

Critical behavior of the Coulomb-glass model in the zero-disorder limit: Ising universality in a system with long-range interactions

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The ordering of charges on half-filled hypercubic lattices is investigated numerically, where electroneutrality is ensured by background charges. This system is equivalent to the $s=1/2$ Ising lattice model with antiferromagnetic $1/r$ interaction. The temperature dependences of specific heat, mean staggered occupation, and of a generalized susceptibility indicate continuous order-disorder phase transitions at finite temperatures in two- and three-dimensional systems. In contrast, the susceptibility of the one-dimensional system exhibits singular behavior at vanishing temperature. For the two- and three-dimensional cases, the critical exponents are obtained by means of a finite-size scaling analysis. Their values are consistent with those of the Ising model with short-range interaction, and they imply that the studied model cannot belong to any other known universality class. Samples of up to 1400, 112^2 , and 22^3 sites are considered for dimensions 1 to 3, respectively.

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I. INTRODUCTION

The long range of electrostatic correlations underlies important physical effects such as screening, charge renormalization, charge orders, and instabilities of plasmas.¹ In Coulomb glasses, disordered systems of localized charges, electrostatic correlations induce the Coulomb gap in the single-particle energy spectrum.² The question under which conditions these glasses exhibit genuine glass transitions has been under controversial debate for a long time.^{3–10,40,41}

Lattices partially occupied by charged particles have been studied as models for ionic fluids, where several phases were identified and an Ising-type liquid-gas critical point was observed.^{11–16} In particular, by means of numerical simulation and finite-size scaling, Luijten *et al.*¹² could clearly rule out this point to belong to any of several alternative universality classes. For a recent review on this field see Ref. 17. In case of full occupancy, such a lattice corresponds to an ionic crystal and provides the zero-disorder limit of the Coulomb-glass problem.

Although the ordering of ionic crystals with decreasing temperature has been studied by several groups, important questions are still open. Analytical^{14–16} and simulation results^{7,18–20} suggest that, for the case of pure Coulomb interaction, staggered (antiferromagnetic) ordering in three-dimensional simple-cubic lattices starts with a continuous phase transition. According to the hierarchical reference theory study by Brognara *et al.*¹³ and the renormalization-group investigation by Ciach,¹⁶ this transition should belong to the short-range Ising universality class in spite of the long-range interaction. This hypothesis is suggested by the transition being the end of a line of Ising transitions in the lattice restricted primitive model, which is reached for complete filling.

We remind the reader, however, that in the case of Ising models with ferromagnetic long-range interactions, the phase transition depends on dimensionality and decay exponent of the interactions. The critical indices can vary from mean-field behavior to that of the short-range Ising universality class via intermediate values.^{21,22}

The case of antiferromagnetic long-range interactions is more subtle due to their inherent frustration. From the corresponding field-theoretic approach for a staggered order, one would expect that the long-distance behavior of the interactions should renormalize to short-range couplings.¹⁴ However, this argument assumes validity of a perturbative expansion around the ground state. Thus, one discounts part of the couplings between charge or higher-order multipole fluctuations that are associated with the defects of the ordered state. In the case of Coulomb-glass systems, the interplay of such fluctuations and quenched disorder is believed to underlie glassy properties. Recently, three different analytical approaches for the screening problem in such disordered electronic systems have been developed, where two of them contain the nondisordered case as natural limit.^{8–10} In this context, precise numerical experiments on the phase transition of lattice models without disorder are called for.

The corroboration of the analytical results on the ordering of ionic crystals by numerical studies is very difficult due to the long-range interaction: Studying samples of up to 12^3 sites, Almarza and Enciso¹⁸ observed their data for simple-cubic lattices to be consistent with the assumption of short-range Ising universality. However, they could not determine the critical exponents directly because the samples were still too small. A considerable progress was reached in Refs. 19 and 20, where samples of up to 18^3 sites were considered, so that critical exponents could be obtained by finite-size scaling. The exponent values were found to be very close to the data for the short-range Ising model, but this work was presented only in a short form. Moreover, further enlarging of the sample size and diminishing of the error bars seemed desirable. Finally, Overlin *et al.*⁷ studied the influence of positional disorder at samples of up to 8^3 sites and determined the critical exponent of the localization length. For the limiting case of vanishing disorder, their numerical result was consistent with both the short-range Ising and mean-field universality classes.

The effects of unscreened interactions and frustration may become more prominent in dimensions $d=1$ and 2. However, only a few numerical studies have been devoted to the be-

havior of such systems: In a first attempt, Díaz-Sánchez *et al.*⁶ studied samples of up to 26 and 14^2 sites for $d=1$ and 2, respectively, by means of a spin-glass approach. They concluded that a phase transition at finite T exists only for $d=2$, but not for $d=1$. The behavior of considerably larger samples was simulated in Refs. 19 and 20, where a continuous phase transition at finite T was obtained for $d=2$, but not for $d=1$. In the former case, according to the obtained critical exponents, short-range Ising universality seems likely. Moreover, Luo *et al.*²³ considered two-dimensional systems with logarithmic interaction, corresponding to the interaction of homogeneously charged lines. They obtained values of the critical exponents of correlation length and order parameter which clearly differ from the short-range Ising values.

The aim of the present work is twofold: On the one hand, for $d=3$, we numerically investigate the ordering in simple-cubic systems to check the analytical theories mentioned above. The critical exponents of correlation length, order parameter, specific heat, and generalized susceptibility are obtained by finite-size scaling. On the other hand, we extend these studies to the cases $d=1$ and 2. For a preliminary and less detailed version of this work, which was still restricted to the investigation of smaller systems, see Ref. 20.

This paper is organized as follows. In Sec. II, we introduce the model Hamiltonian including the used boundary conditions, and we comment on the applied numerical procedures. Section III presents a qualitative overview of the simulation results, whereas Sec. IV is devoted to a quantitative evaluation of the data sets by means of finite-size scaling. Finally, in Sec. V, the obtained critical exponent values are discussed and compared with previous work.

II. MODEL AND NUMERICAL APPROACH

We numerically investigate the nature of the order-disorder transition in a system of charges considering the minimal model: simple hypercubic lattices are half-filled with particles interacting via the Coulomb potential where background charges $-1/2$ are attached at each site for neutrality,

$$H = \frac{1}{2} \sum_{i \neq j} f_{ij} (n_i - 1/2) (n_j - 1/2) \quad (1)$$

with

$$f_{ij} = 1 / |\mathbf{r}_i - \mathbf{r}_j|. \quad (2)$$

Here $n_\alpha \in \{0, 1\}$ denote the occupation numbers of states localized at sites \mathbf{r}_i within a d -dimensional hypercube of size L^d . Elementary charge, lattice spacing, dielectric constant, and Boltzmann constant are all taken to be 1, so that the temperature T is dimensionless. Due to particle-hole symmetry, canonical and grand canonical Hamiltonians equal each other in this case. When substituting s_i for $n_i - 1/2$, Eqs. (1) and (2) take the form of the $s=1/2$ Ising lattice model with Coulomb interaction of antiferromagnetic character.

