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# High-dimensional lattice gases

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**Abstract.** We investigate the critical behaviour of hard-core lattice gases in four, five and six dimensions by means of Monte Carlo simulations. In order to suppress critical slowing down, we use a geometrical cluster Monte Carlo algorithm. In particular, nearest-neighbour-exclusion lattice gases on simple hypercubic lattices are investigated. These models undergo Ising-like ordering transitions where the majority of the lattice-gas particles settle on one of two sublattices. A finite-size-scaling analysis of the simulation data confirms that these lattice gases display classical critical behaviour. The results agree with the renormalization predictions at and above the upper critical dimensionality. In particular, the predicted value of the Binder cumulant is confirmed.

## 1. Introduction

A gas–liquid system can be modelled by means of hard-core particles, which exclude one another within a non-zero range. A further simplification consists of the restriction of the particle coordinates to the vertices of a regular lattice. Moreover, the ratio of the hard-core radius to the lattice constant can be chosen such that the exclusion is restricted to nearest-neighbour sites. Even in such simplified models phase transitions may occur. For low particle density, particles will be distributed uniformly over the sublattices. For sufficiently high particle density, however, the particles may preferentially occupy one sublattice. In addition to gas–liquid systems, such models can also describe several other phenomena such as the formation of metal alloys, the adsorption of gases on crystal surfaces and intercalation phenomena. In the latter context, the physics of lattice gases is applicable to describing the behaviour of certain types of electric batteries [1]. Lattice-gas models have also found applications in the field of loss networks [2].

Lattice gases with nearest-neighbour exclusion have been studied on a number of different lattices by means of a variety of approaches (see, e.g., [3–16] and references therein). The universal classification of phase transitions in hard-core lattice gases is thus known to depend on the dimensionality, the presence of further interactions and the way in which the lattice can be partitioned into sublattices. For bipartite lattices, and interactions dominated by nearest-neighbour exclusion, the ordering transition is the result of competition between the two

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sublattice densities. The phase transition is thus associated with a breaking of the symmetry between these two sublattices. The staggered density assumes the role of the order parameter. Since it is a scalar, one expects that these critical points belong to the Ising universality class.

In particular, in two dimensions a variety of exact and numerical results are known. Consider the hard-square lattice gas with nearest-neighbour exclusion, and no other interactions, as an example. This model has only one parameter for which one may take the particle density or the activity. In the absence of an exact solution, a variety of numerical approaches has been used to investigate the phase transition. It proved to be surprisingly difficult to confirm the Ising nature by means of series expansions [3]. Later, finite-size scaling provided the expected confirmation [4–7].

However, in the presence of further interactions between the hard-core particles on the square lattice, the nature of the phase transition may change completely, as shown by Baxter's exact solution of an interacting hard-square model [8] that belongs to the tricritical Ising universality class [9]. Even in the absence of such interactions, the nature of the transition still depends on the lattice structure. Baxter's hard-hexagon model [10] consists of particles with nearest-neighbour exclusion on the triangular lattice, and its phase transition belongs to the three-state Potts universality class, in accordance with the fact that the phase transition is associated with symmetry breaking involving *three* competing equivalent sublattice densities.

Next we consider higher numbers of dimensions, but restrict ourselves to particles on bipartite lattices which have, besides nearest-neighbour exclusion, no further interactions. Rather surprisingly, non-Ising behaviour has been reported for the simple-cubic [12] and the body-centred-cubic [13] lattice gases. However, some uncertainty exists due to the absence of corrections to scaling in these analyses. The limited statistical accuracy of the Metropolis-type simulations used allows only the resolution of a limited number of free parameters. Unfortunately, the Wolff [17] algorithm is not applicable to these lattice gases. This problem was solved by means of the geometric cluster algorithm [14, 18] which suppresses critical slowing down in a similar way as the Wolff algorithm does for Ising models. In this way the corrections to scaling could be resolved in these lattice gases; when these are taken into account, the evidence for non-Ising universality vanishes [14, 15].

In this paper we study some higher-dimensional ($d = 4$, 5 and 6) lattice gases with the geometrical cluster Monte Carlo method. Unphysical as these high-dimensional models may seem, they provide a means to test the validity of the renormalization theory which describes systems in arbitrary numbers of dimensions, thus including the physical models in $d \leqslant 3$ dimensions. While it seems reasonable to assume that these lattice gases belong to the same universality classes as the corresponding Ising systems, this remains to be verified for the higher-dimensional lattice gases. Some universal properties of high-dimensional Ising-like models have been derived by Brézin and Zinn-Justin [19]. Recently, some doubts have been raised by Chen and Dohm [20, 21] as to the validity of this derivation, in particular with respect to the structure of the finite-size scaling functions. Despite claims that the Binder cumulant [22] above the upper critical dimensionality might differ from the widely accepted value obtained in [19], no such deviation could be observed in recent Monte Carlo results (see, e.g., [23, 24]) and also a one-loop calculation [20] agreed with the zero-mode result. Furthermore, it was demonstrated in [25], that one-loop calculations of finite-size scaling functions differed significantly from the corresponding Monte Carlo results for the five-dimensional Ising model. Therefore, it is worthwhile to study the behaviour of the Binder cumulant in a different group of high-dimensional models, in the hope of shedding some more light on questions of universality above the upper critical dimensionality.

