to obtain improved Hamiltonians characterized by the fact that the leading correction to scaling is absent in the Wegner expansion of any observable near the critical point. Considering, for instance, the magnetic susceptibility χ , the corresponding Wegner expansion is generally given by¹⁵

$$\chi = Ct^{-\gamma} (1 + a_{0,1}t + a_{0,2}t^2 + \dots + a_{1,1}t^\Delta + a_{1,2}t^{2\Delta} + \dots + b_{1,1}t^{1+\Delta} + b_{1,2}t^{1+2\Delta} + \dots + a_{2,1}t^{\Delta_2} + \dots), \quad (13)$$

where $t \equiv 1 - \beta/\beta_c$ is the reduced temperature. We have neglected additional terms due to other irrelevant operators and terms due to the analytic background present in the free energy.^{16–18} The leading exponent γ and the correction-to-scaling exponents Δ, Δ_2, \dots , are universal, while the ampli-

tudes C , $a_{i,j}$, $b_{i,j}$ are nonuniversal. For three-dimensional XY systems, the value of the leading correction-to-scaling exponent is $\Delta \approx 0.53$,^{5,6,9} and the value of the subleading nonanalytic exponent is $\Delta_2 \approx 1.2$.¹⁹ In the case of improved Hamiltonians the leading correction to scaling vanishes, i.e., $a_{1,1} = 0$ in Eq. (13) (actually $a_{1,i} = 0$ for all i), in the Wegner expansion of any thermodynamic quantity.

Improved Hamiltonians belonging to the XY universality class have been discussed in Refs. 5, 9, and 11. We mention that improved Hamiltonians have also been considered for other universality classes, such as the Ising^{20–23} and Heisenberg universality classes.^{24,25}

III. FINITE-SIZE SCALING

In this section we summarize some basic results concerning FSS in critical phenomena. The starting point of FSS is the scaling behavior of the singular part of the free energy density of a sample of linear size L (see, e.g., Refs. 17 and 26):

$$\mathcal{F}_{\text{sing}}(u_t, u_h, \{u_i\}, L) = L^{-d} \mathcal{F}_{\text{sing}}(u_t L^{y_t}, u_h L^{y_h}, \{u_i L^{y_i}\}), \quad (14)$$

where $u_t \equiv u_1$, $u_h \equiv u_2$, and $\{u_i\}$ with $i \geq 3$ are the scaling fields (which are analytic functions of the Hamiltonian parameters) associated respectively with the reduced temperature t ($u_t \sim t$), magnetic field H ($u_h \sim H$), and the other irrelevant perturbations with $y_i < 0$. The scaling behavior of the interesting thermodynamic quantities can be obtained by performing the appropriate derivatives of Eq. (14), with respect to t and H . Since u_t and u_h are assumed to be the only relevant scaling fields, one may expand with respect to the arguments corresponding to the irrelevant scaling fields. This provides the leading scaling behavior and the power-law scaling corrections.

The RG exponents of the relevant scaling fields u_t and u_h are related to the standard exponents ν and η , i.e., $y_t = 1/\nu$ and $y_h = (d+2-\eta)/2$. The RG exponent $y_3 \equiv -\omega$ [$\Delta = \omega\nu$, cf. Eq. (13)] of the leading irrelevant scaling field u_3 has been estimated by the analysis of high-order FT perturbative expansions,⁶ obtaining $\omega = 0.802(18)$ (ϵ expansion) and $\omega = 0.789(11)$ ($d=3$ expansion) in the case of the three-dimensional XY universality class. Results from lattice techniques are in substantial agreement (see Ref. 4). As we shall see later, our FSS analysis provides the estimate $\omega = 0.785(20)$. Concerning the RG exponents of the next-to-leading scaling corrections [they are related to the scaling-correction exponents of Eq. (13) by $\Delta_2 = -y_4\nu$, etc.], we mention the FT results of Ref. 19: $y_4 = -1.77(7)$ and $y_5 = -1.79(7)$ (y_{421} and y_{422} in their notation) for the three-dimensional (3D) XY model. Note that, at present, there is no independent check of these results. As we shall see, our present MC and HT analyses confirm that the next-to-leading scaling corrections are characterized by a RG exponent $y_4 = -1.8(2)$. There are also corrections due to the violation of rotational invariance by the lattice; the corresponding RG dimension is $y_6 = -2.02(1)$.²⁷ We mention that for some quantities, such as the Binder cumulant and the ratio $R_\xi \equiv \xi/L$, there are also corrections due to the analytic background of

the free energy. This should lead to corrections with $y_7 = -(2-\eta) = -1.9619(2)$ (obtained by using the estimate of η of this work). Finally, in the case of R_ξ , we expect also $O(L^{-2})$ corrections,²⁸ related to the particular definition (22) of ξ .

For vanishing external field H , the behavior of a phenomenological coupling R , i.e., of a quantity that is invariant under RG transformations in the critical limit, can be written in the FSS limit as

$$\begin{aligned} R(L, \beta, \lambda) &= R(u_t L^{y_t}, \{u_i L^{y_i}\}) \\ &= r_0(u_t L^{y_t}) + \sum_k r_{3,k}(u_t L^{y_t}) u_3^k L^{ky_3} + \sum_{i \geq 4} r_i(u_t L^{y_t}) u_i L^{y_i} \\ &\quad + \dots, \end{aligned} \quad (15)$$

where we have singled out the corrections due to the leading irrelevant operator. The functions $r_0(z)$, $r_i(z)$, and $r_{3,k}(z)$ are smooth, finite for $z \rightarrow 0$, and universal once one chooses a specific normalization condition (which must be independent of the Hamiltonian parameters) for the scaling fields. For example, one may define the scaling field u_t by imposing $r'_0(0) = 1$ for a particular phenomenological coupling; then, the function $r_0(z)$ for any given phenomenological coupling R is universal, i.e., independent of the Hamiltonian parameters. The scaling fields $u_t(\beta, \lambda)$ and $u_i(\beta, \lambda)$ are smooth functions of β and λ . For $\beta \rightarrow \beta_c$ we have

$$u_i(\beta, \lambda) \approx c_i(\lambda)t, \quad t \equiv 1 - \beta/\beta_c. \quad (16)$$

All other scaling fields u_i are generically finite for $t=0$. Improved models are characterized by the additional condition that $u_3(t=0) = 0$: in this case, all corrections proportional to $L^{ky_3} = L^{-k\omega}$ vanish at the critical point $t=0$. In the limit $t \rightarrow 0$ and $u_i L^{y_i} \sim t L^{1/\nu} \rightarrow 0$, we can further expand Eq. (15), obtaining

$$\begin{aligned} R(L, \beta, \lambda) &= R^* + r'_0(0)c_f(\lambda)t L^{y_t} \\ &\quad + \sum_i r_i(0)u_i(\beta_c, \lambda)L^{y_i} + O(t^2 L^{2y_t}, L^{2y_3}, tL^{y_t+y_3}), \end{aligned} \quad (17)$$

where $R^* \equiv r_0(0)$. As we already mentioned, in improved models all corrections proportional to L^{ky_3} vanish for $t=0$.

Instead of computing the various quantities at fixed Hamiltonian parameters, one may study the FSS keeping a phenomenological coupling R fixed at a given value R_f . This means that, for each L , one considers $\beta_f(L)$ such that

$$R(L, \beta = \beta_f(L)) = R_f. \quad (18)$$

All interesting thermodynamic quantities are then measured at $\beta = \beta_f(L)$. The pseudocritical temperature $\beta_f(L)$ converges to β_c as $L \rightarrow \infty$. The value R_f can be specified at will, as long as R_f is taken between the high- and low-temperature fixed-point values of R . The choice $R_f = R^*$ (where R^* is the critical-point value) improves the convergence of β_f to β_c for $L \rightarrow \infty$; indeed^{5,22} $\beta_f - \beta_c = O(L^{-1/\nu})$ for generic values of R_f , while $\beta_f - \beta_c = O(L^{-1/\nu-\omega})$ for $R_f = R^*$. This method has several advantages. First, no precise knowledge of β_c is needed. Second, for some observables, the statistical error at fixed R_f is smaller than that at fixed $\beta = \beta_c$.

Typically, the thermal RG exponent $y_t=1/\nu$ is computed from the FSS of the derivative of a phenomenological coupling R with respect to β at β_c . Using Eq. (15) one obtains

$$\begin{aligned} S_R|_{\beta_c} &\equiv \left. \frac{\partial R}{\partial \beta} \right|_{\beta_c} \\ &= -\frac{c(\lambda)}{\beta_c(\lambda)} \left(r'_0(0)L^{y_t} + \sum_{i=3} r'_i(0)u_i(\beta_c)L^{y_t+y_i} \right) \\ &\quad + \sum_{i=3} r_i(0) \frac{du_i}{d\beta}(\beta_c, \lambda)L^{y_i} + \dots \end{aligned} \quad (19)$$

An analogous expansion holds for S_R computed at a fixed phenomenological coupling. The leading corrections scale with L^{y_3} . However, in improved models in which $u_3(\beta_c)=0$, the leading correction is of order L^{y_4} . Note that corrections proportional to $L^{y_3-y_t} \approx L^{-2.3}$ are still present even if the model is improved. If one computes the derivative at β_c , one should also take into account the uncertainty on β_c in the error estimate of ν ; therefore, it is more convenient to evaluate S_R at β_f defined in Eq. (18).

Before concluding the section, we would like to recall three basic assumptions of FSS when considering boundary conditions consistent with translation invariance, such as periodic boundary conditions:¹⁷ (a) $1/L$ is an exact scaling field with no corrections proportional to $1/L^2$, $1/L^3$, etc.; (b) the nonlinear scaling fields have coefficients that are L independent; (c) the analytic background present in the free energy depends on L through exponentially small terms.

The theoretical evidence for these three hypotheses is discussed in Ref. 17. Under these assumptions, there are no analytic $1/L$ corrections. These assumptions can be verified analytically in the two-dimensional Ising model (see, e.g., Refs. 18, 29, and 30 and references therein). As far as we know, all numerical results reported in the literature are in full agreement with assumptions (a), (b), and (c). In particular, there is no evidence of $1/L$ corrections to FSS. As we shall see, the FSS analysis that we shall present in this paper will provide further support to the FSS assumptions, and in particular to the absence of $1/L$ analytic corrections.

IV. MONTE CARLO SIMULATIONS AND FINITE-SIZE SCALING ANALYSES

In this section we present MC simulations that significantly extend those of Ref. 5. The statistics are much larger and we consider larger lattice sizes (the largest lattice has $L=128$). As we shall see, the present MC data allow us to perform a more accurate FSS analysis, achieving a much better control of the next-to-leading scaling corrections, and therefore of the systematic errors related to the subleading scaling corrections.

A. Monte Carlo simulations

We simulated the ϕ^4 and ddXY models on simple cubic lattices of size L^3 with periodic boundary conditions, at several values of the Hamiltonian parameters λ and D , close to

the optimal values λ^* and D^* , at which leading scaling corrections vanish.

The basic algorithm is the same as in our previous numerical study reported in Ref. 5. We use a combination of local and cluster³¹ updates. We perform wall-cluster updates:²¹ we flip all clusters that intersect a plane of the lattice. A cluster update changes only the angle of the variables. An ergodic algorithm is achieved by adding local updates,³² which can also change the length of the spin variables. We use Metropolis and overrelaxation algorithms as local updates, which we alternate with the cluster updates.

The main difference with respect to our previous numerical work⁵ concerns the random number generator. Since we planned to increase the statistics by approximately one order of magnitude, we decided to use a higher-quality random number generator, such as those proposed in Ref. 33. In our MC simulations we used the RANLUX random number generator with luxury level 2. Its main drawback is that it requires much more CPU time than the G05CAF generator of the NAG library³⁴ which we used in Ref. 5. In order to get a good performance, despite the use of the expensive random number generator, we used demonized versions^{35,36} of the update algorithms, which allowed us to save many random numbers.