For reducing finite-size effects, we impose periodic boundary conditions for $d=1$ and 2, modifying f_{ij} according to the minimum image convention.²⁴ For $d=3$, the same ap-

proach would give rise to an unphysical feature: The ground state would be a layered arrangement of charges instead of the expected NaCl structure in case L is a multiple of four.²⁵ Therefore, similar to Ref. 26, we consider the sample to be surrounded by 26 equally occupied cubes in this case,²⁷

$$f_{ij} = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{k=1}^{26} \left(\frac{1}{|\mathbf{r}_i - \mathbf{r}_j - \mathbf{R}_k|} - \frac{1}{|\mathbf{R}_k|} \right). \quad (3)$$

Here, \mathbf{R}_k denotes the shift of the neighboring cube k with respect to the central cube. Similar to the minimum image convention, the correction terms in Eq. (3) efficiently reduce the largest finite-size effect, namely, the difference between the surroundings of sites close to the center of the cube and of sites close to its surface. Compared to the implementation of periodic boundary conditions combined with an Ewald summation, our method has the advantage that it does not introduce the artificial long-range correlations arising from the series of periodic images of the cell. However, in the limit $L \rightarrow \infty$, both approaches should yield the same results (see the comparison with Ref. 7 in Sec. IV).

To obtain ensemble averages of various observables, we follow the Metropolis approach and substitute temporal for ensemble averaging.²⁴ Since only equilibrium properties are of interest here, we are free to choose the dynamics so that the simulation effort is minimized. A cluster Monte Carlo algorithm seems not to be available for the antiferromagnetic Coulomb interaction because of frustration. Thus we select the system modifications to be taken into account by hand: We include one-electron exchange with the ‘‘surroundings,’’ one-electron hops over distances below a certain bound, and two-electron hops changing the occupation of four neighboring sites. The maximum permitted distance of one-electron hops is enlarged when T is lowered.

At high T , we use the original Metropolis method.²⁴ But at low T , we take advantage of the hybrid procedure proposed in Ref. 28, which much accelerates the computations: Similar to the n -fold way algorithm,²⁹ we deterministically calculate the rates of the transitions to all multiparticle states, which are accessible from the current state by means of a single system modification. Thus the dwelling time at the current state can be determined directly, and only one Monte Carlo step is needed per system modification. Moreover, the hybrid procedure connects the deterministic evaluation of weighted sums over all states within a low-energy subset of the configuration space with Monte Carlo sampling of the complementary high-energy subset. These two ideas had proved to be very efficient in studying the specific heat of the Coulomb glass at low temperatures.²⁵

For an efficient error control, we decompose the simulation time considering 100 intervals with integration time τ instead of one interval of length 100τ . In detail, we increase τ step by step performing 50 runs for every τ value. In each of these runs, after starting randomly from one multiparticle state out of a set of previously tabulated low-energy states, the sample is first equilibrated during a time interval $\tau/3$. Then the evolution over two successive time intervals τ is emulated. The obtained ensembles of 100 measuring data for each observable are used to estimate mean values and their

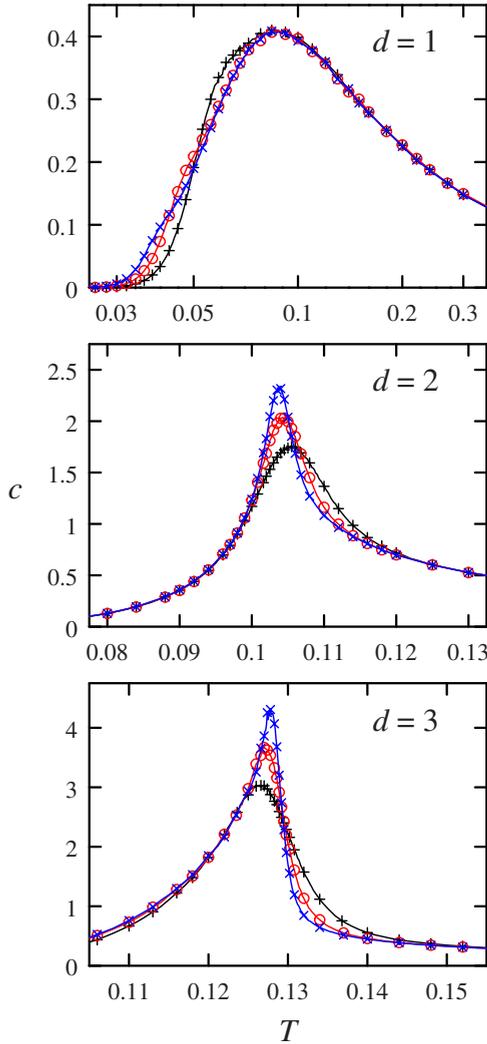


FIG. 1. (Color online) Temperature dependences of the specific heat, $c(T)$, for dimensions $d=1$ to 3 as obtained from simulations of samples of L^d sites. $d=1$: $L=100$ (+), 280 (\circ), and 700 (\times); $d=2$: $L=20$ (+), 34 (\circ), and 58 (\times); $d=3$: $L=8$ (+), 12 (\circ), and 18 (\times). Only a part of the data points forming the curves is marked by symbols, as well as in Figs. 2–4, 6, and 8. The error bars are considerably smaller than the symbol size.

statistical uncertainties, and to check equilibration. Based on these results, it is decided, whether the iteration process can be stopped, or whether τ has to be increased further.

III. QUALITATIVE RESULTS

We now turn to the qualitative behavior of specific heat, order parameter, and susceptibility. The specific heat c was obtained from energy fluctuations utilizing

$$c = (\langle H^2 \rangle - \langle H \rangle^2) / (T^2 L^d), \quad (4)$$

see, e.g., Ref. 30. Figure 1 shows its T and L dependences: For $d=2$ and 3, sharp peaks of increasing height evolve within a small T region as L grows. Away from the peaks, within the T intervals presented, c is almost independent of L . However, for $d=1$, there are only broad rounded peaks