Accurate values for the critical points of the non-interacting hard-core lattice gases are already known for the simple-quadratic and the simple-cubic lattice. When data on critical

points in more than three dimensions become available one might attempt to devise an empirical formula describing the critical points of simple-hypercubic lattice gases in any number of dimensions.

The outline of this paper is as follows. Section 2 defines the models and the Monte Carlo algorithm, and describes the simulations. The numerical data are analysed in sections 3, 4 and 5 for the four-, five- and six-dimensional lattice gases, respectively. In section 6 we apply two mean-field-like (MF) approximations to the phase transitions in these lattice gases, and section 7 concludes with a comparison between the numerical and the theoretical results.

## 2. The Monte Carlo simulations

In order to suppress the critical slowing down in the simulations, we have applied a cluster method similar to that used for the simple-cubic and body-centred-cubic lattice gases [14, 15]. This Monte Carlo algorithm uses a geometric symmetry of the lattice to interchange a pair of lattice-gas variables. If the resulting configuration violates the nearest-neighbour exclusion principle, the trespassing neighbours are also subjected to the symmetry operation and included in the cluster. The cluster-formation process continues until no more violations occur. Unlike the case of hard-core gases in continuous space [26], the cluster-formation process appears to be just on the percolation threshold when applied to a critical system [14]. The cluster method is also applicable and fast in the case of other critical lattice models, such as the Ising model and the tricritical Blume–Capel model [18]. The cluster method presently used corresponds to a special case, namely the absence of finite interactions, of the cluster algorithm of [18].

In a related approach, one may swap particles between two different replicas of the lattices as was recently proposed [27, 28]. Furthermore, this cluster-formation process is also realized in the context of the work of van den Berg and Steif on disagreement percolation [16], where again two replicas of the lattice-gas system are being matched. This work [16] has shown that for bipartite lattices the phase transition coincides with the disagreement percolation threshold, thus explaining why the Monte Carlo cluster formation process just reaches the percolation threshold for two critical lattice gases [14, 15]. This situation resembles the percolation of random clusters [29] and thus of cluster Monte Carlo processes at the Ising or Potts critical point.

A suitable description of $d$-dimensional simple hypercubic lattice gases is by means of variables $s_{\vec{x}}$ that take the value 1 when a particle occupies the lattice site with coordinates $\vec{x} = (x_1, x_2, \ldots, x_d)$, whereas the value $s_{\vec{x}} = 0$ represents the absence of a particle. Including a chemical potential $\mu$ and a nearest-neighbour potential $-K$, we may write the reduced Hamiltonian as

$$-\mathcal{H}/kT = \sum_{\vec{x}} s_{\vec{x}} \left[ \mu + K \sum_{k=1}^{d} s_{\vec{x}+\vec{e}_k} \right] \tag{1}$$

where $\vec{e}_k$ stands for the unit vector in the $k$-direction. Periodic boundary conditions are implicit in the neighbour coordinates: the coordinates $x_k$ are defined modulo the system size $L$. Nearest-neighbour exclusion of the $2d$ adjacent sites occurs in the limit $K \to -\infty$.

We chose the Wolff-like variant of the geometrical cluster method, such that one step consisted of the formation and transformation of one cluster [17]. Random numbers were used to decide whether the transformation involved inversion symmetry with regard to each Cartesian axis. The coordinates of the centre of inversion were also chosen randomly, but such that the geometrical transformation moved the lattice-gas particles from one sublattice to the other. Since these cluster steps conserve the number of particles, and we wish to work in the

grand canonical ensemble, we have also applied Metropolis sweeps. The resulting density fluctuations are expected to reintroduce some critical slowing down, but this effect was not found to be serious in three-dimensional lattice gases [14, 15].

As a generator for the random numbers required in both the Metropolis sweeps and the random choices for the cluster steps, we used a shift-register rule of length 9689 combined with a linear-congruential rule by means of the exclusive-or operation [30]. On the basis of extensive tests [31] involving different cluster algorithms and different Ising-like models, we were confident that this choice does not lead to observable biases. The algorithm indeed passed several tests as mentioned below.

Since we wish to sample the order parameter, i.e. the staggered density,

$$m_{\mathrm{st}} = \frac{1}{L^d} \left\langle \sum_{\vec{x}} s_{\vec{x}} (-1)^{\sum_{k=1}^{d} x_k} \right\rangle \tag{2}$$

the simulations were restricted to even system sizes. From $m_{\mathrm{st}}$ one can calculate the quantity

$$Q_L = \frac{\langle m_{\mathrm{st},L}^2 \rangle^2}{\langle m_{\mathrm{st},L}^4 \rangle} \tag{3}$$

which is related to the Binder cumulant [22]. At low densities the distribution of $m_{\mathrm{st}}$ becomes Gaussian, so that $Q_L$ approaches the value $\frac{1}{3}$, and at high densities the staggered density saturates which corresponds to $Q_L = 1$. At the critical point, $Q_L$ approaches a universal value that may still depend on the dimensionality, the boundary conditions and the aspect ratio of the system. Near this point the curves depicting $Q_L$ as a function of $\mu$ for different $L$ exhibit intersections, from which one can estimate the location of the critical point.

