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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(Dated: June 3, 2009)

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.

PACS numbers: 64.60.F-, 05.70.Jk, 71.10.-w, 02.70.Uu

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.\(^3,4,5,6,7,8,9,10,40,41\)

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.\(^11,12,13,14,15,16\) In particular, by means of numerical simulation and finite-size scaling, Luijten et al. could clearly rule out this point to belong to any of several alternative universality classes.\(^12\) 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\(^11,15,16\) and simulation results\(^7,18,19,20\) 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.

However, we remind 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 underly 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 non-disordered case as natural limit.\(^5,9,10\) In this context, precise numerical experiments on the phase transition of lattice models without disorder are called for.

The corroborations 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 $12^4$ sites, Almarza and Enciso observed their data for simple-cubic lattices to be consistent with the assumption of short-range Ising universality.\(^18\) 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

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sample size and diminishing of the error bars seemed desirable. Finally, Overlin et al. studied the influence of positional disorder at samples of up to $8^3$ sites and determined the critical exponent of the localization length $\lambda$. 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 behavior of such systems: In a first attempt, Diaz-Sanchez et al. 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. 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,

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

with

$$ f_{ij} = 1/|r_i - r_j| \quad . $$

Here $n_{\alpha} \in \{0, 1\}$ denote the occupation numbers of states localized at sites $r_i$ within a $d$-dimensional hypercube of size $L^d$. Elementary charge, lattice spacing, dielectric and Boltzmann constants 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. For $d = 3$, the same approach would give rise to an unphysical feature: The groundstate would be a layered arrangement of charges instead of the expected NaCl structure in case $L$ is a multiple of four. Therefore, similar to Ref. 28, we consider the sample to be surrounded by 26 equally occupied cubes in this case:

$$ f_{ij} = \frac{1}{|r_i - r_j|} + \sum_{k=1}^{26} \left( \frac{1}{|r_i - r_j - R_k|} - \frac{1}{|R_k|} \right) . $$

Here, $R_k$ 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 $L \to \infty$, both approaches should yield the same results, see the comparison with Ref. 28 in Sec. IV.

To obtain ensemble averages of various observables, we follow the Metropolis approach and substitute temporal for ensemble averaging. 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. 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, we deterministically calculate the rates of the transitions to
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 to 4, 6, and 8. The error bars are considerably smaller than the symbol size.

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 $L \to \infty$ explained in the text.

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.

For an efficient error control, we decompose the simulation time considering 100 intervals with integration time $\tau$ instead of one interval of length 100 $\tau$. In detail, we increase $\tau$ step by step performing 50 runs for every $\tau$ 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 $\tau$ is emulated. The obtained ensembles of 100 measuring data for each observable are used to estimate mean values and their statistical uncertainties, and to check equilibration. Based on these results, it is decided, whether the iteration process can be stopped, or whether $\tau$ 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

$$c = \frac{\langle (H^2) - \langle H \rangle^2 \rangle}{T^2 L^d},$$

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 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 as $L$ grows, compare Ref. 25.

Analogously to an antiferromagnet, the order inherent in a charge arrangement $n_i$ can be characterized by the mean staggered occupation $\sigma$ relating to a NaCl structure. 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 $r_i$. 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 increasing $L$. For $d = 2$ and 3, a qualitatively different behavior is found: $|\langle \sigma \rangle|$ 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 $L \to \infty$ 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 $\chi$, 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 $\chi$. On the one hand, for $d = 1$, a broad peak of $\chi(T)$ evolves with increasing $L$ where $T_{\text{max}}$, the temperature of maximum $\chi$, decreases. On the other hand, for $d = 2$ and 3, as $L$ rises, 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. 71112. 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,

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

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

FIG. 4: (Color online) Temperature dependence of the Binder parameter, $Q(T)$, which is related to the mean staggered occupation $\sigma$ by Eq. (7), for $d = 1$ to 3. For the meaning of the symbols see caption of Fig. 1.
which is shown in Fig. 4. 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 $\sigma$ has a bimodal probability distribution, $Q = 1$, whereas, in case of a normal distribution of $\sigma$ 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 $d = 1$.