Most simulations of the ϕ^4 and ddXY models were performed at the estimates of λ^* and D^* obtained in Ref. 5, i.e., $\lambda=2.07$ and $D=1.02$. In addition, we performed simulations at $\lambda=1.9, 2.1, 2.2, 2.3$ for the ϕ^4 model, and at $D=0.9, 1.2$ for the ddXY model. We shall also present some MC simulations of the standard XY model. In total, the MC simulations took approximately 20 years of CPU time on a single 2.0 GHz Opteron processor.

B. Definitions of the measured quantities

The energy density is defined as

$$E = \frac{1}{V} \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y \quad (20)$$

where $V \equiv L^3$. The magnetic susceptibility χ and the correlation length ξ are defined as

$$\chi \equiv \frac{1}{V} \left\langle \left(\sum_x \vec{\phi}_x \right)^2 \right\rangle \quad (21)$$

and

$$\xi \equiv \sqrt{\frac{\chi/F - 1}{4 \sin^2 \pi/L}}, \quad (22)$$

where

$$F \equiv \frac{1}{V} \left\langle \left| \sum_x \exp\left(i \frac{2\pi x_1}{L}\right) \vec{\phi}_x \right|^2 \right\rangle \quad (23)$$

is the Fourier transform of the correlation function at the lowest nonzero momentum.

We also consider several so-called phenomenological couplings, i.e., quantities that, in the critical limit, are invariant under RG transformations. We consider the Binder pa-

parameter U_4 and its sixth-order generalization U_6 , defined as

$$U_{2j} \equiv \frac{\langle (\vec{m}^2)^j \rangle}{\langle \vec{m}^2 \rangle^j}, \quad (24)$$

where $\vec{m} = (1/V) \sum_x \vec{\phi}_x$ is the magnetization of the system. We also consider the ratio $R_Z \equiv Z_a/Z_p$ of the partition function Z_a of a system with antiperiodic boundary conditions in one of the three directions and the partition function Z_p of a system with periodic boundary conditions in all directions. Antiperiodic boundary conditions in the first direction are obtained by changing the sign of the term $\vec{\phi}_x \cdot \vec{\phi}_y$ of the Hamiltonian for links $\langle xy \rangle$ that connect the boundaries, i.e., for $x = (L, x_2, x_3)$ and $y = (1, x_2, x_3)$. Finally, we define the helicity modulus Y . For this purpose we introduce a twisted term in the Hamiltonian. More precisely, we consider the nearest-neighbor sites (x, y) with $x_1 = L, y_1 = 1, x_2 = y_2$, and $x_3 = y_3$, and replace the term $\vec{\phi}_x \cdot \vec{\phi}_y$ in the Hamiltonian with

$$\vec{\phi}_x \cdot R_\varphi \vec{\phi}_y = \phi_x^{(1)} (\phi_y^{(1)} \cos \varphi + \phi_y^{(2)} \sin \varphi) + \phi_x^{(2)} (\phi_y^{(2)} \cos \varphi - \phi_y^{(1)} \sin \varphi), \quad (25)$$

where R_φ is a rotation by an angle φ . The helicity modulus is defined by

$$Y \equiv - \frac{1}{L} \left. \frac{\partial^2 \ln Z(\varphi)}{\partial \varphi^2} \right|_{\varphi=0}. \quad (26)$$

The quantities $U_{2j}, R_Z \equiv Z_a/Z_p, R_\xi \equiv \xi/L$, and $R_Y \equiv YL$ are invariant under RG transformations in the critical limit. Thus, they can be considered as phenomenological couplings. In the following we will generically refer to them by using the symbol R . Finally, we also consider the derivative of the phenomenological couplings with respect to the inverse temperature, i.e.,

$$S_R \equiv \frac{\partial R}{\partial \beta}, \quad (27)$$

which allows us to determine the critical exponent ν through Eq. (19).

C. Determination of the critical temperature

As a first step of the analysis we determine the inverse transition temperature β_c for various values of λ in the ϕ^4 model and of D in the ddXY model. For this purpose we employ the standard Binder-crossing method, i.e., β_c is determined by requiring

$$R(\beta_c, L) = R^* \quad (28)$$

independently of L . Here R is a phenomenological coupling, R^* is its fixed-point value, and corrections to scaling are ignored. In practice we compute $R(\beta, L)$ as Taylor series up to third order around the simulation value β_{run} . We choose as β_{run} our previous best estimate of β_c (see Ref. 5). In the analysis we consider four different phenomenological couplings: $R_Z \equiv Z_a/Z_p, R_\xi \equiv \xi/L, U_4$, and U_6 . We do not use the helicity modulus because it has a poor statistical accuracy for large lattices, which are important to determine β_c .

TABLE I. Estimates of β_c at $\lambda=2.07$ and $D=1.02$ and of the fixed-point value R^* for several dimensionless quantities. Results of fits of the MC data in the range $48 \leq L \leq 128$. For details, see the text.

Quantity	β_c at $\lambda=2.07$	β_c at $D=1.02$	R^*
R_Z	0.5093835(2)[3]	0.5637963(2)[2]	0.3203(1)[3]
R_ξ	0.5093836(2)[3]	0.5637963(2)[2]	0.5924(1)[3]
U_4	0.5093833(3)[1]	0.5637961(3)[1]	1.2431(1)[1]
U_6	0.5093834(3)[2]	0.5637962(3)[2]	1.7509(2)[7]

We first analyze the data at $\lambda=2.07$ for the ϕ^4 model and $D=1.02$ for the ddXY model, for which we have data with higher statistics especially for the largest lattices. We perform fits with Ansatz (28) for the two models separately. The two models provide consistent results for R^* , as required by universality. In order to improve the statistical accuracy, we also perform joint fits of the results for both models, imposing the same value of R^* . In Table I we report our final results, which are taken from joint fits of the results for the two models ($\lambda=2.07$ and $D=1.02$) with $48 \leq L \leq 128$. Systematic errors are estimated by comparison with fits with $24 \leq L \leq 48$, i.e., by evaluating (difference of the two fits)/($2^x - 1$) with $x = 1/\nu + \omega \approx 2.3$ for β_c and $x = \omega \approx 0.8$ for R^* (here we pessimistically assume that leading corrections dominate). The estimates of β_c obtained by using different quantities are all consistent among each other. As our final result we take the one obtained from the data of R_Z : $\beta_c = 0.5093835(2)[3]$ for the ϕ^4 model at $\lambda=2.07$ and $\beta_c = 0.5637963(2)[2]$ for the ddXY model at $D=1.02$, where the number in parentheses is the statistical error, while the number in brackets is the systematic error due to scaling corrections. In Table I we also report the estimates of the fixed-point values R^* of the phenomenological couplings, which improve the results of Ref. 5. For the other values of λ and D considered, we estimate β_c by requiring that $R(\beta_c, L=128) = R^*$; for R^* we use the estimate of R^* reported in Table I. Again, the best estimate is obtained from R_Z ; for this quantity scaling corrections are quite small. The results are reported in Table II, where the number in parentheses is the statistical error, while the number in brackets is the error due to the uncertainty on R^* .

D. FSS at fixed phenomenological coupling R

Instead of performing the FSS analysis at fixed Hamiltonian parameters, one may analyze the data at a fixed value of a given phenomenological coupling R , as discussed in Sec. III. For this purpose we need to compute $R(\beta)$ in the neighborhood of β_c . This could be done by reweighting the MC data obtained in a simulation at $\beta = \beta_{\text{run}} \approx \beta_c$. However, due to our enormous statistics, we could not store all results needed to reweight the data. Instead, we computed the first derivatives of $R(\beta)$ with respect to β and determined $R(\beta)$ by using its third-order Taylor expansion around β_{run} . We checked that this is by far enough for our purpose. If we do not use the reweighting technique, it is enough to store bin

TABLE II. Estimates of β_c for several values of λ and D , from the FSS analysis of the MC data, and from the fit of MC data of χ and ξ in the HT phase using bIA1 approximants of the 22nd-order HT series (MC HT) of χ and ξ (see Sec. V B). The results for $\lambda = 2.00$ (ϕ^4 model) and $D=0.90, 1.03$ (ddXY model) are taken from Ref. 5.

Model	FSS	MC HT from χ	MC HT from ξ
ϕ^4 , $\lambda=1.90$	0.5105799(4)[3]		
ϕ^4 , $\lambda=2.00$	0.5099049(15)		
ϕ^4 , $\lambda=2.07$	0.5093835(2)[3]		
ϕ^4 , $\lambda=2.10$	0.5091503(3)[3]	0.5091504(4)	0.5091504(4)
ϕ^4 , $\lambda=2.20$	0.5083355(3)[4]	0.5083361(4)	0.5083363(4)
ddXY, $D=0.90$	0.5764582(15)[9]		
ddXY, $D=1.02$	0.5637963(2)[2]	0.5637956(6)	0.5637970(7)
ddXY, $D=1.03$	0.5627975(7)[7]		
ddXY, $D=1.20$	0.5470376(17)[6]	0.5470383(6)	0.5470392(7)
Standard XY	0.4541652(5)[6] ^a		

^aThis estimate is obtained from a fit with $R_Z(\beta_c, L) = R_Z^* + cL^{-\omega}$, with $L_{\min} = 32$, fixing $R_Z^* = 0.3203$ and $\omega = 0.785$. This result is consistent with $\beta_c = 0.4541659(10)$ given in Ref. 37.

averages of the different quantities, significantly reducing the amount of needed disk space. Given $R(\beta)$, one determines the value β_f such that $R(\beta = \beta_f) = R_f$. All interesting observables are then measured at β_f ; their errors at fixed $R = R_f$ are determined by a standard jackknife analysis. For compatibility with our previous study,⁵ we choose $R_{Z,f} = 0.3202$ and $R_{\xi,f} = 0.5925$.

This method has the advantage that it does not require a precise knowledge of the critical value β_c . But there is another nice side effect: for some observables the statistical errors at fixed R_f are smaller than those at fixed β (close to β_c). This is due to cross correlations and to a reduction of the effective autocorrelation times. For example, we find

$$\frac{\text{err}[\chi|\beta_c]}{\text{err}[\chi|R_Z=0.3202]} \approx 3.2, \quad \frac{\text{err}[\chi|\beta_c]}{\text{err}[\chi|R_\xi=0.5925]} \approx 4.5,$$

$$\frac{\text{err}[U_4|\beta_c]}{\text{err}[U_4|R_Z=0.3202]} \approx 1.9, \quad \frac{\text{err}[U_4|\beta_c]}{\text{err}[U_4|R_\xi=0.5925]} \approx 1.6 \quad (29)$$

for the ddXY model, with a very small L dependence (within the last figure of the above-reported numbers). In the case of the ϕ^4 model we find slightly smaller improvements for the same quantities. We also mention that the gain is marginal for the derivatives of R considered in this paper. A reduction of the statistical errors when some quantities are measured at a fixed R has also been observed in other models.³⁸

E. The leading correction-to-scaling exponent ω

In order to study corrections to scaling, we analyze the value of a phenomenological coupling R_1 at a fixed value of a second coupling R_2 . If β_f is determined by $R_2(\beta_f) = R_{2,f}$, we consider

$$\bar{R}_1 \equiv R_1(\beta_f) \quad (30)$$

(the dependence on L is understood hereafter). Note that^{5,22} the large- L limit of \bar{R}_1 is universal but depends on $R_{2,f}$ (it differs from the critical value R_1^* , unless $R_{2,f} = R_2^*$). Neglecting scaling corrections in Eq. (15), we have $R_1 = r_{1,0}[c(\lambda)tL^{\nu_t}]$ and $R_2 = r_{2,0}[c(\lambda)tL^{\nu_t}]$ where $r_{1,0}(z)$ and $r_{2,0}(z)$ are universal functions. Fixing $R_2 = R_{2,f}$ corresponds to fixing a particular trajectory in the t, L plane, given by $c(\lambda)tL^{\nu_t} = z_f$ where z_f is the solution of the equation $R_{2,f} = r_{2,0}(z_f)$. Along this trajectory $R_1 = \bar{R}_1 = r_{1,0}(z_f)$ which shows the universality of \bar{R}_1 .