The 64 Mbyte memories of our computing equipment, consisting of a few PCs and workstations, imposed a further restriction on the system sizes. Since each lattice site uses several integers, the total number of lattice sites may not exceed a few million. The simulation lengths are summarized in table 1. This table presents the number of millions of samples taken

**Table 1.** Length of Monte Carlo runs for the four-, five- and six-dimensional Ising models, in millions of sampled configurations (MS). Before taking each sample, one Metropolis sweep and a number GC (also shown) of geometrical cluster steps were executed. In a few cases the values of MS and GC shown here represent a weighted average over runs with a different number of cluster steps.

| | $d = 4$ | | $d = 5$ | | $d = 6$ | |
|---|---|---|---|---|---|---|
| $L$ | MS | GC | MS | GC | MS | GC |
| 2 | 400 | 2 | 200 | 1 | 200 | 1 |
| 4 | 48 | 4 | 14.4 | 50 | 20 | 20 |
| 6 | 32 | 6 | 9.4 | 75 | 10 | 50 |
| 8 | 24 | 8 | 7.2 | 100 | 7.0 | 100 |
| 10 | 20 | 10 | 4.0 | 125 | 3.4 | 200 |
| 12 | 16 | 12 | 2.2 | 150 | 1.1 | 400 |
| 14 | 13.7 | 14 | 1.8 | 800 | | |
| 16 | 12 | 16 | 1.1 | 1200 | | |
| 18 | 10.7 | 18 | 0.5 | 1600 | | |
| 20 | 9.6 | 20 | 1.0 | 1000 | | |
| 24 | 8 | 24 | | | | |
| 28 | 6.9 | 28 | | | | |
| 32 | 6 | 32 | | | | |

per system size, and the number of geometrical cluster steps that were done in addition to one Metropolis sweep before taking a new sample. As mentioned above, one geometrical cluster step means the formation and geometrical transformation of one cluster. The first sample was taken after at least 1000 Metropolis sweeps and the accompanying number of cluster updates. All data were taken close to the critical points, but sufficient variation of $\mu$ was present to estimate the $\mu$ dependence of the relevant finite-size scaling functions in lowest order. The Monte Carlo calculations were checked for internal consistency when the number of cluster steps per Metropolis sweep was varied. Further consistency checks are described in appendix B for systems of size $2^d$. These checks use exact results for $Q$, and the remarkable equivalence of the $2^6$ lattice with the periodic $4^3$ lattice.

## 3. Four dimensions

The renormalization-group theory of the $\phi^4$ model yields useful information of the finite-size scaling form of the amplitude ratio $Q$ and other quantities. The renormalization flow at $d = 4$ is found to become anomalously slow near the critical fixed point. This translates into a very slow finite-size convergence of the various quantities, involving small powers of logarithms of the linear system size $L$. As a result, it is not possible to determine many independent parameters in the fit. We thus make use of the theoretical predictions for the critical exponents, including the powers of the logarithms. Later we will attempt verification of the exponents. Expanding the finite-size scaling function for $Q$, we expect the following behaviour [32]:

$$Q_L(\mu) = Q + \sum_{k=1,2,\ldots} p_k \left\{ L^{y_t} (\ln L)^{\zeta_t} \left[ \mu - \mu_c + v \frac{L^{-y_t}}{(\ln L)^{2/3}} \right] \right\}^k + q_1 L^{d-2y_h} + \cdots + q_3 / \ln L + \cdots \tag{4}$$

with $d = 4$, $\zeta_t = \frac{1}{6}$, $y_h = 3$ and $y_t = 2$. As in the case of the $d = 4$ Ising model [32], the 'shift' term with amplitude $v$ seems unimportant, and was taken to be zero. Discarding system sizes of 4 or smaller, and taking into account terms with $k = 1$, 2 and 3, we find a satisfactory fit leading to $Q = 0.461 \pm 0.005$ and $\mu_c = -0.538\,32 \pm 0.000\,03$. Two-sigma error bars are quoted to account for the slow convergence. This result is in good agreement with the renormalization prediction $Q = 0.4569\ldots$. Assuming that this is indeed the exact value, we fix $Q$ accordingly and find $\mu_c = -0.538\,33 \pm 0.000\,02$ as a somewhat more accurate value for the critical point.