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 $n \to \infty$.) 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 $T_{\text{max}}$ 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 $T_{\text{max}}(L)$ likely vanish as $L \to \infty$. 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 $3\sigma$ 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 $L \to \infty$, long-range order should be destroyed by thermal excitations at arbitrarily small, but finite $T$ 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. However, for numerical convenience, we consider the quantities

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

and

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

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.
earity problem by considering has to be taken into account. We approach this nonlin-
scaling analysis is based on the critical exponents, which are numerically obtained from
fluence of deviations from scaling on the values of the range
a, d
L = 3, already the study of samples with L ∼ 12 yields
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 \(\nu = (\ln|a_d|/\ln L)^{-1}\). The advantage of this approach is a meaningful control of convergence with 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, \(\nu\) 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 \(\nu\), which were obtained from the fits safely fulfilling this requirement. Additionally, these values are included in Fig. 9.
This graph implies several conclusions: The \(\nu\) values converge rapidly with increasing sample size so that, for \(d = 3\), already the study of samples with \(L ∼ 12\) yields

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**Figure 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.

**Figure 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 +, ×, and • see caption of Fig. 1; • (green/gray) refers to \(L = 112\) and \(22\) for \(d = 2\) and \(3\), respectively.

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**Table I**

| \(L\)  | \(a_d(L)\) | \(T_{c,2}(L)\) | \(T_{c,3}(L)\) |
|-------|-------------|----------------|----------------|
| 16    |             |                |                |
| 24    |             |                |                |
| 34    |             |                |                |
| 48    |             |                |                |
| 68    |             |                |                |
| 88    |             |                |                |
| 112   |             |                |                |

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**Footnotes**

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interactions for \( L = 4, 6, \) and 8.\)

Finally, according to Fig. 3, the green (gray) symbols \( \nu \) give upper and lower bounds of the corresponding exponents or exponent ratios, see text. Values for the Ising model with short-range interactions \( L = 8, 10, 12, 14, 16, 18, 20, \) and 22. The error bar represents \( \sigma \), where the 3σ interval is marked.

Thus the good agreement between our result of a power-law fit, \( 0.633(4) \), and the known Ising value \( 0.630 \), supports Ising universality and clearly excludes mean-field behavior. For comparison, the green (gray) symbols \( \times \) mark the known values of the Ising model with short-range interactions for \( L = \infty \), see Tab. I.

\( \nu \) 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, \( \nu \approx 0.588 \), compare Ref. 12. Also for \( d = 2 \), our \( \nu \) 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. got the somewhat lower value \( 0.55 \pm 0.1 \) from simulations for \( L = 4, 6, \) and 8.\( \frac{2}{3} \).

In obtaining \( T_{c,d}(L) \) from \( q_d(T_{c,d}(L), L) = q_{0,d} \), a deviation \( \delta \) of \( q_{0,d} \) from the \( L \to \infty \) 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\( \pm \)3. 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 \( \nu \); 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”\( \frac{2}{3} \). 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).\( \frac{3}{3} \) This supports the hypothetical Ising criticality inferred from the value of \( \nu \).

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 \( L \to \infty \).

Our \( T_{c,3} \) value is consistent with the result 0.128±0.005 in Ref. 7, which was obtained for considerably smaller

\begin{table}[h]
\centering
\caption{Finite-size scaling results for the critical exponents of specific heat, mean staggered occupation, susceptibility, and correlation length, \( \alpha \), \( \beta \), \( \gamma \), and \( \nu \), 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 \( \alpha/\nu \)), 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\( \frac{3}{3} \) are included for comparison. Parentheses and brackets give 3σ random errors and total errors, respectively, referring to the last given digit of the value.}
\begin{tabular}{llllll}
\hline
\textbf{Quantity} & \textbf{d} & \textbf{L region} & \textbf{method} & \textbf{Coulomb} & \textbf{s.-r. Ising} \\
\hline
\( \alpha/\nu \) & 2 & 28 – 112 & d & -0.02(4) & 0 (ln) \\
\( \alpha/\nu \) & 2 & 34 – 112 & i & -0.03(5) & 0 (ln) \\
\( \beta/\nu \) & 2 & 48 – 112 & d & 0.131(21) & 1/8 \\
\( \beta/\nu \) & 2 & 48 – 112 & i & 0.129(8) & 1/8 \\
\( \gamma/\nu \) & 2 & 48 – 112 & i & 1.742(15) & 7/4 \\
\( \nu \) & 2 & 34 – 112 & d & 0.103(25) & 1 \\
\( \alpha/\nu \) & 3 & 10 – 22 & d & 0.09(9) & 0.174(8) \\
\( \alpha/\nu \) & 3 & 10 – 22 & i & 0.158(21) & 0.174(8) \\
\( \beta/\nu \) & 3 & 14 – 22 & d & 0.506(7) & 0.51820(8) \\
\( \beta/\nu \) & 3 & 14 – 22 & i & 0.514(5) & 0.51820(8) \\
\( \gamma/\nu \) & 3 & 14 – 22 & i & 1.973(10) & 1.96361(15) \\
\( \nu \) & 3 & 8 – 22 & d & 0.633(4) & 0.63012(16) \\
\hline
\end{tabular}
\end{table}
symbols see caption of Fig. 9.