The phenomenological couplings that we consider are U_4 , U_6 , $R_Z \equiv Z_a/Z_p$, $R_\xi \equiv \xi/L$, and $R_Y \equiv YL$.

In the ϕ^4 model we define

$$\Delta(\lambda_1, \lambda_2) \equiv \bar{R}_1(\lambda_2) - \bar{R}_1(\lambda_1), \quad (31)$$

and analogously for the ddXY model, replacing λ with D . Since

$$\bar{R}_1(\lambda) = \bar{R}_1^* + c(\lambda)L^{-\omega} + \dots, \quad (32)$$

we perform fits with the most simple *Ansatz*

$$\Delta(\lambda_1, \lambda_2) = \Delta c L^{-\omega}, \quad \Delta c = c(\lambda_2) - c(\lambda_1), \quad (33)$$

and analogously for the ddXY model. A selection of such fits is given in Table III, where we report only results for \bar{U}_4 and \bar{R}_Y at a fixed value of either R_Z or R_ξ . Very similar results are obtained by using \bar{U}_6 instead of \bar{U}_4 . \bar{R}_ξ at a fixed value of R_Z is not very useful, because corrections to scaling and statistical errors are relatively large. In order to get an idea of the corrections to scaling, we give results for the fit intervals $5 \leq L \leq 12$ and $10 \leq L \leq 24$. The difference of the two results provides a rough estimate of the error due to next-to-leading corrections to scaling. As our final result we quote

TABLE III. Fits to *Ansatz* (33), using the data at $\lambda_1 = 1.9$ and $\lambda_2 = 2.3$ in the case of the ϕ^4 model and $D_1 = 0.9$ and $D_2 = 1.2$ in the case of the ddXY model. L_{\min} and L_{\max} are the minimal and maximal lattice sizes that have been included in the fit. DOF is the number of degrees of freedom of the fit.

Model	R_1	R_2	L_{\min}	L_{\max}	Δc	ω	χ^2/DOF
ϕ^4	U_4	R_Z	5	12	-0.0209(2)	0.825(4)	0.8
			10	24	-0.0200(5)	0.804(10)	1.1
	U_4	R_ξ	5	12	-0.0210(2)	0.775(4)	0.5
			10	24	-0.0215(5)	0.785(10)	1.4
	R_Y	R_Z	5	12	-0.0053(1)	0.722(9)	1.4
			10	24	-0.0060(5)	0.775(37)	0.7
ddXY	U_4	R_Z	5	12	-0.0355(2)	0.782(3)	0.7
			10	24	-0.0349(6)	0.775(7)	0.9
	U_4	R_ξ	5	12	-0.0365(2)	0.739(3)	4.3
			10	24	-0.0386(7)	0.764(7)	0.6
	R_Y	R_Z	5	12	-0.0099(1)	0.708(5)	3.6
			10	24	-0.0115(7)	0.773(25)	0.9

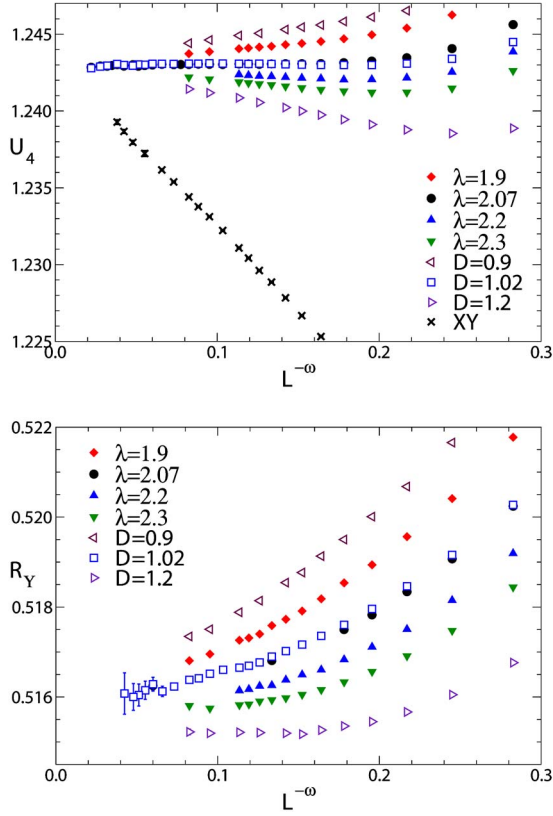


FIG. 2. (Color online) \bar{U}_4 (above) and \bar{R}_Y (below) at fixed $R_Z = 0.3202$ for various values of λ (ϕ^4 model), D (ddXY model), and the standard XY model, vs $L^{-\omega}$ with $\omega=0.785$.

$$\omega = 0.785(20), \quad (34)$$

which includes (almost) all results for the interval $10 \leq L \leq 24$.

F. Determination of λ^* and D^*

To begin with, in Fig. 2 we show results for \bar{U}_4 and \bar{R}_Y at fixed $R_Z = 0.3202$, for various values of λ in the ϕ^4 model, of D in the ddXY model, and in the standard XY model, vs $L^{-\omega}$ with $\omega=0.785$. They show a clear evidence of the leading scaling corrections, and of the existence of optimal values λ^*, D^* of λ and D for which they are suppressed. We also note that \bar{R}_Y is subject to larger next-to-leading scaling corrections; we shall return to this point later.

In order to determine λ^* and D^* , we mainly use our data generated for $\lambda=2.07$ and $D=1.02$. We fit them using various *Ansätze*. The most simple one is

$$\bar{R} = \bar{R}^* + cL^{-\omega}, \quad (35)$$

where \bar{R} is defined in Eq. (30). Equation (35) includes only leading corrections to scaling; we fix $\omega=0.785$ as previously obtained. We may also include subleading corrections to scaling. As we mentioned in Sec. III, there are several scaling corrections that have similar exponents with $1.8 \leq \omega_i \leq 2.0$. Of course, it is impossible to distinguish these correction terms and in the fits we have included a single effective

next-to-leading term with an exponent that we still indicate, for notational simplicity, with ω_2 . Thus, we consider

$$\bar{R} = \bar{R}^* + cL^{-\omega} + eL^{-\omega_2}, \quad (36)$$

and use either $\omega_2=1.8$ or $\omega_2=2$.

We first perform fits of types (35) and (36) for the two models ϕ^4 and ddXY separately. As \bar{R} we consider \bar{U}_4 at fixed R_Z , \bar{U}_4 at fixed R_ξ , \bar{U}_6 at fixed R_Z , \bar{U}_6 at fixed R_ξ , and \bar{R}_Y at fixed R_Z . The results for \bar{R}^* are, as required by universality, consistent for the two models. Hence we take our final results from joint fits of the results for both models. For instance, in a joint fit with *Ansatz* (35) there are three free parameters: \bar{R}^* and two correction-to-scaling amplitudes, one for the ϕ^4 and one for the ddXY model.

In order to determine λ^* (and analogously D^*), we assume $c(\lambda)$ to be linear in the neighborhood of λ^* and write

$$c(\lambda) \approx c_1(\lambda - \lambda^*), \quad (37)$$

so that

$$\lambda^* = \lambda - \frac{1}{c_1}c(\lambda). \quad (38)$$

We use $\lambda=2.07$, the value for which we have most of the simulations, and determine c_1 by using

$$c_1 = \left. \frac{\partial c}{\partial \lambda} \right|_{\lambda=\lambda^*} \approx \frac{c(\lambda=2.3) - c(\lambda=1.9)}{2.3 - 1.9}. \quad (39)$$

In the ddXY model we use the same formulas with $D=1.02$ and

$$c_1 = \left. \frac{\partial c}{\partial D} \right|_{D=D^*} \approx \frac{c(D=1.2) - c(D=0.9)}{1.2 - 0.9}. \quad (40)$$

In order to determine $c(\lambda)$ and $c(D)$, we fix $\omega=0.785$ (and, to estimate errors, $\omega=0.765$, $\omega=0.805$). The results of the fits with *Ansatz* (33) for $\omega=0.785$ are summarized in Table IV. The final estimate is taken from the fits with $12 \leq L \leq 24$. The comparison with the fits with $6 \leq L \leq 12$ gives us an idea of the error due to subleading corrections. It is small enough to be ignored in the following.

We also checked whether the linear approximation is sufficiently accurate by determining the derivatives (39) and (40) from other pairs of values of λ and D . The error due to the linear extrapolation is approximately 10%, which is negligible for the purpose of determining λ^* and D^* . In Fig. 3 we plot the results for λ^* and D^* as functions of the L_{\min} used in the fits to (35) and (36). The results of the fits to Eq. (35) show a systematic drift and become stable only for $L_{\min}=30$. This systematic variation is mostly due to the next-to-leading corrections and indeed fits to Eq. (36) are less dependent on L_{\min} and give fully consistent results. As our final results we quote

$$\lambda^* = 2.15(5), \quad D^* = 1.06(2), \quad (41)$$

which correspond to

TABLE IV. Fits to *Ansatz* (33) as in Table III, but keeping ω fixed. $\Delta c \equiv c(\lambda=2.3) - c(\lambda=1.9)$ for the ϕ^4 model and $\Delta c \equiv c(D=1.2) - c(D=0.9)$ for the ddXY model.

Model	R_1	R_2	ω	L_{\min}	L_{\max}	Δc	χ^2/DOF	
ϕ^4	U_4	R_Z	0.785	6	12	-0.01925(3)	5.8	
				12	24	-0.01898(5)	1.5	
		0.805	6	12	-0.02006(3)	1.5		
			12	24	-0.02002(5)	1.2		
	0.765	6	12	-0.01847(3)	13.6			
				12	24	-0.01799(5)	2.4	
		U_4	R_ξ	0.785	6	12	-0.02145(3)	0.2
					12	24	-0.02145(5)	1.6
	U_6	R_Z	0.785	6	12	-0.0688(1)	7.7	
				12	24	-0.0678(2)	1.5	
	U_6	R_ξ	0.785	6	12	-0.0763(1)	0.2	
				12	24	-0.0763(2)	1.6	
R_Y	R_Z	0.785	6	12	-0.00608(2)	2.5		
			12	24	-0.00615(5)	0.8		
	U_4	R_Z	0.785	6	12	-0.03576(3)	0.8	
				12	24	-0.03578(8)	0.9	
ddXY	0.805	6	12	-0.03727(3)	6.5			
				12	24	-0.03774(8)	3.4	
	0.765	6	12	-0.03431(3)	4.4			
				12	24	-0.03393(7)	0.2	
U_4	R_ξ	0.785	6	12	-0.04021(4)	12.7		
			12	24	-0.04077(9)	1.0		
	U_6	R_Z	0.785	6	12	-0.1271(1)	1.7	
				12	24	-0.1276(3)	1.2	
U_6	R_ξ	0.785	6	12	-0.1423(1)	22.3		
			12	24	-0.1447(3)	1.3		
R_Y	R_Z	0.785	6	12	-0.01157(2)	7.2		
			12	24	-0.01177(8)	1.2		

$$\left(\bar{U}_4|_{R_Z=0.3202}\right)^* = 1.242\,81(10),$$

$$\left(\bar{U}_4|_{R_\xi=0.5925}\right)^* = 1.242\,77(10). \quad (42)$$

Consistent results for λ^* and D^* are obtained by analyzing \bar{U}_6 at $R_Z=0.3202$ and $R_\xi=0.5925$. Note that the estimates of λ^* and D^* are slightly larger than those obtained in our previous work,⁵ where we reported $\lambda^*=2.07(5)$ and $D^*=1.02(2)$. Since the larger statistics and larger lattice sizes allow us to achieve a better control of all sources of systematic errors, and in particular of the next-to-leading scaling corrections, we are confident that the estimates (41) are now correct with the quoted errors (which are as large as those reported in our previous work).