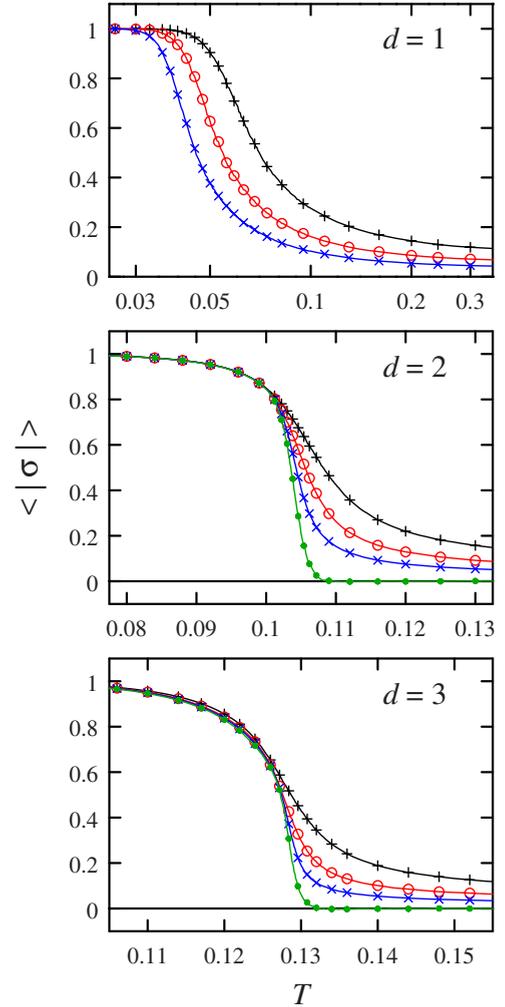


FIG. 2. (Color online) Temperature dependence of the average absolute value of the mean staggered occupation, $\langle |\sigma| \rangle(T)$, which is defined by Eq. (5) for $d=1$ to 3. For the meaning of the symbols +, \circ , and \times see caption of Fig. 1; \bullet marks the extrapolation $L \rightarrow \infty$ explained in the text.

with L -independent height—a logarithmic T scale is used for $d=1$, in contrast to the linear scales for $d=2$ and 3, which display far smaller T intervals. For $d=1$, finite-size effects are restricted to low T where the reliability bound decreases with increasing L (compare Ref. 25).

Analogously to an antiferromagnet, the order inherent in a charge arrangement n_i can be characterized by the mean staggered occupation σ relating to a NaCl structure.³ For $d=3$,

$$\sigma = \frac{1}{L^d} \sum_i (-1)^{x_i + y_i + z_i} (2n_i - 1), \quad (5)$$

where x_i , y_i , and z_i denote the (integer) components of \mathbf{r}_i . Thus we consider the ensemble average of the absolute value of the mean staggered occupation $\langle |\sigma| \rangle$ as order parameter. T and L dependences of $\langle |\sigma| \rangle$ are shown in Fig. 2. For $d=1$, a rapid decrease of $\langle |\sigma| \rangle$ with increasing T occurs already clearly below the temperature of maximum c (same T scales in Figs. 1 and 2). This marked decrease shifts to lower T with

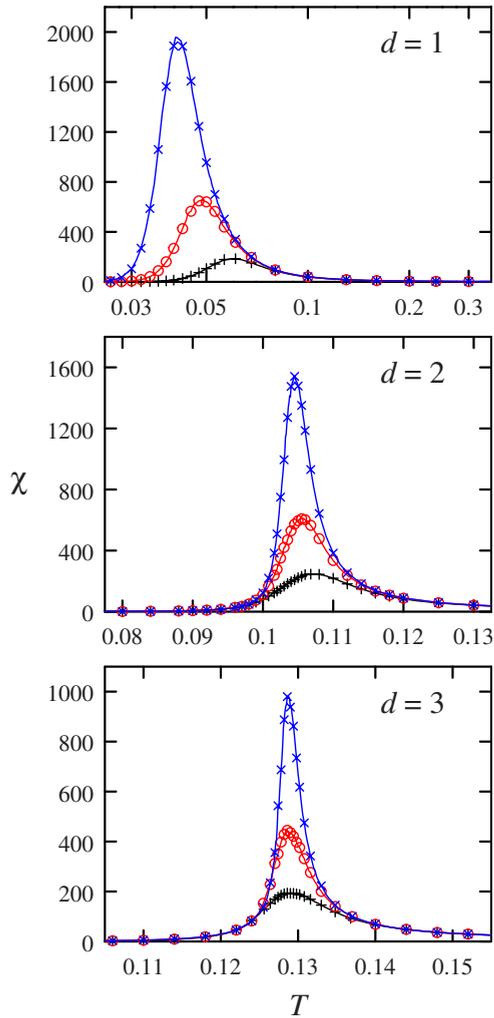


FIG. 3. (Color online) Temperature dependence of the susceptibility, $\chi(T)$, which is related to the mean staggered occupation σ by Eq. (6), for $d=1$ to 3. For the meaning of the symbols see caption of Fig. 1.

increasing L . For $d=2$ and 3, a qualitatively different behavior is found: the order parameter $\langle|\sigma|\rangle$ decreases rapidly just in that T region where the peak of $c(T)$ evolves, and the T interval of rapidly diminishing $\langle|\sigma|\rangle$ shrinks as L rises. In these cases, the extrapolation $L \rightarrow \infty$ by means of $\langle|\sigma|\rangle(T, L) = \langle|\sigma|\rangle(T, \infty) + A(T)/L^{d/2}$ seems natural. Based on the $\langle|\sigma|\rangle(T, L)$ data for $L=34$ and 58 in case $d=2$, and for $L=12$ and 18 in case $d=3$, it yields almost sharp transitions. However, this extrapolation is of limited accuracy in the immediate vicinity of the transition.

The generalized susceptibility χ , which is related to the response of $\langle|\sigma|\rangle$ to a staggered field, is given by

$$\chi = L^d (\langle\sigma^2\rangle - \langle|\sigma|\rangle^2) / T \quad (6)$$

(see Ref. 31). Figure 3 shows T and L dependences of χ . On the one hand, for $d=1$, a broad peak of $\chi(T)$ evolves with increasing L , where T_{\max} , the temperature of maximum χ , decreases. On the other hand, for $d=2$ and 3, as L rises,

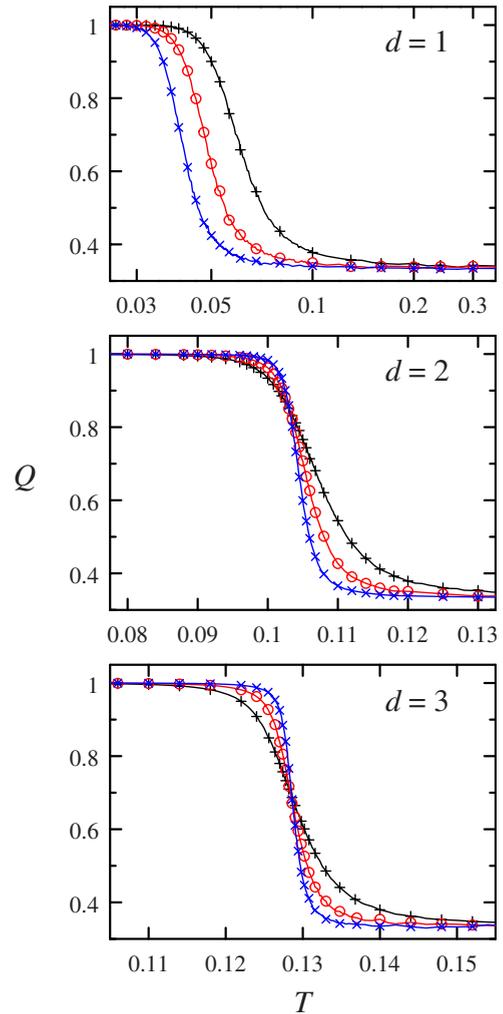


FIG. 4. (Color online) Temperature dependence of the Binder parameter, $Q(T)$, which is related to the mean staggered occupation σ by Eq. (7), for $d=1$ to 3. For the meaning of the symbols see caption of Fig. 1.

a narrow peak grows in just that T region where $c(T, L)$ has such a feature.