The renormalization prediction for the finite-size scaling behaviour of the staggered compressibility $\chi_L(\mu)$ is

$$\chi_L(\mu) = L^{2y_h - d} (\ln L)^{2\zeta_h} \left( \sum_{k=0,1,2,\ldots} a_k \left\{ L^{y_t} (\ln L)^{\zeta_t} \left[ \mu - \mu_c + v \frac{L^{-y_t}}{(\ln L)^{2/3}} \right] \right\}^k + b_1 / \ln L + b_2 / (\ln L)^2 + \cdots \right) \tag{5}$$

with $\zeta_h = \frac{1}{4}$. The numerical data do not allow us to simultaneously determine all exponents involved, and we left only one exponent free at a time. First, we applied a least-squares procedure with $\zeta_h$, $\zeta_t$, $y_t$ fixed at their renormalization predictions and $\mu_c$ as found from the analysis of $Q$. Furthermore, the so-called shift of the critical temperature was omitted again, i.e. we set $v = 0$. This yielded $y_h = 2.992 \pm 0.007$ for $L_{\min} = 6$ and $y_h = 3.000 \pm 0.012$ for $L_{\min} = 8$. Next, we fixed $y_h = 3$ and let $\zeta_h$ free. This yielded $\zeta_h = 0.231 \pm 0.014$ for $L_{\min} = 6$ and $\zeta_h = 0.247 \pm 0.017$ for $L_{\min} = 8$. Both estimates agree well with the renormalization prediction.

Also the particle density $\rho$ was subjected to a finite-size analysis. The renormalization theory predicts for this energy-like quantity

$$\rho_L(\mu) = c_0 + \cdots + L^{y_t-d}(\ln L)^{\zeta_t}\left(b_1/\ln L + b_2/(\ln L)^2 + \cdots \right.$$
$$\left. + \sum_{k=0,1,2,\ldots} a_k \left\{ L^{y_t}(\ln L)^{\zeta_t}\left[\mu - \mu_c + v\frac{L^{-y_t}}{(\ln L)^{2/3}}\right]\right\}^k \right). \tag{6}$$

Using the value of $\mu_c$ found above, and solving for $y_t$ in the least-squares fit, we obtain $y_t = 1.998 \pm 0.008$ for $L_{\min} = 6$, again in agreement with the theory.

## 4. Five dimensions

For $d > 4$, the renormalization-group theory of the $\phi^4$ model predicts that the logarithmic factors in $L$ disappear: they transform into powers of $L$ with exponents proportional to $4 - d$. Although the situation thus seems not to be as difficult as for $d = 4$, the convergence is still rather slow when $d$ is close to 4. Expansion of the theoretically calculated finite-size scaling function for $Q$ in powers of $L$ and $\mu - \mu_c$ yields, for $d > 4$ (see, e.g., [23]),

$$Q_L(\mu) = Q + \sum_{k=1,2,\ldots} p_k \left\{ L^{y_t^*}\left[\mu - \mu_c + vL^{y_i-y_t}\right]\right\}^k + q_1 L^{d-2y_h^*} + \cdots + q_3 L^{y_i} + \cdots \tag{7}$$

with $y_i = 4 - d$, $y_h^* = y_h - y_i/4$, $y_t^* = y_t - y_i/2$, $y_h = (d + 2)/2$ and $y_t = 2$. A least-squares fit to the data for $d = 5$, in which the exponents were kept fixed, system sizes $L \geqslant 4$ were used, and three terms in the sum on $k$ were included, yielded $Q = 0.454 \pm 0.003$ and $\mu_c = -0.909\,83 \pm 0.000\,02$. The expected value $Q = 0.4569\ldots$ agrees well with our result. We thus assumed the validity of the theoretical prediction for $Q$ in order to obtain an improved estimate of $\mu_c$. However, the results are still slightly dependent on possible additional terms in equation (7) such as one proportional to $L^{2y_i}$. After a considerable number of fits, our resulting best estimate is $\mu_c = -0.909\,82 \pm 0.000\,02$.

The following finite-size expansion for the density was used:

$$\rho_L(\mu) = c_0 + \cdots + L^{y_t^*-d}\left\{ \sum_{k=0,1,2,\ldots} a_k \left[L^{y_t^*}\left(\mu - \mu_c + vL^{y_i-y_t}\right)\right]^k + b_1 L^{y_i} + b_2 L^{2y_i} + \cdots \right\}. \tag{8}$$

Since a cross term proportional to $(\mu - \mu_c)L^{y_i}$ is absent in this formula, the data points for small $L$ used in the fits were restricted to a narrow range: $|\mu - \mu_c| < 0.005$ for $L = 4$ and $|\mu - \mu_c| < 0.015$ for $L = 6$. Satisfactory least-squares fits to the numerical data appear to be possible without the terms proportional to $v$ and $b_2$, and these were assumed to be negligible. A fit to the data for $L \geqslant 4$, with $y_i$ fixed at its renormalization prediction $-1$ and $\mu_c$ fixed at the value just found, yielded $y_t^* = 2.503 \pm 0.010$, in agreement with the theoretical value $y_t^* = \frac{5}{2}$.