We also performed some MC simulations of the standard XY model up to lattice size $L=96$. Using the estimates for ω and \bar{U}_4^* obtained above, one-parameter fits of the MC data give (taking data for $24 \leq L \leq 96$)

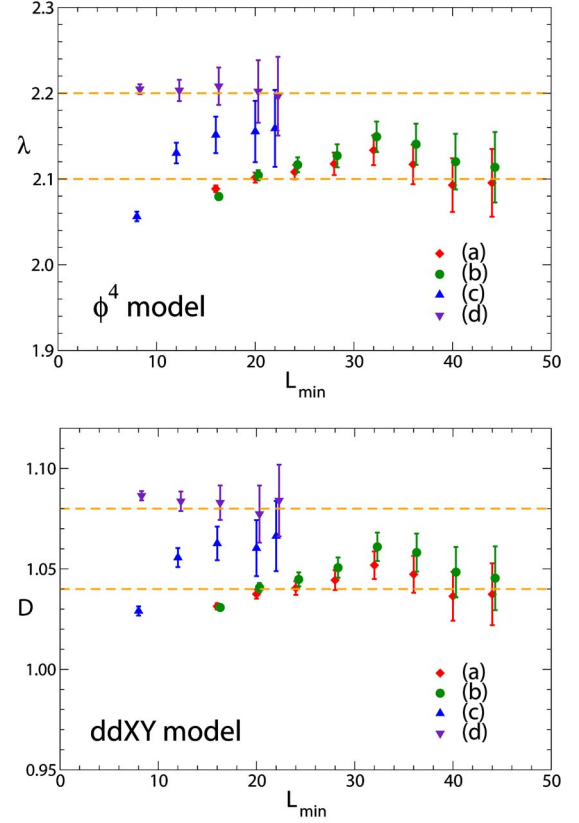


FIG. 3. (Color online) Determination of λ^* and D^* from joint fits of both ϕ^4 and ddXY models: (a) results from fits of \bar{U}_4 at $R_Z=0.3202$ to $a+cL^{-\omega}$ with $\omega=0.785$; (b) results from fits of \bar{U}_4 at $R_\xi=0.5925$ to $a+cL^{-\omega}$ with $\omega=0.785$; (c) results from fits of \bar{U}_4 at $R_Z=0.3202$ to $a+cL^{-\omega}+eL^{-\omega_2}$ with $\omega=0.785$, $\omega_2=1.8$; (d) results from fits of \bar{U}_4 at $R_\xi=0.5925$ to $a+cL^{-\omega}+eL^{-\omega_2}$ with $\omega=0.785$, $\omega_2=1.8$. The dashed lines indicate our final estimates.

$$\bar{U}_4|_{R_Z=0.3202} = 1.242\,81 - 0.1014(4)L^{-0.785} \quad (43)$$

and

$$\bar{U}_4|_{R_\xi=0.5925} = 1.242\,77 - 0.1138(4)L^{-0.785}. \quad (44)$$

We can use these results to obtain a conservative upper bound on the ratios $|c(\lambda=2.15)/c(XY)|$ and $|c(D=1.06)/c(XY)|$ that are independent of the quantity one is considering. Using the estimate of the linear coefficient c_1 and taking into account that the error on λ^* is ± 0.05 , we infer that the leading scaling-correction amplitude of U_4 at $R_Z=0.3202$ for $\lambda=2.15$ satisfies $|c(\lambda=2.15)| < 0.0024$. The same bound is obtained in the ddXY model for $c(D=1.06)$. This implies $|c(\lambda=2.15)/c(XY)| < 0.0024/0.1014 \approx 1/42$ and an analogous bound for $|c(D=1.06)/c(XY)|$. A similar calculation also shows that $|c(\lambda=2.07)|$ and $|c(D=1.02)|$ are at least 20 times smaller than $|c(XY)|$.

G. Next-to-leading scaling corrections

In this section we present evidence of next-to-leading scaling corrections characterized by an exponent $\omega_{\text{hlo}} \approx 2$, as

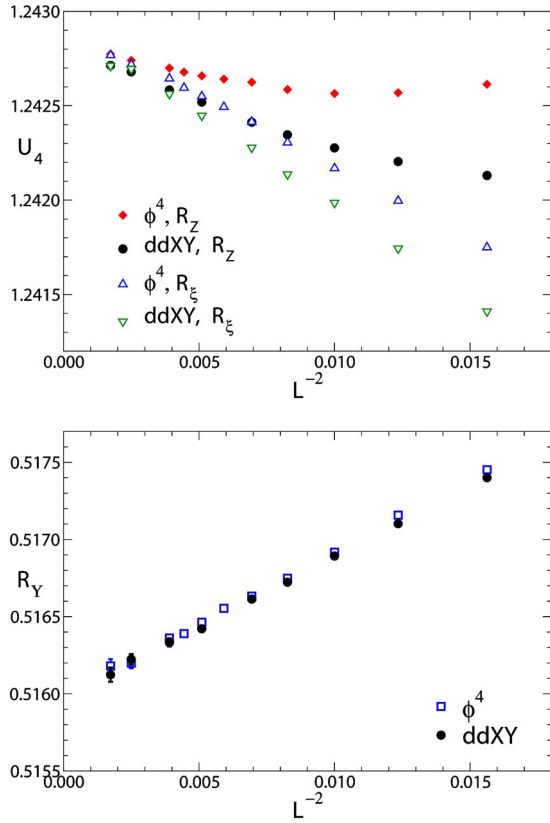


FIG. 4. (Color online) Estimates of the improved quantity (45) in the case of the Binder cumulant U_4 at $R_Z=0.3202$ and $R_\xi=0.5925$ (above), and of R_Y at $R_Z=0.3202$ (below), vs L^{-2} .

expected due to the presence of several irrelevant perturbations with $y \approx -2$, as discussed in Sec. III. In particular, this provides robust evidence of the absence of $1/L$ analytic corrections (see the discussion at the end of Sec. III).

We first construct improved variables for $\bar{U}_4|_{R_Z=0.3202}$, $\bar{U}_4|_{R_\xi=0.5925}$, and $\bar{R}_Y|_{R_Z=0.3202}$, which do not have leading scaling corrections. In the ddXY model (analogous formulas hold in the ϕ^4 model by replacing D with λ) we consider

$$\bar{R}_{\text{imp}} \approx \bar{R}(D_1)^x \bar{R}(D_2)^{1-x}. \quad (45)$$

Expanding \bar{R} as in Eq. (35) and using a linear approximation for $c(D)$, $c(D) \approx c_1(D - D^*)$, as in the previous section, we obtain for $L \rightarrow \infty$

$$\bar{R}_{\text{imp}} \approx \bar{R}^* \left(1 + \frac{c_1}{\bar{R}^* L^\omega} [x D_1 + (1-x) D_2 - D^*] + \dots \right). \quad (46)$$

Thus, if we take $x = x^* = (D^* - D_2)/(D_1 - D_2)$, the leading scaling correction cancels. In the ddXY model we use the data at $D_1=1.02$ and $D_2=1.2$, while in the ϕ^4 model we combine our data for $\lambda_1=1.9$ and $\lambda_2=2.3$.

In Fig. 4 we show the improved combination (45) in the case of the Binder cumulant \bar{U}_4 as a function of L^{-2} . For $\bar{U}_4|_{R_\xi=0.5925}$ we observe straight lines to a good approxima-

tion. On the other hand, for $\bar{U}_4|_{R_Z=0.3202}$ there is a clear bending of the curves, indicating that, in the given range of lattice sizes, corrections with exponent $\omega' > 2$ are contributing significantly. We should note that these results do not provide completely independent information, since we have already used $\omega_2 \approx 2$ as input in the determination of D^* and λ^* in the previous section. Therefore, they only provide a consistency check. This is not the case for $R_Y \equiv YL$, since it was not used for the determination of D^* and λ^* . In Fig. 4, $\bar{R}_Y|_{R_Z=0.3202}$ is plotted as a function of L^{-2} . We clearly observe a straight line. Hence corrections with $\omega_2 \approx 2$ clearly dominate in the whole range of lattice sizes that are shown. There are no leading corrections to scaling and, as expected from general RG arguments, also no corrections proportional to L^{-1} . If there were a correction proportional to L^{-1} , the ratio of its amplitude with the amplitude of the correction proportional to $L^{-\omega}$ (i.e., the leading one) would not be the same in different quantities. In other words, if corrections proportional to L^{-1} and $L^{-\omega}$ effectively cancel for U_4 at our estimates of D^* , λ^* and for the range of values of L considered, there is no reason why this should also happen for R_Y . Hence we conclude that our numerical results confirm the theoretical argument that no L^{-1} corrections are present in FSS for periodic boundary conditions.

H. The critical exponent ν

Here, we compute the critical exponent ν from a FSS analysis of the derivative $S_1 \equiv \partial R_1 / \partial \beta$ at a fixed value of another (or the same) phenomenological coupling R_2 .

For this purpose we define an improved quantity that does not have leading scaling corrections. Since S_1 behaves as

$$S_1 = a(\lambda) L^{1/\nu} [1 + c(\lambda) L^{-\omega} + \dots] \quad (47)$$

for $L \rightarrow \infty$, if we take $\lambda \approx \lambda^*$, so that $c(\lambda)$ is small and the linear approximation $c(\lambda) \approx c_1(\lambda - \lambda^*)$ works well, an improved variable is simply

$$S_{1,\text{imp}}(\lambda) \approx S_1(\lambda) [1 - c_1(\lambda - \lambda^*) L^{-\omega}]. \quad (48)$$

We compute c_1 using

$$c_1 = \left. \frac{\partial c}{\partial \lambda} \right|_{\lambda=\lambda^*} \approx \frac{c(\lambda_1) - c(\lambda_2)}{\lambda_1 - \lambda_2}, \quad (49)$$

where λ_1 and λ_2 are sufficiently close to λ^* so that the linear approximation works well. We estimate the difference $c(\lambda_1) - c(\lambda_2)$ from fits of

$$\begin{aligned} \Delta S_1(\lambda_1, \lambda_2) &\equiv \frac{S_1(\lambda_2)|_{R_2=\text{const}}}{S_1(\lambda_1)|_{R_2=\text{const}}} \\ &= \frac{a(\lambda_2)}{a(\lambda_1)} \{1 + [c(\lambda_2) - c(\lambda_1)] L^{-\omega} + \dots\}. \end{aligned} \quad (50)$$

In the ϕ^4 model we take $\lambda_1=1.9$, $\lambda_2=2.3$, and $\lambda=2.07$ and fix $\omega=0.785$. The same formulas hold in the ddXY model: we take $D_1=0.9$, $D_2=1.2$, $D=1.02$.

TABLE V. Fits to *Ansatz* (50) of S_{U_4} at $R_Z=0.3202$ for the ddXY model, where we have used $D_1=0.9$ and $D_2=1.2$. We fix $\omega=0.785$. L_{\min} and L_{\max} are the minimal and maximal lattice sizes included in the fit.