Hence, according to the described behavior of $c(T, L)$, $\langle|\sigma|\rangle(T, L)$, and $\chi(T, L)$, a phase transition likely occurs for $d=2$ and 3, for $d=3$ in agreement with Refs. 7, 11, and 12. However, for $d=1$, in spite of the long-range interaction, there seems to be no phase transition at finite T .

This conclusion is confirmed by the behavior of the Binder parameter, the fourth-moment ratio,

$$Q = \langle\sigma^2\rangle^2 / \langle\sigma^4\rangle, \quad (7)$$

which is shown in Fig. 4.¹² This quantity is directly derived from the Binder cumulant $1 - \langle\sigma^4\rangle / (3\langle\sigma^2\rangle^2)$ and exhibits similar features: In the ordered phase, where σ has a bimodal probability distribution, $Q=1$, whereas, in case of a normal distribution of σ in the disordered phase, $Q=1/3$. A common intersection point of the $Q(T)$ curves for various system sizes indicates a phase transition. According to Fig. 4, such points seem to exist for $d=2$ and 3, but not for $d=1$.

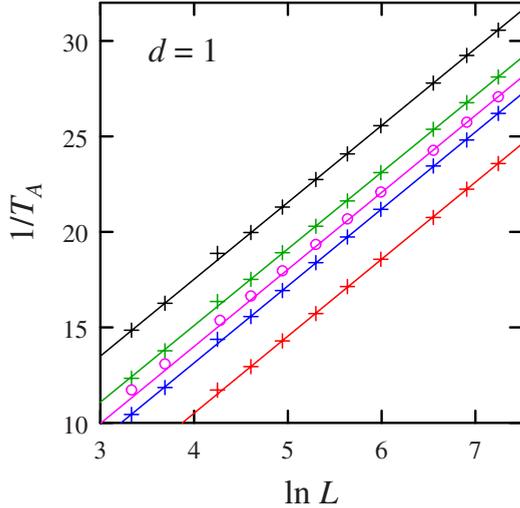


FIG. 5. (Color online) Size dependence of the solution T_A of $Q(T_A, L) = A$ for $d=1$ in a $1/T_A$ versus $\ln L$ plot. From top to bottom, the crosses are related to $A=0.90, 0.75, 0.60,$ and 0.45 . The maximum temperatures T_{\max} of $\chi(T, L)$ are included as circles for comparison. Error bars are omitted since they are considerably smaller than the symbol size. The straight lines correspond to linear regression in this representation for $L \geq 100$ in case of T_A , and for $L \geq 700$ in case of T_{\max} .

IV. QUANTITATIVE ANALYSIS BY MEANS OF FINITE-SIZE SCALING

Consider first the one-dimensional case: Careful inspection of Fig. 4 leads to the conclusion that, although there seems to be no common intersection point of the $Q(T)$ curves, simple scaling $Q(T, L) = Q(T/L^p)$ is unlikely because of the L dependence of the slope in this graph. Thus, to perform a detailed analysis, we numerically solved $Q(T_A, L) = A$ for $A=0.45, 0.60, 0.75,$ and 0.90 . The resulting $T_A(L)$ are presented in a $1/T_A$ versus $\ln L$ plot in Fig. 5.

Figure 5 shows that, with high precision, $1/T_A$ is a linear function of $\ln L$ for all considered A values. (The tiny deviation at $L=70$ arises from a small systematic shift of the $Q(T, L)$ curves for $L=4n$, where n is integer, in comparison to the curves with $L=4n+2$. This shift vanishes as $n \rightarrow \infty$.) Moreover, it is remarkable that the slope of the linear function is independent of A within the accuracy of the simulations. Finally, with increasing L , the L dependence of the maximum temperature T_{\max} of the susceptibility seems to tend to the same behavior as $T_A(L)$.

Due to the linear dependences in Fig. 5, $T_A(L)$ and $T_{\max}(L)$ likely vanish as $L \rightarrow \infty$. This is confirmed by the parallelism of the regression lines, a second argument against the intersection of $Q(T, L = \text{const})$ curves at finite T . As a consequence of these two observations, $Q(T, L)$ is expected to depend only on the composed quantity $z = T_0/T - \ln L$ with $T_0 = 0.2484(8)$, where the uncertainty denotes the 3σ bound of the random deviation. This reduction is confirmed by Fig. 6, which shows the corresponding master curve made up of $Q(T, L = \text{const})$ curves with $L=40, 100, 280, 700,$ and 1400 .

Thus, in the limit $L = \infty$, long-range order should be destroyed by thermal excitations at arbitrarily small, but finite

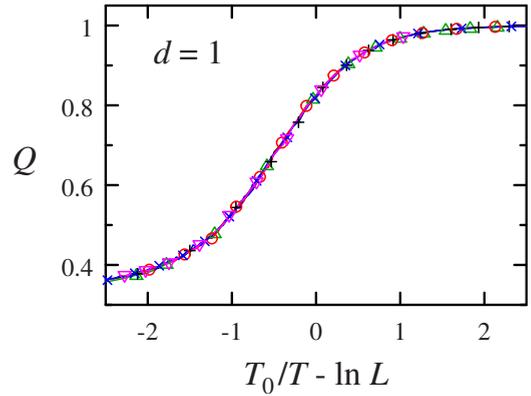


FIG. 6. (Color online) Check for $d=1$ whether $Q(T, L)$ depends only on the composed quantity $z = T_0/T - \ln L$ where $T_0 = 0.2484$. The symbols $\Delta, +, \circ, \times,$ and ∇ stand for $L=40, 100, 280, 700,$ and 1400 , respectively.

T although the considered model exhibits a long-range interaction.

One may ask whether the logarithmic relation indicates that the antiferromagnetic Coulomb interaction is a marginal case for $d=1$. Thus we performed additional simulations for the antiferromagnetic $1/r^{1/2}$ interaction which decays more slowly. These studies yielded similar results: Considering samples of up to 1000 sites, we could not find a clue of a phase transition at finite T . However, on the one hand, $1/T_A$ rises with increasing L slightly faster than as a linear function of $\ln L$, and, on the other hand, small deviations from the parallelism of the dependences of $1/T_A$ on $\ln L$ for different A are present.