The staggered compressibility is expected to behave like

$$\chi_L(\mu) = L^{2y_h^*-d}\left( \sum_{k=0,1,2,\ldots} a_k \left\{ L^{y_t^*}\left[(\mu - \mu_c)(1 + sL^{y_i}) + vL^{y_i-y_t}\right]\right\}^k \right.$$
$$\left. + b_1 L^{y_i} + b_2 L^{2y_i} + \cdots \right). \tag{9}$$

A fit to the data for $L \geqslant 4$ yielded $y_h^* = 3.70 \pm 0.03$ which is close to the expected value $y_h^* = \frac{15}{4}$. Variations in the number of free parameters in the fit formula led to similar results, within a few times $10^{-2}$ from $\frac{15}{4}$, in those cases where the residual was acceptable. For instance, neglecting the terms proportional to $s$ and $v$, we obtained a satisfactory fit for $L \geqslant 8$, leading to $y_h^* = 3.75 \pm 0.02$. This agrees well with the theoretical prediction and also with the result $y_h^* = 3.748 \pm 0.009$ for the five-dimensional Ising model in [32].

## 5. Six dimensions

According to the renormalization prediction, the corrections to scaling will converge faster than in five dimensions, but our range of available system sizes is now restricted to $L \leqslant 12$. We have fitted equation (7) with $d = 6$, taking three terms in the sum on $k$, to the Monte Carlo data for $L \geqslant 4$. This led to the results $\mu_c = -1.176\,97 \pm 0.000\,03$ and $Q = 0.454 \pm 0.003$. The result for $Q$ is again in a good agreement with the expected value $Q = 0.4569\ldots$. Assuming exact validity of this number we obtain $\mu_c = -1.176\,95 \pm 0.000\,02$ for the critical point.

The finite-size data for the nearest-neighbour sum could be matched by equation (8) with $d = 6$, within reasonable statistical margins. Since a cross term such as that with amplitude $s$ in equation (9) was not taken into account here, the fit was restricted to data points close to the critical point: $|\mu - \mu_c| < 0.01$. The $\chi^2$ criterion allowed us to neglect the term proportional to $v$. The fit for $L \geqslant 4$ then yielded $y_t^* = 3.011 \pm 0.014$, close to the theoretical value $y_t^* = 3$.

The staggered compressibility data with $L \geqslant 4$ could be well described by equation (9). The terms with amplitudes $s$ and $v$ were necessary to obtain an acceptable $\chi^2$, but the rapidly decaying one with amplitude $b_2$ seemed insignificant and was omitted. The least-squares fit yielded $y_h^* = 4.51 \pm 0.02$, in accordance with the expected value $y_h^* = \frac{9}{2}$.

## 6. Classical approximations

The results found above for the high-dimensional lattice gases agree nicely with the renormalization scenario. Accordingly, the critical exponents and the amplitude ratio $Q$ assume the 'classical' or mean-field-like values. One may thus wonder to what extent non-universal properties such as the critical point, can be reproduced by classical theories. For this reason we present two such classical analyses of the nearest-neighbour exclusion lattice gas.

Both analyses have the following notation in common. Every site has $q$ nearest-neighbour sites. The particle density $\rho$ is controlled by assigning a Boltzmann weight $\exp(\mu)$ to every occupied site. Furthermore, the lattice consists of two sublattices, such that the two sites of each nearest-neighbour pair occupy different sublattices. In the ordered phase, the particle densities $\rho_1$ and $\rho_2$ on the two sublattices are different.

### *6.1. Mean-field-like description*

Assuming the absence of correlations, one can express the probability of occupation of a site of sublattice 1, i.e. $\rho_1$, in $\rho_2$ and vice versa. The analysis of these self-consistency equations is given in appendix A and leads to the result that a mean-field-like transition occurs at a critical density

$$\rho_c = \frac{1}{q+1} \tag{10}$$

and the corresponding chemical potential $\mu_c$ is determined by

$$\exp(-\mu_c) = \frac{q^q}{(q+1)^{q-1}} - 1. \tag{11}$$

### *6.2. Bethe-lattice approximation*

Another type of classical approximation involves the replacement of the real lattice by the Bethe lattice (BL) having the same number $q$ of nearest neighbours per site. The hierarchical nature of the Bethe lattice allows the description of the partition sum by means of a recursion relation from which one may read the breaking of the sublattice symmetry. For more details of a general nature see, e.g., [11]. The necessary derivations are given in appendix A. They predict a mean-field-like transition when the density reaches the critical value

$$\rho_c = \frac{1}{q} \tag{12}$$

and the value of the chemical potential satisfies

$$\exp(-\mu_c) = \frac{(q-2)^q}{(q-1)^{q-1}}. \tag{13}$$

The two approximations formulated above display the mean-field like property that the results depend only on the lattice structure via the number of nearest neighbours.