L_{\min}	L_{\max}	$a(D=1.2)/a(D=0.9)$	$c(D=1.2)-c(D=0.9)$	χ^2/DOF
6	12	0.9811(4)	-0.0735(18)	1.4
6	24	0.9809(2)	-0.0723(12)	1.0
8	24	0.9806(3)	-0.0699(21)	0.9
10	24	0.9803(5)	-0.0677(33)	1.1
12	24	0.9803(7)	-0.0672(54)	0.3

As an example, let us discuss the determination of the linear coefficient c_1 for S_{U_4} at $R_Z=0.3202$. In Table V we report some results of fits with *Ansatz* (50). They are quite stable when L_{\min} and L_{\max} are varied. This indicates that leading scaling corrections dominate in the difference and that subleading corrections vary little with D . As our final result we take

$$c(D=1.2) - c(D=0.9) = -0.067(7), \quad (51)$$

which should take into account both statistical and systematic errors. The error due to the uncertainty on ω as well as the error due to the linear approximation are negligible. We repeat this procedure for all quantities of interest. Typically, the amplitude differences analogous to (51) can be deter-

mined with an error of approximately 10% for the ddXY model and 15% for the ϕ^4 model.

To determine ν , we fitted the data of $S_1=S_{U_4}$ at $R_2=R_Z=0.3202$ to

$$S_1|_{R_2=\text{const}} \equiv \left. \frac{\partial R_1}{\partial \beta} \right|_{R_2=\text{const}} = aL^{1/\nu} \quad (52)$$

and

$$S_1|_{R_2=\text{const}} = aL^{1/\nu}(1 + eL^{-\omega_2}), \quad (53)$$

where we consider either $\omega_2=1.8$ or $\omega_2=2$. Assuming that there are no leading scaling corrections, the fits of the original data at $\lambda=2.07$ and $D=1.02$ give the result $\nu=0.67181(12)$ and $0.67195(13)$ for $\lambda=2.07$ and $D=1.02$, respectively. The errors take into account the results obtained by using the two *Ansätze* and the L_{\min} dependence.

In order to evaluate the effect of the residual leading corrections to scaling, we repeat the same fits for $S_{1,\text{imp}}$ computed by using Eq. (48). We obtain estimates of ν that are smaller by roughly 0.0002. This change depends slightly on the *Ansatz* and L_{\min} . These results allow us to give an effective estimate of ν as a function of D and λ , the λ and D dependence being due to the residual leading corrections to scaling that are not taken into account in the fit. Since the estimates of the improved quantities correspond approximately to those that would be obtained by using data at $\lambda=\lambda^*$ or $D=D^*$, we obtain

$$\nu = \begin{cases} 0.67181(12) - 0.0022(3) \times (\lambda - 2.07) & \text{for the } \phi^4 \text{ model,} \\ 0.67195(13) - 0.0061(9) \times (D - 1.02) & \text{for the ddXY model.} \end{cases} \quad (54)$$

The λ and D dependence is that corresponding to the fit without corrections with $L_{\min}=16$. The error on the linear coefficient is due to the error on c_1 [cf. Eq. (48)]. Using the estimates $\lambda^*=2.15(5)$ and $D^*=1.06(2)$, we obtain the results

$$\nu = \begin{cases} 0.67163(12)[11] & \text{for the } \phi^4 \text{ model,} \\ 0.67171(13)[12] & \text{for the ddXY model,} \end{cases} \quad (56)$$

where the first error is statistical and the second one is due to the uncertainty on λ^* and D^* . The analysis of S_{U_4} at $R_\xi=0.5925$ gives analogous results. Other quantities provide consistent, but less precise, estimates.

Finally, we analyze the derivative $S_{R_Y} \equiv \partial R_Y / \partial \beta$ of the helicity modulus. In this case subleading corrections are smaller when considering the data at $\beta=\beta_c$, rather than at a fixed phenomenological coupling. Since we have only a few data for the ϕ^4 model at $\lambda=2.07$, we give results only for the ddXY model. We first compute the improved slopes $S_{R_Y,\text{imp}}$ by using Eq. (48). Fits to the *Ansatz* $S=aL^{1/\nu}$ have a small χ^2/DOF already from rather small L_{\min} , indicating that subleading corrections are rather small in this quantity. Fitting

the data with $16 \leq L \leq 128$, we obtain $\nu=0.67200(15)$ at $D=1.02$ and $\nu=0.67173(15)$ at $D=1.06$ (more precisely, for the improved quantity $S_{R_Y,\text{imp}}$). Therefore, taking also into account the error on D^* , we might quote $\nu=0.6717(3)$ as a final result of this analysis, which agrees with the results (56) and (57). We have also checked the dependence of this result on the estimate of β_c , finding that the error due to the uncertainty of β_c is definitely smaller than the error on ν quoted above.

I. Eliminating leading scaling corrections from the derivative of phenomenological couplings

We now consider a combination of the derivative $S_i \equiv \partial R_i / \partial \beta$ of two phenomenological couplings R_i , at β_c or at fixed R_j ,

$$|S_1(\lambda)|^p |S_2(\lambda)|^{1-p}, \quad (58)$$

and show that one can choose a value p such that this quantity is improved—no leading corrections to scaling—for any

λ or D . Moreover, the computation of p does not rely on any estimate of ω .

For $L \rightarrow \infty$, S_i at β_c or at a fixed R_j , behaves as

$$S_i(\lambda) = a_i(\lambda)L^{1/\nu}[1 + c_i(\lambda)L^{-\omega} + \dots]. \quad (59)$$

Therefore, we have

$$\begin{aligned} & |S_1(\lambda)|^p |S_2(\lambda)|^{1-p} \\ &= |a_1(\lambda)|^p |a_2(\lambda)|^{1-p} \\ & \times L^{1/\nu} \{1 + [pc_1(\lambda) + (1-p)c_2(\lambda)]L^{-\omega} + \dots\}. \end{aligned} \quad (60)$$

An improved quantity is obtained by taking $p=p^*$, where

$$p^*c_1(\lambda) + (1-p^*)c_2(\lambda) = 0. \quad (61)$$

Note that, since the ratios $c_1(\lambda)/c_2(\lambda)$ are universal, thus independent of λ (or D), also the optimal value p^* is universal.

Now we show how p^* can be accurately computed. We consider ratios of $S_i(\lambda)$ at different values of λ :

$$\frac{S_i(\lambda_2)}{S_i(\lambda_1)} = \frac{a_i(\lambda_2)}{a_i(\lambda_1)} \{1 + [c_i(\lambda_2) - c_i(\lambda_1)]L^{-\omega} + \dots\}. \quad (62)$$

Due to the universality of the amplitude ratios we have

$$\frac{c_2(\lambda_1)}{c_1(\lambda_1)} = \frac{c_2(\lambda_2)}{c_1(\lambda_2)} = \frac{c_2(\lambda_2) - c_2(\lambda_1)}{c_1(\lambda_2) - c_1(\lambda_1)}. \quad (63)$$

Therefore,

$$\begin{aligned} & \left[\frac{S_1(\lambda_2)}{S_1(\lambda_1)} \right]^p \left[\frac{S_2(\lambda_2)}{S_2(\lambda_1)} \right]^{1-p} \\ &= \left[\frac{a_1(\lambda_2)}{a_1(\lambda_1)} \right]^p \left[\frac{a_2(\lambda_2)}{a_2(\lambda_1)} \right]^{1-p} (1 + \{p[c_1(\lambda_2) - c_1(\lambda_1)] \\ & + (1-p)[c_2(\lambda_2) - c_2(\lambda_1)]\}L^{-\omega} + \dots). \end{aligned} \quad (64)$$

We can obtain the desired value of p^* by imposing that the combination

$$\left[\frac{S_1(\lambda_2)}{S_1(\lambda_1)} \right]^p \left[\frac{S_2(\lambda_2)}{S_2(\lambda_1)} \right]^{1-p} \quad (65)$$

is L independent. This procedure does not require any knowledge of ω and assumes only that leading scaling corrections dominate in the considered range of lattice sizes.

The optimal pair of slopes S_i turns out to be

$$S_1 = \left. \frac{\partial R_Z}{\partial \beta} \right|_{R_Z=0.3202}, \quad S_2 = \left. \frac{\partial U_4}{\partial \beta} \right|_{R_Z=0.3202}, \quad (66)$$

essentially because the amplitudes of their leading scaling corrections have opposite signs. In order to determine the corresponding value of p^* , we perform fits with *Ansatz* (65) using the data at $\lambda_1=1.9$ and $\lambda_2=2.3$ for the ϕ^4 model, and at $D_1=0.9$ and $D_2=1.2$ for the ddXY model. Some results are reported in Table VI. The estimates of p^* from the two models are consistent, as required by universality. We take $p^*=0.72(3)$ as our final estimate (from fits with $L_{\min}=8$, while the error is estimated by varying the fit range).

TABLE VI. Fits to *Ansatz* (65) of the improved combination of S_{U_4} and S_{R_Z} at $R_Z=0.3202$. L_{\min} and L_{\max} are the minimal and maximal lattice sizes included in the fit. For a detailed discussion, see the text.

Model	L_{\min}	L_{\max}	p^*	χ^2/DOF
ϕ^4	6	12	0.703(11)	0.93
	8	24	0.718(11)	1.37
	12	24	0.744(30)	1.61
ddXY	6	12	0.736(6)	1.87
	8	24	0.720(8)	1.29
	12	24	0.702(19)	0.02

Using this estimate for p^* , we construct the improved combinations (60) at $\lambda=2.07$ for the ϕ^4 model and at $D=1.02$ for the ddXY model. Since these values of λ and D are close to the optimal values λ^* and D^* , leading scaling corrections are quite small. Therefore, the uncertainty on p^* is negligible with respect to the final error of our estimate for ν . In Fig. 5 we show results for the exponent ν obtained by fits to the functions $aL^{1/\nu}$ and to $aL^{1/\nu}(1+eL^{-\omega_2})$ with $\omega_2=1.8$, for several values of L_{\min} . Guided by Fig. 5, we take

$$\nu = \begin{cases} 0.6718(2) & \text{for the } \phi^4 \text{ model,} \\ 0.6717(3) & \text{for the ddXY model} \end{cases} \quad (67)$$

as our final estimates. Moreover, combined fits applied to both ϕ^4 and ddXY models give the estimate $\nu=0.6718(2)$.

As a further check, we apply this method to the standard XY model, where leading corrections to scaling are large. In Fig. 6 we show results for the critical exponent ν from MC simulations of the standard XY model up to $L=96$, as obtained by fits to the simple *Ansatz* $S=aL^{1/\nu}$ of the data of S_{R_Z} at $R_Z=0.3202$, S_{U_4} at $R_Z=0.3202$, and their combination (60) at $p=p^*=0.72$. The first two sets of results clearly disagree with the estimate of ν from improved Hamiltonians and also between themselves (thus, they are inconsistent). Instead, the analysis of their improved combination provides perfectly consistent results, giving further support for the validity of the method and confirming the accurate determination of p^* .