We turn now to the two- and three-dimensional cases: Here, the quantitative evaluation of our simulation data consists in a finite-size scaling analysis.^{32,33} However, for numerical convenience, we consider the quantities

$$q_2 = -\ln(1 - Q) \quad (8)$$

and

$$q_3 = -\tan(\pi(1 - 1.5Q)) \quad (9)$$

for $d=2$ and 3 , respectively, instead of Q . The $q_d(T)$ have small curvature in the vicinity of the transition. This behavior alleviates a precise interpolation.

Figure 7 shows $q_d(T)$ for various L values. For $d=2$, there clearly is a common intersection point of the curves for different L at the critical temperature $T_{c,2}$. However, for $d=3$, only a tendency toward such a behavior is seen although the widths of the T intervals for both cases as well as the ranges of numbers of sites L^d are comparable.

The corresponding corrections to scaling can be taken into account to a large extent in a simple way: Following Ref. 34, we define a size-dependent critical temperature $T_{c,d}(L)$ by the demand $q_d(T_{c,d}(L), L) = q_{0,d}$, where the $q_{0,d}$ are appropriate constants, which are fixed below. Scaling of $q_d(T)$ curves for different L with respect to $T - T_{c,d}(L)$ yields very good data collapse. Figure 8 demonstrates this observation, showing plots of $Q(T, L)$ versus $t = a_d(L)[T - T_{c,d}(L)]$ based on the parameter values obtained below. In our study, referring to

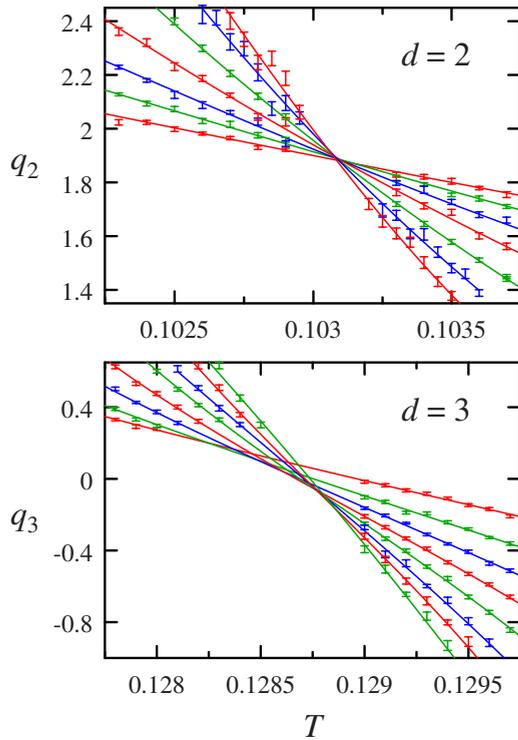


FIG. 7. (Color online) Temperature dependence of q_d , related to the Binder parameter Q by Eqs. (8) and (9), in the close vicinity of the transition for $d=2$ and 3. According to increasing modulus of the slope, the curves refer to $L=16, 24, 34, 48, 68, 88$, and 112 for $d=2$, and to $L=8, 10, 12, 14, 16, 18, 20$, and 22 for $d=3$. The error bars denote the 1σ region. For clarity, data points in the intersection regions are omitted.

$T_{c,d}(L)$ instead of $T_{c,d}(\infty)$ proved to considerably reduce the influence of deviations from scaling on the values of the critical exponents, which are numerically obtained from samples of finite size.

Figure 8 simultaneously shows that $Q(t)$ has a substantial curvature within the crucial region—our finite-size scaling analysis is based on the Q intervals $[0.75, 0.91]$ and $[0.45, 0.80]$ for $d=2$ and 3, respectively. However, to reach a high accuracy of the critical exponents, very precise $a_d(L)$ values are needed so that a broad t range has to be taken into account. We approach this nonlinearity problem by considering $q_d(t)$ instead of Q on the one hand, and by approximating $q_d(t)$ by polynomials of third degree, $q_{0,d} + t + b_d t^2 + c_d t^3$, on the other hand.

We evaluated our $q_d(T, L)$ data by a series of regression studies of the T and L dependences: First, the only weakly L -dependent parameters b_d and c_d of the polynomial ansatz were adjusted, after this the $a_d(L)$ and $T_{c,d}(L)$ values were determined.

Both for the cases $d=2$ and 3, the relations $a_d(L)$ only weakly deviate from power laws, $a_d(L) \propto L^p$, so that they are not graphically depicted here. Based on the $a_d(L)$ data, the value of the critical exponent of the correlation length, $\nu = 1/p$, can be obtained in two ways. First, it can be directly calculated by numerical differentiation by means of the midpoint formula utilizing $\nu = (d \ln|a_d| / d \ln L)^{-1}$. The advantage of this approach is a meaningful control of convergence with

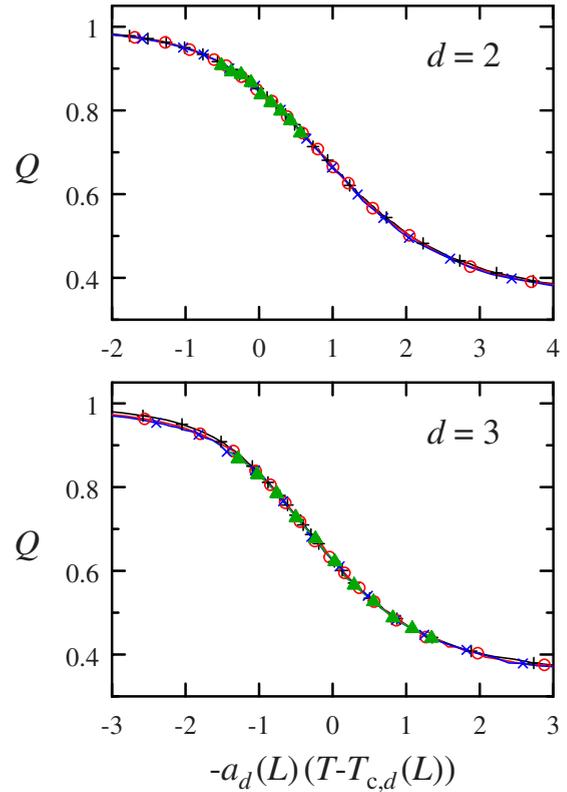


FIG. 8. (Color online) Scaling check for $Q(T, L)$: The adjustment of the parameters $a_d(L)$ and $T_{c,d}(L)$ is described in the text. Scaling is indicated by the agreement of the nonlinear contributions to $Q(T, L = \text{const})$ for various L in these plots. For the meaning of the symbols $+$, \circ , and \times see caption of Fig. 1; \blacktriangle refers to $L = 112$ and 22 for $d=2$ and 3, respectively.

increasing L . Figure 9 shows such results from the consideration of pairs of sixth-next and next-nearest neighbors in the sequence of sample sizes for $d=2$ and 3, respectively. Second, ν can be determined by means of power-law fits, taking into account various L intervals. This method yields more precise estimates of the exponents. For consistency, the mean-square deviation of these fits must be understandable as resulting from random errors alone. Table I presents the most precise results for ν , which were obtained from the fits safely fulfilling this requirement. Additionally, these values are included in Fig. 9.