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 $L$.

samples. This coincidence, together with the approximate agreement of the values of $\nu$, 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. [1]. Moreover, comparing with analytical theories, we mention that the nonlinear screening theory by Pankov and Dobrosavljević underestimates our “exact” $T_{c, 3}$ value by 26% whereas a study by Malik and Kumar, 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 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 $\nu$. However, while the effective $\gamma/\nu$ converges quite rapidly with increasing $L$, see Fig. 11, the determination of the limit of $\beta/\nu$ as $L \to \infty$ in Fig. 12 is hindered by slow convergence: Within a fixed $L$ interval, the relative change of the effective $\beta$ is considerably larger than the variations of the effective $\nu$ and $\gamma$. 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 $d = 3$, 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 $\beta/\nu$ can be obtained from the value of $\gamma/\nu$ utilizing the Widom relation, $2 = \alpha + 2\beta + \gamma$, and the hyperscaling relation, $2 - \alpha = d\nu$. These equations imply $\beta/\nu = (d - \gamma/\nu)/2$. Corresponding results are included in Fig. 12, as well as in Tab. I, additionally to the results of the power-law fits.
Table I shows that our $\beta/\nu$ data are very close to the exponent ratios $\alpha/\nu$ 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 $\chi$, the analysis of $c$ is more difficult: Exponent values obtained by means of numerical differentiation converge only very slowly with increasing $L$, 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 $c(T_{\nu},L) = a + bL^p$ with $p = \alpha/\nu$ similar to Ref. 39. Moreover, in order to avoid numerical problems, we approximated $c(T_{\nu},L)$ by $\frac{1}{\alpha/\nu} \frac{1}{L^d} (L^p - 1)/p$ instead of by $a + bL^p$. Results for $\alpha/\nu$, which were obtained in this way, are included in Tab. I and Fig. 14.

Alternatively, $\alpha/\nu$ was calculated by means of the hyperscaling relation utilizing the $\nu$ results, which were obtained by numerical differentiation. These $\alpha/\nu$ values exhibit a far better convergence than the directly obtained $\alpha/\nu$ 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 Tab. I.

FIG. 14: (Color online) Approximations of the critical exponent ratios $\alpha/\nu$ 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, blue (gray) symbols • denote values, which were obtained by means of the hyperscaling relation from $\nu$ data in Fig. 9, marked by ○ there. The dashed lines are included only as guide to the eye in order to demonstrate the considerable $L$ dependence of the exponent ratio $\alpha/\nu$ obtained by numerical differentiation.

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 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 Tab. 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 Tab. 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 3$\sigma$ bounds. Simultaneously, our data satisfy the hyperscaling relation which implies the quantity $2/\nu - \alpha/\nu - d$ to equal zero: In this case, Tab. 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 $\alpha$ 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 Tab. I. Thus our set of the critical exponent values satisfies all consistency criteria.

Among the critical exponents, $\nu$ exhibits the best convergence with increasing sample size. The values given in Tab. I are consistent with the assumption that the studied phase transition belongs to 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 $\nu$. Moreover, the supposed Ising universality is supported by the values of the critical exponents $\alpha$, $\beta$, and $\gamma$ 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 belong 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.

Acknowledgments

We thank A. Ciach, H. Eschrig, M.E. Fisher, B. Kramer, T. Nattermann, M. Richter, M. Schreiber,
R.H. Swendsen, and T. Vojta for helpful discussions and literature hints.

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27. A 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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