J. The critical exponent ν from the finite-size scaling of the energy density

We also derive estimates of ν from the FSS of the energy density. On finite lattices of size L^3 , the free energy density behaves as

$$f(\beta, L) = f_{ns}(\beta) + f_s(\beta, L), \quad (69)$$

where the nonsingular part of the free energy density f_{ns} does not depend on L , apart from exponentially small contributions. The singular part is expected to behave as

$$f_s(\beta, L) = L^{-d} g(tL^{1/\nu}, u_3L^{-\omega}, \dots). \quad (70)$$

The energy density is obtained by taking the derivative with respect to β ,

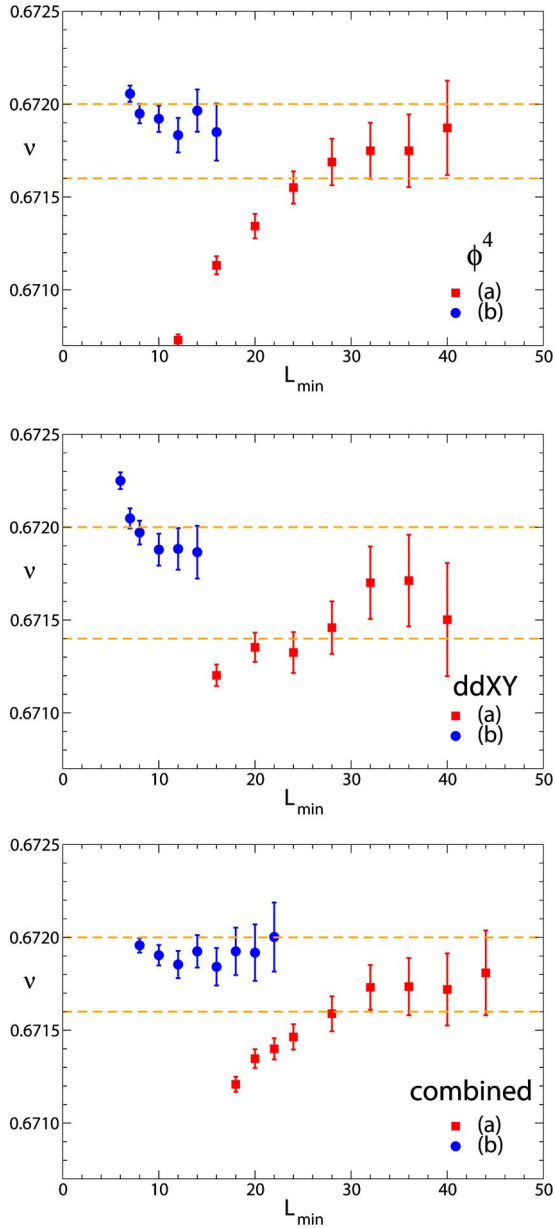


FIG. 5. (Color online) Results for the exponent ν obtained by fits of the improved combination (58) using the quantities (66), for several values of L_{\min} : (a) to $aL^{1/\nu}$ and (b) to $aL^{1/\nu}(1+eL^{-\omega_2})$ with $\omega_2=1.8$.

$$E(\beta, L) = E_{ns}(\beta) + L^{-d+1/\nu} g_e(tL^{1/\nu}, u_3 L^{-\omega}, \dots) + \dots \quad (71)$$

Setting $\beta = \beta_c$,⁴⁰ we obtain for $L \rightarrow \infty$ the expansion

$$E(\beta_c, L) = E_{ns}(\beta_c) + aL^{-d+1/\nu}(1 + cL^{-\omega}) + \dots \quad (72)$$

In Fig. 7 we show the results of the fits to Eq. (72) without correction terms (i.e., with $c=0$) for the ϕ^4 and ddXY models, respectively, at $\lambda=2.07$ and $D=1.02$. Our final estimates of ν from the scaling of the energy density (obtained from fits of data for $12 \leq L \leq 128$) are

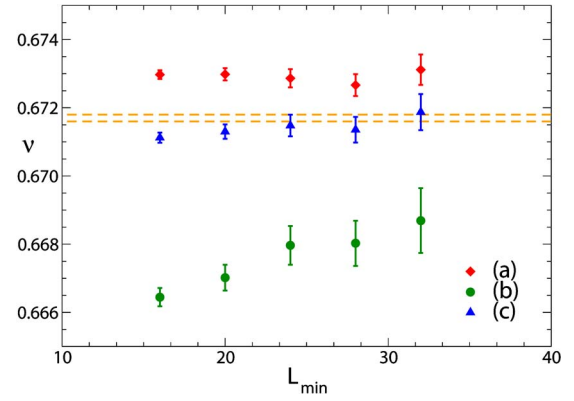


FIG. 6. (Color online) Results for the critical exponent ν from MC simulations of the standard XY model, as obtained by fits of the data of the derivative of R_Z at $R_Z=0.3202$ (a), the derivative of U_4 at $R_Z=0.3202$ (b), and by using the method that combines them to eliminate the residual leading scaling corrections (c). The two dashed lines correspond to our final estimate $\nu=0.6717(1)$.

$$\nu = \begin{cases} 0.6717(2) & \text{for the } \phi^4 \text{ model,} \\ 0.6715(3) & \text{for the ddXY model.} \end{cases} \quad (73)$$

Our data at $\lambda=1.9, 2.3$ in the case of the ϕ^4 model and $D=0.9, 1.2$ for the ddXY model are not sufficient to get a reliable estimate of the systematic error due to the leading scaling corrections. However, we can estimate it by a comparison with the standard XY model. Fitting the data of the standard XY model to the simplest *Ansatz* without scaling corrections (using the value of β_c reported in Table II and data for $8 \leq L \leq 96$), we obtain $\nu=0.6701(2)$, i.e., the exponent is underestimated by approximately 0.0015. We may use this difference to estimate the leading scaling-correction amplitude in the improved model. Taking into account that the largest lattice for the XY model has $L=96$ instead of $L=128$, we obtain $c \approx 0.0015 \times (128/96)^{-0.785} = 0.0012$, where we have also taken into account the difference of the sizes L used in the fits. Since the leading correction amplitudes at $D=1.02$ and $\lambda=2.07$ should be smaller by a factor of approximately 20 than in the standard XY model, we may have

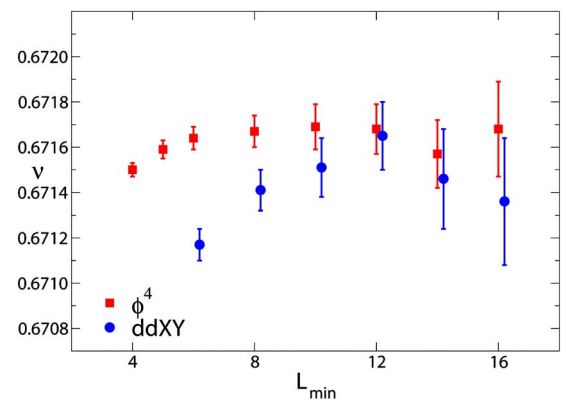


FIG. 7. (Color online) Results of fits for the FSS of the energy for the ϕ^4 model at $\lambda=2.07$ and the ddXY model at $D=1.02$.

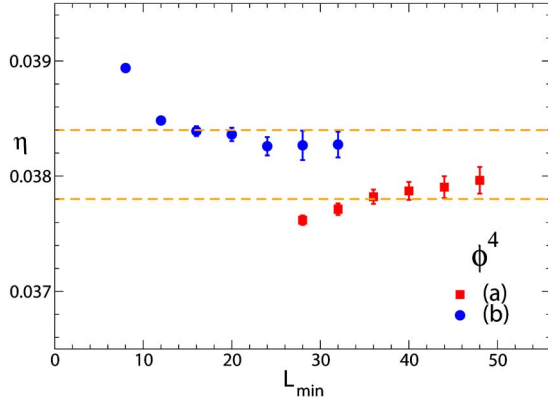


FIG. 8. (Color online) Results for the exponent η obtained by fits of χ_{imp} for several values of L_{min} : (a) to $aL^{1/\nu}$ and (b) to $aL^{1/\nu}(1+eL^{-\omega_2})$ with $\omega_2=1.8$. The dashed lines indicate our final FSS estimate $\eta=0.0381(3)$.

a shift by 0.000 06 in our estimates (73) and (74) for ν due to leading corrections, which is much smaller than their errors.

K. The critical exponent η

We compute the critical exponent η from the FSS behavior of the magnetic susceptibility χ either at $R_Z=0.3202$ or at $R_\xi=0.5925$. As in the analyses of the derivatives S_R , we first compute an improved quantity for χ that does not have leading scaling corrections. Since

$$\chi = aL^{2-\eta}(1 + cL^{-\omega} + \dots), \quad (75)$$

close to the improved value λ^* where c is small and a linear approximation $c(\lambda) = c_1(\lambda - \lambda^*)$ suffices, we can take

$$\chi_{\text{imp}} = \chi(\lambda)[1 - c(\lambda)L^{-\omega}] \approx \chi(\lambda)[1 - c_1(\lambda - \lambda^*)L^{-\omega}]. \quad (76)$$

To compute c_1 we consider the ratio

$$\frac{\chi(\lambda_2)|_{R_Z=0.3202}}{\chi(\lambda_1)|_{R_Z=0.3202}} \approx \frac{a(\lambda_2)}{a(\lambda_1)} \{1 + [c(\lambda_2) - c(\lambda_1)]L^{-\omega} + \dots\} \quad (77)$$

with $\lambda_1=1.9$ and $\lambda_2=2.3$. Fits to Eq. (77) allow us to estimate

$$c_1 = \left. \frac{\partial c}{\partial \lambda} \right|_{\lambda=\lambda^*} \approx \frac{c(\lambda=2.3) - c(\lambda=1.9)}{2.3 - 1.9}. \quad (78)$$

Analogous equations can be written for the ddXY model and at fixed R_ξ .

Then, we fitted the data for the improved χ [we use $\lambda=2.07$ in Eq. (76)] using the *Ansätze*

$$\chi_{\text{imp}}|_{R_Z=0.3202} = aL^{2-\eta}, \quad (79)$$

$$\chi_{\text{imp}}|_{R_Z=0.3202} = aL^{2-\eta}(1 + eL^{-\omega_2}), \quad (80)$$

where we fix either $\omega_2=1.8$ or $\omega_2=2$. In Fig. 8 we show the results of the fits of $\chi_{\text{imp}}|_{R_Z=0.3202}$ for the ϕ^4 model vs the

minimum value L_{min} of L allowed in the fits. Similar results are obtained for the ddXY model, using $D=1.02$ in Eq. (76). In all cases, the fits with *Ansatz* (79) have a large χ^2/DOF for $L_{\text{min}} \leq 40$. Moreover, the resulting values of η appear to slightly increase with increasing L_{min} . In contrast, the fits allowing for subleading corrections are more stable and give a χ^2/DOF close to 1 already for $L_{\text{min}} \geq 10$. We also mention that fixing R_ξ instead of R_Z gives slightly lower values for η , by about 0.000 05 for the fit to (79), and 0.000 15 for the fits to (80). A comparison of $\lambda=2.07$ and $\lambda=2.15$ indicates that a possible error due to the uncertainty of λ^* should be approximately 0.000 05. Our final FSS estimate obtained from both ϕ^4 and ddXY models is

$$\eta = 0.0381(3). \quad (81)$$

V. CRITICAL EXPONENTS FROM IMPROVED HIGH-TEMPERATURE EXPANSIONS

A. High-temperature expansions

High-temperature expansion in powers of the inverse temperature β is one of the most effective lattice approaches to investigate the critical behavior in the HT phase. We consider a general class of models defined on a simple cubic lattice by the Hamiltonian

$$\mathcal{H} = -\beta \sum_{\langle xy \rangle} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x V(\vec{\phi}^2), \quad (82)$$

where $\beta \equiv 1/T$, $\langle xy \rangle$ indicates nearest-neighbor sites, $\vec{\phi}_x = (\phi_x^{(1)}, \phi_x^{(2)})$ is a two-component real variable, and $V(\vec{\phi}^2)$ is a generic potential satisfying appropriate stability constraints.