This graph implies several conclusions: The ν values converge rapidly with increasing sample size so that for $d=3$, already the study of samples with $L \approx 12$ yields ν values, which are very close to the results for $L \approx 20$. Thus the good agreement between our result of a power-law fit, 0.633(4), and the known Ising value 0.630, suggests that the considered model may belong to the Ising universality class. This hypothesis is supported by our result 0.633(4) clearly differing from the mean-field value 0.5, from the Heisenberg value 0.71, and from exponents of the alternative “nearby” models XY, $\nu=0.670$, and self-avoiding walks, $\nu=0.588$ (compare Ref. 12). Also for $d=2$, our ν value supports Ising universality and clearly excludes mean-field behavior. Finally, according to Fig. 9, it is not surprising that for $d=3$, Overlin *et al.*⁷ got the somewhat lower value 0.55 ± 0.1 from simulations for $L=4, 6$, and 8.

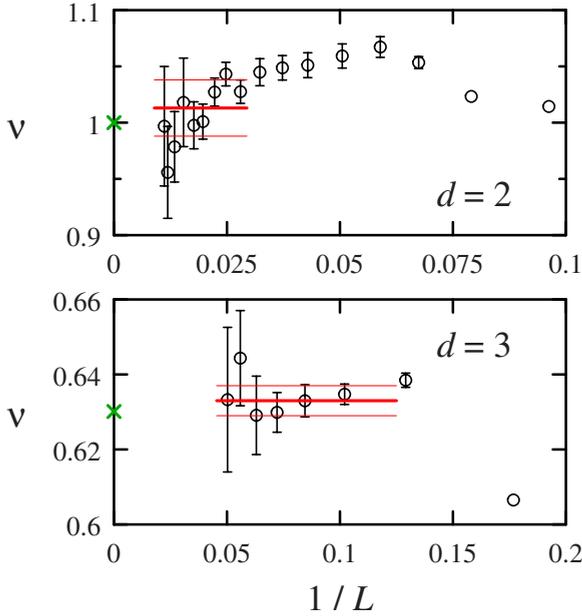


FIG. 9. (Color online) Approximations of the critical exponent ν versus sample size. The symbols \circ denote values which were obtained by numerical differentiation (see text). The corresponding error bars denote the 1σ regions. The thick red (gray) lines represent results of power-law fits, where their extension visualizes the evaluated L interval. The thin red (gray) lines give upper and lower bounds of the corresponding 3σ intervals. For comparison, the green (gray) symbols \times mark the known values of the Ising model with short-range interactions for $L=\infty$ (see Table I).

In obtaining $T_{c,d}(L)$ from $q_d(T_{c,d}(L), L) = q_{0,d}$, a deviation δ of $q_{0,d}$ from the $L \rightarrow \infty$ limit of the solution of $q_d(T, 2L) = q_d(T, L)$ gives rise to a contribution $\delta/a_d(L)$ to $T_{c,d}(L)$. We

fix $q_{0,d}$ by the demand that this term vanishes: $q_{0,2} = 1.892(8)$ and $q_{0,3} = -0.200(19)$, corresponding to the Q values $0.8492(12)$ and $0.625(4)$, respectively. For $d=2$, the critical Q value slightly, but significantly deviates from the analytical result for the $L=\infty$ limit of the short-range Ising model with periodic boundary conditions 0.856216 .³⁵ But this is not a strong counterargument to the considered model belonging to the Ising universality class, as it is suggested by the value of ν : It is known that the critical Q value is a very sensitive quantity which depends on the boundary conditions, and that “universality of the critical cumulant holds in a rather restricted sense, when compared to universality of critical exponents.”³⁶ Nevertheless, for $d=3$, our critical Q value perfectly agrees with the value for the Ising model with short-range interaction and periodic boundary conditions, $0.6233(4)$.³⁷ This supports the hypothetical Ising criticality inferred from the value of ν .

The remaining higher-order corrections in $T_{c,d}(L)$ originate from imperfection of finite-size scaling. Comparing several empirical approximations, we observed that over a wide L range, they are almost proportional to $a_d(L)^{-2}$ (see Fig. 10). Corresponding extrapolations yield the following values of $T_{c,d}(\infty)$: $0.103082(9)$ and $0.128838(17)$ for $d=2$ and 3 , respectively. The confidence intervals include the 3σ random errors and cautious estimates for the systematic uncertainty of the extrapolation $L \rightarrow \infty$.

Our $T_{c,3}$ value is consistent with the result 0.128 ± 0.005 in Ref. 7, which was obtained for considerably smaller samples. This coincidence, together with the approximate agreement of the values of ν , confirms an assumption from Sec. II. It shows that, within the accuracy of the simulation, our treatment of the surroundings of the sample yields the same results as the Ewald summation performed in Ref. 7. Moreover, comparing with analytical theories, we mention

TABLE I. Finite-size scaling results for the critical exponents of specific heat, mean staggered occupation, susceptibility, and correlation length, α , β , γ , and ν , respectively. To retain numerical precision, we mostly present exponent ratios instead of the exponents themselves. The data were obtained by two alternative methods, either directly (marked as d) by power-law fits (modified by a constant term in the case of α/ν), or indirectly (marked as i) via Widom and hyperscaling relations from power-law fits yielding other exponents or exponent ratios, see text. Values for the Ising model with short-range interaction (Refs. 33 and 38) are included for comparison. Parentheses and brackets give 3σ random errors and total errors, respectively, referring to the last given digit of the value.

Quantity	d	L region	Method	Coulomb	Short-range Ising
α/ν	2	28–112	d	-0.02(4)	0 (ln)
α/ν	2	34–112	i	-0.03(5)	0 (ln)
β/ν	2	48–112	d	0.1318(21)	1/8
β/ν	2	48–112	i	0.129(8)	1/8
γ/ν	2	48–112	d	1.742(15)	7/4
ν	2	34–112	d	1.013(25)	1
α/ν	3	10–22	d	0.09(9)	0.1740 [8]
α/ν	3	8–22	i	0.158(21)	0.1740 [8]
β/ν	3	14–22	d	0.506(7)	0.51820 [8]
β/ν	3	14–22	i	0.514(5)	0.51820 [8]
γ/ν	3	14–22	d	1.973(10)	1.96361 [15]
ν	3	8–22	d	0.633(4)	0.63012 [16]