## 7. Discussion

In sections 3–5 we have already observed that the universal parameters $Q$, $y_h^*$ and $y_t^*$ agree well with the theoretical predictions for Ising-like models. Together with results obtained earlier for the four- and five-dimensional Ising model [24, 32], these findings are in a complete agreement with the work of Brézin and Zinn-Justin [19]. The mean-field-like estimates for the critical density and the corresponding chemical potential, as obtained in the previous subsection, can be compared with various numerical results for $(d = q/2)$-dimensional simple hypercubic lattice gases. Results for $d = 2$ have been obtained by means of a transfer-matrix analysis [33] and for $d = 3$ we make use of the Monte Carlo results obtained via the geometric cluster algorithm in [14], and of new simulation data to improve the accuracy. The analysis of the Binder cumulant yields $Q_c = 0.6226 \pm 0.0011$, in good agreement with the expected universal value $Q_c = 0.6233$ [31], and $\mu_c = 0.054\,48 \pm 0.000\,03$. Assuming universality, and fixing the value of $Q$ accordingly, yields $\mu_c = 0.054\,50 \pm 0.000\,01$. For $4 \leqslant d \leqslant 6$ we quote the Monte Carlo results obtained above. Table 2 summarizes the 'mean-field' and Bethe-lattice values of $\mu_c$ as well as the numerical results for $\mu_c$.

With increasing number of dimensions, the 'MF' and 'BL' results are seen to approach the values of the numerical calculations, in accordance with expectation. Because correlations are

**Table 2.** 'Mean-field', Bethe-lattice and Monte Carlo results for the critical chemical potential.

| $d$ | $\mu_c$ (MF) | $\mu_c$ (BL) | $\mu_c$ (numerical) |
|---|---|---|---|
| 2 | −0.046 884 | 0.523 248 | 1.344 015 1004(8) |
| 3 | −0.574 356 | −0.270 577 | 0.054 50(2) |
| 4 | −0.919 366 | −0.712 705 | −0.538 33(2) |
| 5 | −1.175 875 | −1.019 394 | −0.909 82(2) |
| 6 | −1.380 039 | −1.254 173 | −1.176 95(2) |

**Table 3.** 'Mean-field', Bethe-lattice and Monte Carlo results for the critical density.

| $d$ | $\rho_c$(MF) | $\rho_c$(BL) | $\rho_c$ (numerical) |
|---|---|---|---|
| 2 | $\frac{1}{5}$ | $\frac{1}{4}$ | 0.367 743 000(5) |
| 3 | $\frac{1}{7}$ | $\frac{1}{6}$ | 0.210 490(3) |
| 4 | $\frac{1}{9}$ | $\frac{1}{8}$ | 0.143 334(3) |
| 5 | $\frac{1}{11}$ | $\frac{1}{10}$ | 0.109 392(2) |
| 6 | $\frac{1}{13}$ | $\frac{1}{12}$ | 0.088 948(2) |

neglected in mean-field-like treatments one expects the cluster density to be underestimated. The clusters will therefore percolate at a lower value of $\mu$. Indeed, the Monte Carlo results for $\mu_c$ are higher than both the 'MF' and 'BL' values, where it is noted that the Bethe-lattice approach yields generally better estimates than the mean-field approximation. Van den Berg and Steif [16] have shown that the critical activity of the lattice gas is at least $P_c/(1 - P_c)$, where $P_c$ is the critical probability for site percolation on the graph. This lower bound [16] is lower than the Bethe-lattice value for the cases shown in table 2.

Table 3 shows the 'mean-field' and Bethe-lattice values of $\rho_c$ as well as numerical results for $\rho_c$. The error estimates in the last decimal place are shown in parentheses. These errors include the uncertainty margin in the critical point. Also here, one observes that the agreement between the different entries improves with increasing dimensionality, and that the results of the Bethe-lattice approach are better than those of the mean-field approximation.

Finally, we present a formula that describes the numerical data for the critical points in $d = 2$ to 6 dimensions. Since both equations (11) and (13) can be expanded in $d = q/2$ as $\exp(-\mu_c) = [2(d-1)/e](1 - \sum_{i=1}^{\infty} a_i d^{-i})$ we may choose a Padé form:

$$\exp(-\mu_c) = \frac{2(d-1)}{e} \frac{1 + a_1 d^{-1} + a_2 d^{-2}}{1 + b_1 d^{-1} + b_2 d^{-2}}. \tag{14}$$

The numerical results for the critical points are approximately reproduced by $a_1 = -1.985\,20$, $a_2 = 0.995\,95$, $b_1 = -1.614\,57$ and $b_2 = 2.122\,43$. However, the differences, which amount to a few times $10^{-4}$, exceed the numerical accuracies listed in table 2. For large $d$, equation (14) reproduces the expected mean-field-like dependence on the number of neighbours. Apart from that, there is no reason to assign more than just a phenomenological meaning to it. We remark that in an analysis of the Ising critical points, the formula presented by Galam and Mauger [34] does not obey the expected dependence when the number of neighbours becomes large.

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## Appendix A

Consider a bipartite lattice gas where each site has $q$ nearest neighbours, and with sublattice densities $\rho_1$ and $\rho_2$ governed by an activity $\exp(\mu)$ per particle.