Using the linked-cluster expansion technique (see Refs. 5 and 39 for details), we extended the HT computations of Ref. 5 by adding a few terms in the HT series. The two main steps of the algorithm are the generation of the graphs and the evaluation of the contribution of each graph. The first step is limited by memory, and was performed on a computer with 16 Gbytes of RAM. The second step is limited by processing time; it was parallelized and required approximately 4 years of CPU time on a single 2.0 GHz Opteron processor. We computed the 22nd-order HT expansion of the magnetic susceptibility and of the second moment of the two-point function

$$\chi = \sum_x \langle \phi_\alpha(0) \phi_\alpha(x) \rangle,$$

$$m_2 = \sum_x x^2 \langle \phi_\alpha(0) \phi_\alpha(x) \rangle, \quad (83)$$

and therefore, of the second-moment correlation length

$$\xi^2 = \frac{m_2}{6\chi}. \quad (84)$$

Moreover, we computed the HT expansion of some zero-momentum connected $2j$ -point Green's functions χ_{2j} ,

$$\chi_{2j} = \sum_{x_2, \dots, x_{2j}} \langle \phi_{\alpha_1}(0) \phi_{\alpha_1}(x_2) \cdots \phi_{\alpha_j}(x_{2j-1}) \phi_{\alpha_j}(x_{2j}) \rangle_c \quad (85)$$

($\chi = \chi_2$). We computed χ_4 to 20th order, χ_6 and χ_8 to 18th order.

The HT series for the general model (82) are reported in Ref. 14. In the following we will restrict ourselves to the ϕ^4 and ddXY models [cf. Eqs. (9) and (10)].

B. Critical exponents from the analysis of the HT expansion of improved models

In our analysis of the HT series we consider quasideagonal first-, second-, and third-order integral approximants (IA1's, IA2's, and IA3's, respectively), and in particular biased IA n 's (bIA n 's) using the most precise available estimate of β_c . The FSS estimates of β_c are reported in Table II. We refer to Ref. 5, and in particular to its Appendix B, for details on the HT analysis and the precise definition of the various integral approximants. A review of methods for the analysis of HT series can be found in Ref. 41.

The leading nonanalytic corrections are the dominant source of systematic errors in HT studies. Indeed, nonanalytic corrections introduce large and dangerously undetectable systematic deviations in the results of the analysis. Integral approximants can in principle cope with an asymptotic behavior of the form (13); however, in practice, they are not very effective when applied to the series of moderate length available today. As shown in Refs. 5, 23, and 25, analyses of the HT series for the improved models lead to a significant improvement in the estimates of the critical exponents and of other infinite-volume HT quantities. The crux of the method is a precise determination of the improved value of the parameter appearing in the Hamiltonian. In this respect FSS techniques appear quite effective, as we have shown in the preceding section. A further improvement is achieved by biasing the HT analysis using the available estimates of β_c .

Our working hypothesis is that, with the series of current length, the systematic errors, i.e., the systematic deviations that are not taken into account in the HT analysis, are largely due to the leading nonanalytic corrections, especially when they are characterized by a relatively small exponent, as is the case in the 3D XY universality class where $\Delta = \omega\nu \approx 0.53$. Therefore, improved models are expected to give results with smaller and, more importantly, reliable error estimates. The systematic errors in our analyses are related either to next-to-leading nonanalytic scaling corrections or to our approximate knowledge of λ^* and D^* . Since $\Delta_2 = \omega_2\nu \approx 1.2$, we will assume that next-to-leading corrections do not play much role, and we will take into account only the residual leading corrections proportional to $\lambda - \lambda^*$ ($D - D^*$ for the ddXY model). Of course, this hypothesis requires stringent checks. A nontrivial check is achieved by comparing the results obtained using different improved models: If the hypothesis is correct, they should agree within error bars.

As an additional check of our results we compare IA1's of the 22nd-order HT series of χ and ξ^2 with high-statistics MC results. We simulated the ϕ^4 model at $\lambda = 2.1, 2.2$ and the

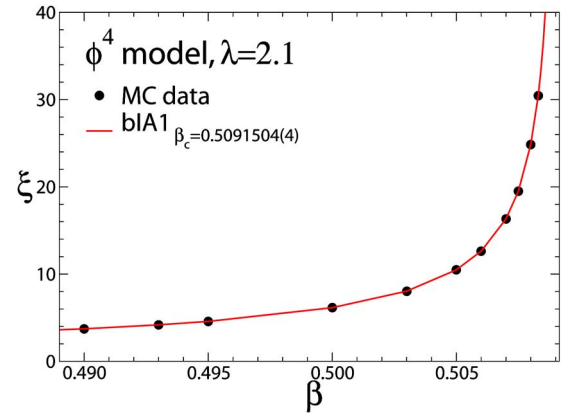


FIG. 9. (Color online) High-temperature MC data for the correlation length of the ϕ^4 model at $\lambda=2.1$, and the result of the fit using bIA1 of the 22nd-order HT series of ξ^2 .

ddXY model at $D=1.02, 1.2$ in the HT phase ($\beta < \beta_c$). We alternate single-cluster updates and local Metropolis and overrelaxation updates. In order to obtain negligible finite-size effects (i.e., orders of magnitude smaller than the statistical errors), we used lattices of size $L > 10\xi$ throughout. We obtained infinite-volume estimates up to $\xi \approx 30$ on a 350^3 lattice.

In Fig. 9 we show MC data for the ϕ^4 model at $\lambda=2.1$ from $\beta=0.493$, where $\xi=4.1825(2)$, to the largest β value $\beta=0.5083$, where $\xi=30.453(10)$. bIA1's using the FSS estimate $\beta_c=0.5091503(5)$ provide perfectly consistent results, for example $\xi=30.449(1)[7]$, where the first error is related to the spread of the approximants and the second one to the uncertainty on β_c . We also obtain an independent estimate of β_c by fitting the MC data of ξ to bIA1's with β_c taken as a free parameter. The resulting estimate $\beta_c=0.5091504(4)$ (with $\chi^2/\text{DOF} \approx 0.9$) is perfectly consistent with the FSS estimate. The corresponding curve is drawn in Fig. 9. An identical result, i.e., $\beta_c=0.5091504(4)$, is found by fitting the MC data of χ , which shows that the agreement with the FSS analysis is not just by chance. We performed similar analyses also for $\lambda=2.2$, and in the case of the ddXY model for $D=1.02$ and 1.20 . The results denoted by MC+HT are reported in Table II. The comparison with the FSS estimates is satisfactory overall. This successful analysis should be contrasted with the case of the standard XY model, where the fit of the MC results in the HT phase by bIA1 does not provide acceptable results: indeed, most of the approximants are defective. This fact may be explained by the presence of sizable leading scaling corrections.

In order to determine the critical exponents γ and ν , we analyze the 22nd-order series of χ and 21st-order series of ξ^2/β , respectively, using bIA n 's with $n=1, 2, 3$ biased at the best available estimate of β_c . Estimates of the exponent η can be obtained by using the scaling relation $\eta=2-\gamma/\nu$. More precise estimates of the product $\eta\nu$ can be obtained by using the so-called critical-point renormalization method (CPRM) applied to the series of χ and ξ^2/β (see Ref. 5 for details). For the ϕ^4 and ddXY models we performed analyses at different values of the λ and D to determine the dependence of the effective exponents on λ and D due to the

TABLE VII. Results for the exponents γ , ν , and $\eta\nu$ as obtained by using bIAn.

Model	β_c	Approximants	γ	ν	$\eta\nu$ from CPRM
ϕ^4 , $\lambda=1.90$	0.5105799(7)	bIA1	1.31718(3)[10]	0.67116(10)[3]	0.02531(4)
		bIA2	1.31726(8)[12]	0.67119(5)[3]	0.02527(10)
		bIA3	1.31723(3)[11]	0.67118(14)[4]	0.02528(5)
ϕ^4 , $\lambda=2.07$	0.5093835(5)	bIA1	1.31757(2)[7]	0.67153(4)[3]	0.02553(5)
		bIA2	1.31759(4)[7]	0.67155(6)[3]	0.02552(12)
		bIA3	1.31758(2)[7]	0.67153(5)[3]	0.02552(4)
ϕ^4 , $\lambda=2.10$	0.5091504(4)	bIA1	1.31767(3)[6]	0.67160(3)[2]	0.02557(5)
		bIA2	1.31769(5)[5]	0.67163(6)[2]	0.02556(12)
		bIA3	1.31767(3)[5]	0.67160(4)[2]	0.02556(5)
ϕ^4 , $\lambda=2.20$	0.5083355(7)	bIA1	1.31787(2)[8]	0.67178(2)[5]	0.02569(6)
		bIA2	1.31789(5)[10]	0.67181(7)[5]	0.02567(12)
		bIA3	1.31788(5)[9]	0.67179(4)[4]	0.02569(5)
ddXY, $D=1.02$	0.5637963(4)	bIA1	1.31757(15)[5]	0.67141(4)[3]	0.02547(5)
		bIA2	1.31746(9)[4]	0.67143(6)[2]	0.02550(23)
		bIA3	1.31745(12)[5]	0.67149(9)[3]	0.02533(19)
ddXY, $D=1.03$	0.5627975(13)	bIA1	1.31767(15)[15]	0.67148(4)[7]	0.02550(4)
		bIA2	1.31756(9)[14]	0.67150(5)[6]	0.02552(23)
		bIA3	1.31755(10)[15]	0.67155(8)[9]	0.02537(18)
ddXY, $D=1.20$	0.5470388(11)	bIA1	1.31871(5)[14]	0.67227(8)[7]	0.02602(4)
		bIA2	1.31872(11)[13]	0.67232(10)[6]	0.02597(28)
		bIA3	1.31868(13)[13]	0.67224(10)[8]	0.02575(52)

residual leading corrections to scaling that are not taken into account in the analysis. In Table VII we report some intermediate results, i.e., the results for each bIAn analysis, which will then lead us to our final estimates reported below. We closely follow Ref. 5, so we refer to it for details. We only mention that the set of bIAn's that we consider are those with $q=2$, $s=1/2$, $n_\sigma=2$ in the definitions reported in Ref. 5.

In the case of the ϕ^4 model, using the results of the bIAn analysis at $\lambda=2.10$ and $\lambda=2.20$, and assuming a linear dependence on λ in between, we obtain the IHT results

$$\begin{aligned}\nu &= 0.671\ 61(4)[2] + 0.0018(\lambda - 2.10), \\ \gamma &= 1.317\ 68(3)[5] + 0.0021(\lambda - 2.10), \\ \eta\nu &= 0.025\ 56(5) + 0.0013(\lambda - 2.10).\end{aligned}\quad (86)$$

The central value at $\lambda=2.1$ is taken from the bIA2 and bIA3 analyses, the number in parentheses is basically the spread of the approximants at $\lambda=2.10$ using the central value of β_c [we use $\beta_c=0.509\ 150\ 4(4)$], while the number in brackets gives the systematic error due to the uncertainty on β_c . The dependence of the results on the chosen value of λ is estimated by assuming a linear dependence, and evaluating the coefficient from the results for $\lambda=2.2$ and $\lambda=2.1$, i.e., from the ratio $[Q(\lambda=2.2)-Q(\lambda=2.1)]/0.1$, where Q represents the quantity at hand. Consistent results are obtained by using the pair of values 2.07, 2.20 or 1.90, 2.10 instead of 2.10, 2.20. In the case of the ddXY model, using the results of the bIAn analysis at $D=1.02$ and 1.20, we obtain

$$\nu = 0.671\ 45(6)[2] + 0.0046(D - 1.02),$$

$$\gamma = 1.317\ 46(11)[5] + 0.0070(D - 1.02),$$

$$\eta\nu = 0.025\ 47(14) + 0.0031(D - 1.02).\quad (87)$$

An alternative and more straightforward analysis of HT series is represented by the matching method, which was applied in Refs. 23 and 42 for the two- and three-dimensional Ising models. The idea is to generate sequences of estimates by fitting the expansion coefficients with their asymptotic form. By adding a sufficiently large number of terms one may improve the convergence, although, of course, the procedure becomes unstable if the number of terms included is too large compared to the number of available terms. The estimates of the critical exponents from this analysis are consistent with the bIAn results and with the fact that the ϕ^4 model at $\lambda \approx 2.1$ and the ddXY model at $D \approx 1.1$ are approximately improved, i.e., the coefficients of the leading scaling corrections are consistent with zero. However, the results of this analysis are not sufficiently stable and precise to improve the estimates already obtained.