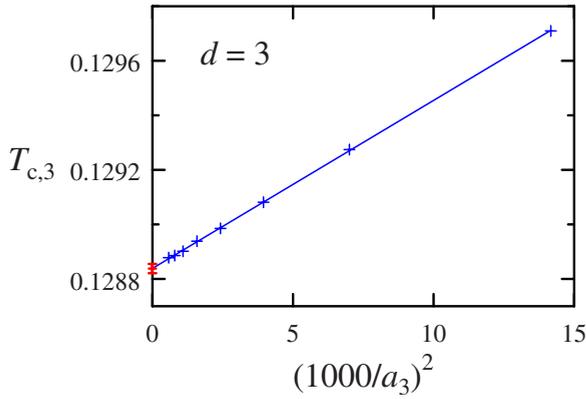


FIG. 10. (Color online) Relation between $a_3(L)$ and $T_{c,3}(L)$ for $q_{0,3} = -0.200$. With increasing a_3 , the data points refer to $L=8, 10, 12, 14, 16, 18, 20$, and 22 . The error bar represents our extrapolation $L \rightarrow \infty$, where the 3σ interval is marked.

that the nonlinear screening theory by Pankov and Dobrosavljević⁸ underestimates our “exact” $T_{c,3}$ value by 26%, whereas a study by Malik and Kumar,¹⁰ which utilizes the replica method, overestimates $T_{c,3}$ by roughly a factor 1.5 when using the random-phase approximation, and by more than a factor 3 for the Hartree approximation.

The analysis of $\chi(T, L)$, $\langle |\sigma| \rangle(T, L)$, and $c(T, L)$ was performed similarly to the evaluation of $q_d(T, L)$: We considered $\ln \chi$, $\ln \langle |\sigma| \rangle$, and $\ln c$ as functions of t and L . For not too large $|t|$, as $L \rightarrow \infty$, scaling implies that each of these quantities is decomposable into a sum of two functions depending only on t and L , respectively. However, for the L regions considered here, this hypothesis proved to be well fulfilled only for $\ln \chi$. In the cases of $\ln c$ and $\ln \langle |\sigma| \rangle$, there is a clear tendency toward such a behavior, but small deviations cannot be neglected. Thus we approximated $\ln \chi$, $\ln \langle |\sigma| \rangle$, and $\ln c$ by polynomials in t of third order, taking advantage of universalities in the coefficients as far as possible. This regression provides precise values for the observables at $t=0$. Simultaneously, we obtained the confidence intervals taking into account the uncertainties in the individual measurements of the observables and in the $T_{c,d}(L)$ values.

The interpolated $\chi(T_{c,d}(L), L)$ and $\langle |\sigma| \rangle(T_{c,d}(L), L)$ were analyzed by means of power-law fits, where proportionality to $L^{\gamma/\nu}$ and $L^{-\beta/\nu}$, respectively, was presumed. These studies were performed analogously to the determination of ν . However, while the effective γ/ν converges quite rapidly with increasing L , see Fig. 11, the determination of the limit of β/ν as $L \rightarrow \infty$ in Fig. 12 is hindered by slow convergence: Within a fixed L interval, the relative change of the effective β is considerably larger than the variations in the effective ν and γ . The reason of this slow convergence is understood by inspection of Fig. 13. Although this graph shows high-quality power-law behavior above $L \approx 30$ and $L \approx 10$ for $d=2$ and 3 , respectively, the uncertainty of the slope is rather large since, due to the small relative change of $\langle |\sigma| \rangle$, small deviations from the power law may considerably shift the exponent value.

Alternatively, the value of β/ν can be obtained from the value of γ/ν utilizing the Widom relation, $2 = \alpha + 2\beta + \gamma$, and the hyperscaling relation, $2 - \alpha = d\nu$. These equations imply

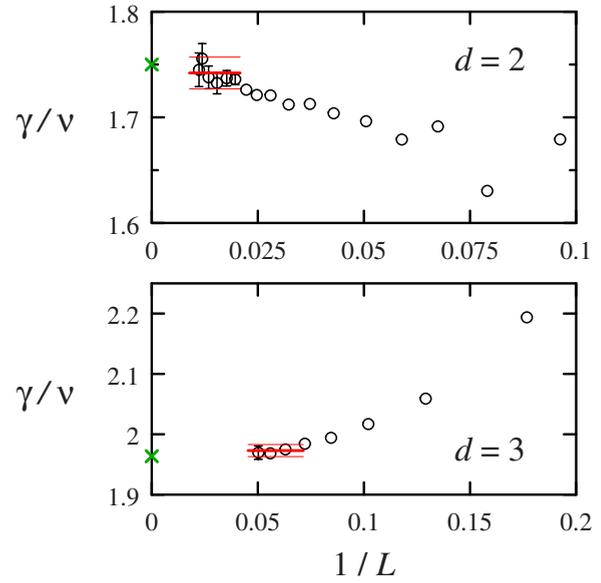


FIG. 11. (Color online) Approximations of the critical exponent ratios γ/ν versus sample size. For the meaning of the symbols see caption of Fig. 9.

$\beta/\nu = (d - \gamma/\nu)/2$. Corresponding results are included in Fig. 12, as well as in Table I, additionally to the results of the power-law fits.

Table I shows that our β/ν data are very close to the exponent ratios for the short-range Ising model, where the results of the indirect approach deviate somewhat less from the Ising values than the data obtained directly by means of power-law fits.

Compared to the study of $\langle |\sigma| \rangle$ and χ , the analysis of c is more difficult: Exponent values obtained by means of numerical differentiation converge only very slowly with in-

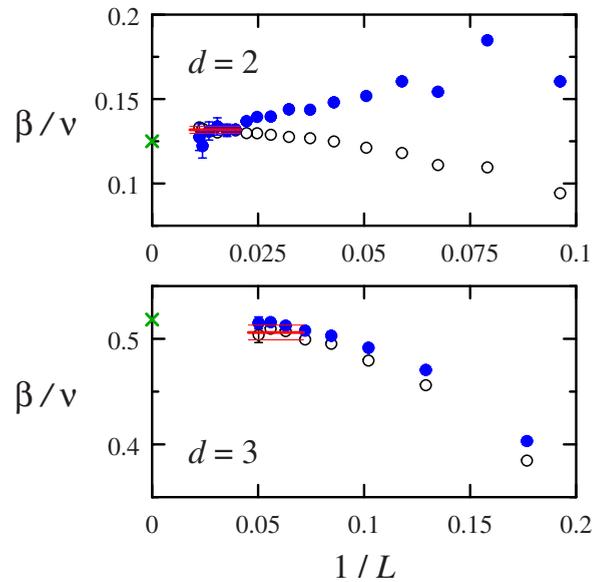


FIG. 12. (Color online) Approximations of the critical exponent ratios β/ν versus sample size. The meaning of most symbols is defined in the caption of Fig. 9. Here, additionally, the symbols \bullet denote values, which were obtained by means of the Widom and hyperscaling relations from γ/ν data in Fig. 11, marked by \circ there.