*Mean-field-like analysis*

We assume that the probabilities of occupation of the sites on sublattice 2 are independent. The probability that no nearest-neighbour site of a site on sublattice 1 is occupied is thus $p_1 = (1 - \rho_2)^q$, so that the density on sublattice 1 is

$$\rho_1 = (1 - \rho_2)^q/(1 + \exp[-\mu]). \tag{A1}$$

On the basis of symmetry we also have

$$\rho_2 = (1 - \rho_1)^q/(1 + \exp[-\mu]). \tag{A2}$$

These two equations represent the condition of self-consistency for the particle densities. We find one solution to these equations with $\rho_{st} \equiv \rho_1 - \rho_2 = 0$. At low densities this is the stable solution. At higher densities we find two symmetry-breaking solutions with $\rho_{st} \neq 0$, e.g. $\rho_1 = 1$, $\rho_2 = 0$ for the case $\mu = \infty$. These are the stable solutions at high densities. In the limit $\rho_{st} \to 0$ the difference between equations (A1) and (A2) becomes

$$\rho_{st} = \frac{d(1 - \rho)^q}{d\rho} \frac{\rho_{st}}{1 + \exp(-\mu)} + \cdots \tag{A3}$$

where we have omitted third and higher powers of $\rho_{st}$. Thus, a mean-field like transition occurs at

$$\frac{q(1 - \rho)^{q-1}}{1 + \exp(-\mu_c)} = 1. \tag{A4}$$

Combination with the self-consistency equation for the dilute phase, i.e. $\rho = (1 - \rho^q)/(1 + \exp[-\mu])$, yields the critical density $\rho_c = 1/(q + 1)$. The corresponding chemical potential is determined by $\exp(-\mu_c) = q^q/(q + 1)^{q-1} - 1$.

*Bethe-lattice approximation*

Let $Z_{1,n}$ be the restricted partition sum of a length-$n$ branch of the Bethe lattice, starting with an occupied site; and let $Z_{0,n}$ be such a sum for a branch growing from an empty site. A recursion follows when we connect $q - 1$ such branches to a new site:

$$Z_{1,n+1} = e^{\mu} Z_{0,n}^{q-1}$$

$$Z_{0,n+1} = (Z_{0,n} + Z_{1,n})^{q-1}.$$

We express this recursion using the new variable $x_n \equiv Z_{0,n}/Z_{1,n}$ as

$$x_{n+1} = e^{-\mu} \left(1 + \frac{1}{x_n}\right)^{q-1}. \tag{A5}$$

A fixed point of this recursion occurs for

$$e^{\mu} x_{fp}^q = (x_{fp} + 1)^{q-1}. \tag{A6}$$

Since the derivative of the right-hand side of equation (A5) with respect to $x_n$ is negative, the recursion oscillates about the fixed point. Marginal stability, associated with the symmetry-breaking phase transition, occurs for $dx_{n+1}/dx_n = -1$ which leads to

$$e^{\mu} x_{fp}^q = (q - 1)(x_{fp} + 1)^{q-2}. \tag{A7}$$

Combination with equation (A6) yields $x_{\rm fp} = q - 2$. Substitution in the fixed-point equation leads to the critical activity

$$\exp(\mu_{\rm c}) = (q-1)^{q-1}/(q-2)^q. \tag{A8}$$

In order to find the critical density $\rho_{\rm c}$ at a site far from the outer surface, we connect $q$ branches to that site. The expectation value becomes

$$\rho_{\rm c} = \frac{{\rm e}^{\mu} Z_{0,n}^q}{(Z_{0,n} + Z_{1,n})^q + {\rm e}^{\mu} Z_{0,n}^q} = \frac{{\rm e}^{\mu} x_n^q}{(1+x_n)^q + {\rm e}^{\mu} x_n^q}. \tag{A9}$$

Substitution of equation (A6) and $x_{\rm fp} = q - 2$ yields $\rho_{\rm c} = 1/q$.

## Appendix B

In order to calculate the partition sum of a hard-core lattice gas on a bipartite lattice, one may treat the variables on sublattice 1 as independent ones, and restrict the sum on the variables on sublattice 2 to obey the nearest-neighbour exclusion. Approximations can be obtained by allowing only a limited number of particles on sublattice 1. Since the resulting sum in particular covers the densest configurations, it may be taken as a high-density approximation. When more particles are allowed on sublattice 1, the quality of the approximation improves and, in the case of a finite lattice, it will eventually include all configurations and thus become exact.