Estimates of the critical exponents can be then obtained by evaluating Eqs. (86) and (87) at the FSS estimates of λ^* , i.e., $\lambda^*=2.15(5)$, and D^* , i.e., $D^*=1.06(2)$, where the residual effect of the leading scaling correction should vanish. We refer to these results as MC+IHT estimates. For the ϕ^4 theory we obtain

$$\begin{aligned}\nu &= 0.671\,70(4)[2]\{9\}, \\ \gamma &= 1.317\,79(3)[5]\{11\}, \\ \eta &= 0.038\,16(7)\{10\}\end{aligned}\quad (88)$$

and using the scaling and hyperscaling relations

$$\begin{aligned}\alpha &= 2 - 3\nu = -0.015\,10(12)[6]\{27\}, \\ \eta &= 2 - \gamma/\nu = 0.038\,13(15)\{10\}.\end{aligned}\quad (89)$$

The error due to the uncertainty on λ^* is reported in braces. For the ddXY model we obtain

$$\begin{aligned}\nu &= 0.671\,63(6)[2]\{9\}, \\ \gamma &= 1.317\,74(11)[5]\{14\}, \\ \eta &= 0.038\,11(20)\{9\},\end{aligned}\quad (90)$$

and

$$\begin{aligned}\alpha &= -0.014\,89(18)[6]\{27\}, \\ \eta &= 2 - \gamma/\nu = 0.038\,00(25)\{6\}.\end{aligned}\quad (91)$$

There is good agreement between the MC+IHT estimates obtained from the ϕ^4 and ddXY models. We stress that this represents a nontrivial check of the hypotheses underlying the IHT analysis. In particular, this supports our working hypothesis that effects due to next-to-leading nonanalytic corrections are negligible. Finally, estimates of the critical exponents δ and β can be obtained using the hyperscaling relations $\delta = (5 - \eta)/(1 + \eta)$ and $\beta = \nu(1 + \eta)/2$.

C. Combining IHT and FSS analyses

Critical exponents can be also estimated by comparing Eqs. (86) and (87) with the analogous FSS results (54) and (55) obtained from the MC data of S_{U_4} . We note that the coefficients that give the dependence on λ and D in the IHT and FSS expressions have opposite signs. Therefore, the results of the two analyses agree only in a relatively small λ (or D) interval. This is shown in Fig. 10. This comparison provides an estimate of ν that is independent of the determination of the optimal values λ^* , D^* . Taking the values consistent with both the IHT and FSS analyses as estimates of ν , we obtain the following FSS+IHT results

$$\nu = \begin{cases} 0.67168(10) & \text{for the } \phi^4 \text{ model,} \\ 0.67167(15) & \text{for the ddXY model.} \end{cases}\quad (92)$$

$$\nu = \begin{cases} 0.67168(10) & \text{for the } \phi^4 \text{ model,} \\ 0.67167(15) & \text{for the ddXY model.} \end{cases}\quad (93)$$

The good agreement between the two results nicely supports our estimates of the errors. The FSS+IHT results represent our most precise estimates of the critical exponent ν . Corresponding estimates of α can be obtained using the scaling relation $\alpha = 2 - 3\nu$.

Note that this analysis also provides alternative estimates of λ^* and D^* . The intersection region in Fig. 10 indicates $\lambda^* = 2.14(5)$ and $D^* = 1.07(3)$, which are in good agreement with those obtained in Sec. IV F.

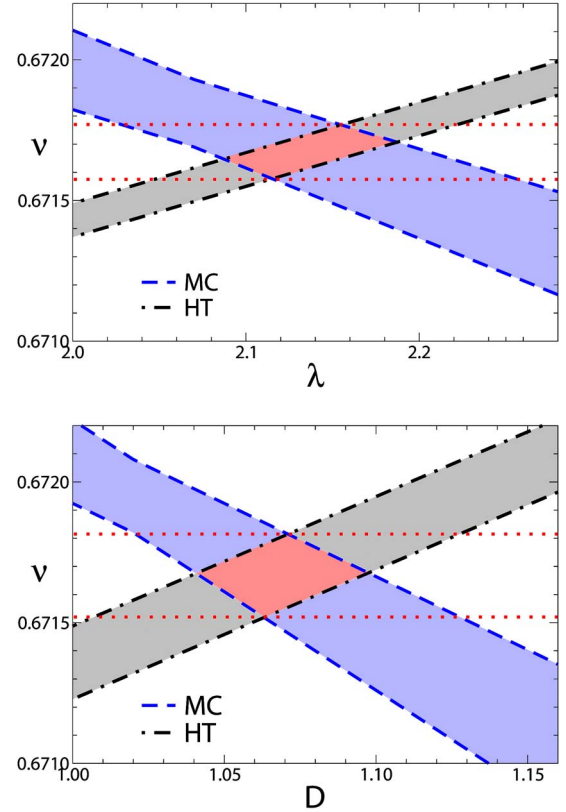


FIG. 10. (Color online) Comparison of the HT and FSS results for the critical exponent ν as a function of the parameters λ , D around their optimal values. The dotted lines correspond to the estimates of ν that are consistent with both the IHT and FSS analyses.

D. Universal amplitude ratios

Using HT methods, it is possible to compute the first coefficients g_{2j} and r_{2j} appearing in the small-magnetization expansion of the Helmholtz free energy and of the equation of state.⁴ Indeed, these quantities can be expressed in terms of zero-momentum $2j$ correlation functions and of the correlation length. They are defined as

$$g_4 \equiv -\frac{3}{2} \frac{\chi_4}{\chi^2 \xi^3}, \quad (94)$$

and

$$r_6 \equiv 10 - \frac{10}{9} \frac{\chi_6 \chi_2}{\chi^4},$$

$$r_8 \equiv 280 - \frac{560}{9} \frac{\chi_6 \chi_2}{\chi^4} + \frac{35}{27} \frac{\chi_8 \chi_2^2}{\chi^3}, \quad (95)$$

etc.

Using their extended HT series, we update the estimates of g_4 , r_6 , and r_8 obtained in Ref. 5. Consider a universal amplitude ratio A which, for $t \equiv 1 - \beta/\beta_c \rightarrow 0$, behaves as

$$A(t) = A^* + c_1 t^\Delta + c_2 t^{\Delta^2} + \cdots + a_1 t + a_2 t^2 + \cdots. \quad (96)$$

TABLE VIII. Estimates of the fixed-point value of g_4 from the 20th-order HT series of $\beta^{3/2}g_4$. The error due to the uncertainty of β_c is negligible.

Model	g_4	ζ
ϕ^4 , $\lambda=2.07$	21.149(5)	1.13(6)
ϕ^4 , $\lambda=2.10$	21.153(4)	1.16(6)
ϕ^4 , $\lambda=2.20$	21.167(4)	1.28(7)
ddXY, $D=0.90$	21.13(7)	0.9(2)
ddXY, $D=1.02$	21.15(3)	1.1(4)
ddXY, $D=1.03$	21.15(3)	1.1(3)
ddXY, $D=1.20$	21.22(2)	2.5(1.1)

In order to determine A^* from the HT series of $A(t)$, we consider bIA1's, whose behavior at β_c is given by^{5,41}

$$f(\beta)(1 - \beta/\beta_c)^\zeta + g(\beta), \quad (97)$$

where $f(\beta)$ and $g(\beta)$ are regular at β_c , except when ζ is a nonnegative integer. In the case we are considering, ζ is positive and therefore $A^* = g(\beta_c)$. Moreover, for improved Hamiltonians we expect $\zeta = \Delta_2 \approx 1.2$, instead of $\zeta = \Delta \approx 0.53$.

In the case of g_4 we analyze the series $\beta^{3/2}g_4 = \sum_{i=0}^{20} a_i \beta^i$. In Table VIII we report some results for several values of λ and D . Assuming a linear dependence on λ , D around their optimal values, we find

$$g_4 = 21.153(4) + 0.14(\lambda - 2.10) \quad (98)$$

for the ϕ^4 model, and

$$g_4 = 21.15(3) + 0.4(D - 1.03) \quad (99)$$

for the ddXY model. We estimate the critical value of g_4 by evaluating the above expressions at λ^* and D^* . We obtain respectively,

$$g_4 = 21.160(4)\{7\}, \quad g_4 = 21.16(3)\{1\}, \quad (100)$$

where the error in braces is related to the uncertainty on the estimates of λ^* and D^* . We consider $g_4 = 21.16(1)$ as our final estimate. This significantly improves our earlier result⁵ $g_4 = 21.14(6)$ and is fully consistent with the FT estimate $g_4 = 21.16(5)$ obtained from an analysis of six-loop perturbative

series.^{6,43} Other results for g_4 can be found in Ref. 4. The results for the nonanalytic exponent ζ , reported in Table VIII, give

$$\zeta = 1.16(6) + 1.3(\lambda - 2.10) \quad (101)$$

in the case of the ϕ^4 model. Evaluating ζ at $\lambda = \lambda^*$ we obtain an estimate of Δ_2 , i.e., $\Delta_2 = 1.23(6)\{7\}$, corresponding to $\omega_2 = 1.83(19)$. A consistent, but less precise, estimate can be obtained from the results for the ddXY model.

It is worth mentioning some results obtained for the analysis of the HT series of g_4 in the standard XY model. Using bIA1's, biased so that $\beta_c = 0.454\,165\,2(11)$ and $\Delta = 0.527(13)$ [corresponding to $\omega = 0.785(20)$], we obtain $g_4 = 21.12(5)$, which is in good agreement with the estimate obtained from the improved models. Moreover, if we analyze the same series biasing $\beta_c = 0.454\,165\,2(11)$ and $g_4 = 21.16(1)$ and taking scaling-correction exponent Δ as a free parameter, we obtain the estimate $\Delta = 0.56(5)$, which is in agreement with the result obtained from the FSS analysis.

Similar analyses applied to the 18th-order HT series of r_6 and r_8 provide the estimates $r_6 = 1.96(2)$ and $r_8 = 1.5(1)$, which substantially confirm those obtained in Ref. 5. These results can be used to compute approximations of the critical equation of state, using the method outlined in Refs. 5 and 44, which is based on an appropriate analytic continuation in the t, H space. Using our estimates of α , η , r_6 , and r_8 , we obtain results for the critical equation of state and universal amplitude ratios that are substantially equivalent to those obtained in Ref. 5, essentially because our HT results do not significantly improve the estimates of r_6, r_8 , and no precise and reliable estimates of the higher-order coefficients r_{2j} are available. Therefore we do not provide further details. We only report the result $R_\alpha \equiv (1 - A^+/A^-)/\alpha = 4.3(2)$ which is relevant for the superfluid transition in ^4He . For comparison, we mention the FT result⁴⁵ $R_\alpha = 4.43(8)$, the numerical MC results $R_\alpha = 4.20(5)$ (Ref. 46) and $R_\alpha = 4.01(5)$,⁴⁷ and the experimental estimate $R_\alpha = 4.154(22)$ reported in Ref. 3.

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