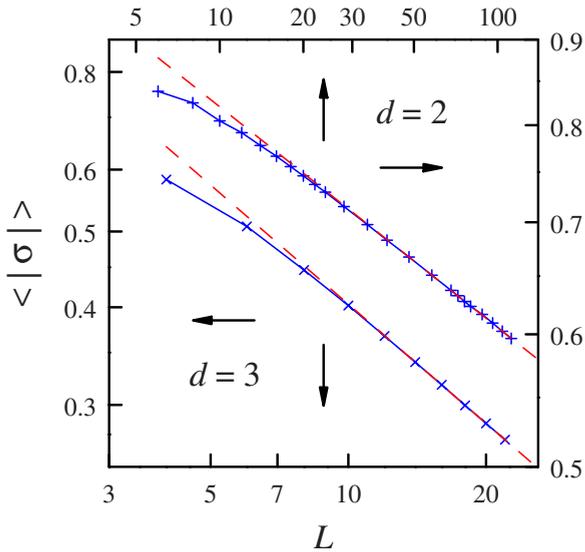


FIG. 13. (Color online) Size dependence of the value of $\langle |\sigma| \rangle$ at the critical temperature $T_{c,d}(L)$ defined in the text. The error bars are considerably smaller than the symbol size, thus they are omitted. The dashed lines represent the fits given in Table I.

creasing L , see Fig. 14, and the mean-square deviations of the power-law fits remain too large. Therefore we took into account a background contribution presuming $c(T_{c,d}(L), L) = a + bL^p$ with $p = \alpha/\nu$ similar to Ref. 39. Moreover, in order to avoid numerical problems, we approximated $c(T_{c,d}(L), L)$ by $\bar{a} + \bar{b}(L^p - 1)/p$ instead of by $a + bL^p$. Results for α/ν ,

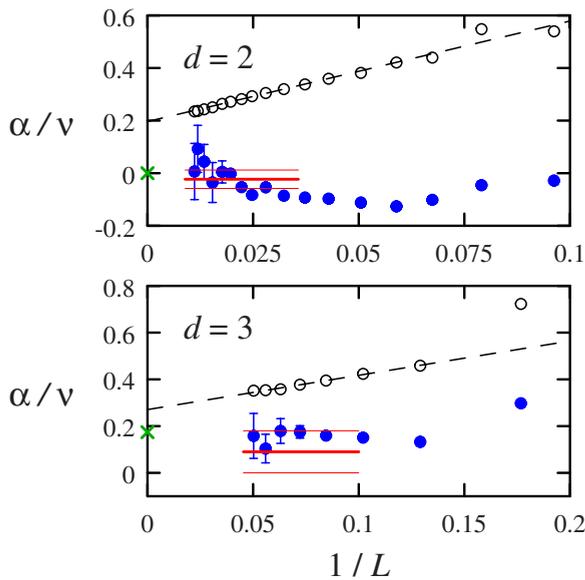


FIG. 14. (Color online) Approximations of the critical exponent ratios α/ν versus sample size. The meaning of most symbols is defined in the caption of Fig. 9. However, in this case, the power-law fit is modified by a background constant (see text). Additionally, the symbols \bullet denote values, which were obtained by means of the hyperscaling relation from ν data in Fig. 9, marked by \circ there. The dashed lines are included only as guide to the eye in order to demonstrate the considerable L dependence of the exponent ratio α/ν obtained by numerical differentiation.

which were determined in this way, are included in Table I and Fig. 14.

Alternatively, α/ν was calculated by means of the hyperscaling relation utilizing the ν results, which were obtained by numerical differentiation. These α/ν values exhibit a far better convergence than the directly obtained α/ν data; this is demonstrated Fig. 14. They agree nicely not only with the results of the modified power-law fits but also with the known values for short-range Ising universality (see Fig. 14 and Table I).

V. DISCUSSION

Summarizing, we have presented a detailed Monte Carlo study of the ordering of charges on a half-filled hypercubic lattice. For one-dimensional systems, the order seems to be destroyed already at arbitrarily small but finite temperature in spite of the long-range character of the interaction. However, for two- and three-dimensional systems, continuous phase transitions occur at finite temperatures. We have determined the critical exponents not only for the correlation length, but also for the specific heat, for the order parameter staggered occupation, as well as for the related susceptibility.

A survey of the exponent values, which we obtained by finite-size scaling, is given in Table I. These data have to be regarded as effective exponents. Due to the finiteness of L , tiny systematic errors are certainly present, presumably the more relevant the smaller the exponent value. Unfortunately, our data set is not sufficient for a convincing estimate of them. Nevertheless, the exponents which we obtained directly by means of power-law fits (modified by a background constant in case of the specific heat) obey the Widom relation, according to which the term $2/\nu - (\alpha/\nu + 2\beta/\nu + \gamma/\nu)$ has to vanish: Presuming the errors in Table I to be independent and random, one obtains $-0.01(6)$ and $0.08(9)$ for $d=2$ and 3, respectively, where the errors are given as 3σ bounds. Simultaneously, our data satisfy the hyperscaling relation, which implies the quantity $2/\nu - \alpha/\nu - d$ to equal zero: In this case, Table I yields $-0.01(6)$ and $0.07(9)$ for $d=2$ and 3, respectively. Together, Widom and hyperscaling relations imply that the expression $2\beta/\nu + \gamma/\nu - d$ vanishes what can be checked with higher precision since α is not included here. For this expression, one obtains the values $0.006(16)$ and $-0.015(17)$ for $d=2$ and 3, respectively, from Table I. Thus our set of the critical exponent values satisfies all consistency criteria.

Among the critical exponents, ν exhibits the best convergence with increasing sample size. The values given in Table I are consistent with the assumption that the studied phase transition belongs to the short-range Ising universality class, in spite of the long-range Coulomb interaction, both for the cases $d=2$ and 3. All other well-known universality classes could clearly be ruled out according to the values of ν . Moreover, the supposed Ising universality is supported by the values of the critical exponents α , β , and γ being likewise consistent with the corresponding critical indices of the Ising model, as well as by the critical values of the Binder parameter Q .

Concluding, in spite of the long-range interaction, the Coulomb system described by Eqs. (1) and (2) seems to be-

long to the same universality class as the Ising model with short-range interaction. This suggests that screening should be highly effective in the ordering process and that the lattice Coulomb-glass model might have the same critical properties as the random-field short-range Ising model.

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- ²⁷A single-particle hop from site i to site j in the central cube, which is accompanied by corresponding hops in the 26 neighboring cubes, modifies the total energy of all 27 cubes not only by the difference of the corresponding single-particle energies. But, moreover, it reduces the total energy by the attraction terms for the 729 pairs of differently occupied participating sites. Simultaneously, the total energy is increased by the repulsion terms of the 702 pairs of equally occupied sites. Focusing only on the energy change related to the central cube, we utilize 1/27 of all these terms as approximation of f_{ij} , namely, the sum of the interaction of the occupied site in the central cube with the empty sites in all cubes, reduced by the sum of the interactions of the occupied site in the central cube with the occupied sites in the neighboring cubes.
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