If sublattice 1 of the lattice is empty, no restrictions apply to the sites of sublattice 2. Thus, in lowest-order approximation the sum becomes

$$Z_0 = -1 + (1 + z z_{\rm st})^{N/2} + \left(1 + \frac{z}{z_{\rm st}}\right)^{N/2}$$

where $z = {\rm e}^{\mu}$, $z_{\rm st} = {\rm e}^{\mu_{\rm st}}$ and $\mu_{\rm st}$ is the staggered chemical potential. If there is one lattice-gas atom on sublattice 1, it prevents $2d$ sites from being occupied, so that

$$Z_1 = -\tfrac{1}{2}N\left(\tfrac{1}{2}N - 2d\right)z^2 + \frac{N}{2}\frac{z}{z_{\rm st}}\left\{-1 + (1 + z z_{\rm st})^{N/2-2d}\right\} + \tfrac{1}{2}N z z_{\rm st}\left\{-1 + \left(1 + \frac{z}{z_{\rm st}}\right)^{N/2-2d}\right\}$$

has to be added to the partition sum. However, periodic boundary conditions may lead to modifications. If, for example, the lattice size in the $x$-direction is 2, the neighbours in the $+x$- and $-x$-directions are the same. We present some results for simple hypercubic lattices of size $2^d$.

For $d = 3$ the presence of one atom prevents the occupation of all sites on the other sublattice but one. Thus

$$Z = -1 + (1 + z z_{\rm st})^4 + \left(1 + \frac{z}{z_{\rm st}}\right)^4 + 4z^2.$$

After taking the appropriate derivatives with respect to $\mu_{\rm st}$ we obtain the second and fourth moments of the staggered density and

$$Q = \frac{8z\left(1 + 6z + 9z^2 + 4z^3\right)^2}{\left(2\,(1+z)^4 + 4z^2 - 1\right)\left(1 + 24z + 81z^2 + 64z^3\right)}.$$

For the case $d = 4$ even more particles are needed on sublattice 1 in order to prevent the population of sublattice 2. We obtain

$$Z = -1 + (1 + zz_{st})^8 + \left(1 + \frac{z}{z_{st}}\right)^8 + 8\frac{z}{z_{st}}\left\{-1 + (1 + zz_{st})^4\right\}$$
$$+8zz_{st}\left\{-1 - 4\frac{z}{z_{st}} + \left(1 + \frac{z}{z_{st}}\right)^4\right\} + 24z^4.$$

With increasing dimensionality, the calculation of $Q$ tends to become lengthy, and it was therefore done by computer algebra. Also the formula for $Q$ becomes lengthy, and we present the result only in numerical form: $Q = 0.442\,735\,6114$ for $\mu = -0.538$. The result of our Monte Carlo calculation with $\mu = 0.538$ was $Q = 0.442\,75(2)$.

The partition sum for the $L = 2$ system in $d = 5$ is

$$Z = -1 + (1 + zz_{st})^{16} + \left(1 + \frac{z}{z_{st}}\right)^{16} + 16zz_{st}\left\{-1 - 11\frac{z}{z_{st}} + \left(1 + \frac{z}{z_{st}}\right)^{11}\right\}$$
$$+16\frac{z}{z_{st}}\left\{-1 + (1 + zz_{st})^{11}\right\} + 80z^2z_{st}^2\left\{-1 - 8\frac{z}{z_{st}} - 28\left(\frac{z}{z_{st}}\right)^2 + \left(1 + \frac{z}{z_{st}}\right)^8\right\}$$
$$+80\left(\frac{z}{z_{st}}\right)^2\left\{-1 - 8zz_{st} + (1 + zz_{st})^8\right\}$$
$$+40z^2z_{st}^2\left\{-1 - 6\frac{z}{z_{st}} - 15\left(\frac{z}{z_{st}}\right)^2 + \left(1 + \frac{z}{z_{st}}\right)^6\right\}$$
$$+40\left(\frac{z}{z_{st}}\right)^2\left\{-1 - 6zz_{st} + (1 + zz_{st})^6\right\} + 160\frac{z^7}{z_{st}}\left\{15 + 6\frac{z}{z_{st}} + \left(\frac{z}{z_{st}}\right)^2\right\}$$
$$+160\left(\frac{z}{z_{st}}\right)^3\left\{-1 - 6zz_{st} - 15z^2z_{st}^2 + (1 + zz_{st})^6\right\} + 240\frac{z^7}{z_{st}}\left(5 + \frac{z}{z_{st}}\right)$$
$$+240z^6\left\{10 + 5zz_{st} + z^2z_{st}^2\right\} + 160z^6 + 80\frac{z^9}{z_{st}} + 80z^9z_{st} + 980z^8 + 16z^{10}.$$

After some further computer algebra and numerical operations we obtain $Q = 0.393\,120\,3291$ for $\mu = -0.91$. From the Monte Carlo calculation we obtained the value $Q = 0.393\,09(3)$ for this value of $\mu$.

The numerical results for the $2^6$ system were checked in a different way. For this purpose we made use of the equivalence of the $2^6$ lattice (without periodic boundaries, but this is immaterial for the present hard-core lattice gas) with the periodic $4^3$ lattice [35]. The meaning of this equivalence is that a one-to-one mapping between the sites of both lattices exists, such that nearest neighbours remain nearest neighbours. As a test of the Monte Carlo program, we performed runs of $10^8$ cycles for both systems. At $\mu = -1.177$ we obtained $Q = 0.366\,98(3)$ for the $2^6$ lattice and $Q = 0.366\,94(5)$ for the $4^3$ lattice.

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