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Dependence of Lattice Gas Properties on Mesh Size*

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The way in which the properties of a lattice gas converge to the properties of a real gas as the number of sites covered per particle is increased, till configuration space is a continuum, is investigated. Only for one-dimensional hard lines have the properties been worked out exactly for any mesh size, with the result that at any density the free volume per particle must span at least 50 lattice sites for the lattice gas pressure to approximate the real gas pressure within 1%. In the limit of close packing the lattice gas leads to an incorrect asymptotic form of the pressure for any finite mesh size. The virial coefficients for a lattice gas with a coarse spacing can be shown to differ in order of magnitude from the real gas coefficients. Inequalities between the real gas configurational integral and the lattice gas configurational sum can be established in any number of dimensions. Finally, by relating lattice and real gas results, an approximate way is found to predict properties of real gases in two and three dimensions from lattice results alone.

1. INTRODUCTION

THE term "lattice gas" is in fact a misnomer since a real gas is not realistically described by placing particles on a lattice whose mesh size is comparable to the average nearest-neighbor separation. The lattice model corresponds to a trapezoidal rule evaluation of the configurational integral, and it must therefore be anticipated that noticeable errors in the thermodynamic functions result whenever the lattice spacing is comparable in magnitude to the characteristic length of the interparticle potential. The lattice model has, of course, been introduced because the properties of it are more easily calculable then those of a real gas, as most dramatically illustrated by the demonstration of the condensation phenomenon. The phase transition for a two-dimensional lattice gas whose particles have a repulsive core and an attractive nearest-neighbor attraction is one of the few that can be rigorously established.

Nevertheless, the fundamental question remains of how well lattice gas properties approximate real gas properties and, in particular, whether phase transitions or their order are not artifacts of the model. As the mesh is made finer relative to a given interparticle spacing a better approximation of the real gas is obtained; but, if this mesh size has to be quite fine for accurate representation of a real gas, then the mathematical simplicity of the model is lost.

At very low densities in the conventional lattice theory many lattice sites cover the volume accessible to the particles, and the lattice model gives an accurate description of the real gas. However, at higher densities, for hard particles, the numbers of occupied and unoccupied sites are usually comparable; thus the volume accessible to the particles (free volume) is poorly approximated. This is the situation at the density of the gas–liquid phase transition. Even worse, at still higher densities the occupied sites outnumber the unoccupied sites. In addition, at high densities regions of phase space are tenuously connected by narrow

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channels, and the coarse lattice theory cannot be expected to give even a qualitatively correct description. The crude approximation to the phase space volume might affect, in particular, the solid–fluid phase transition in the model.

Up to now exact lattice gas properties have been determined in two dimensions when the repulsive core of the particles covers a single site, and the density is half the close-packed density.[1] It has been possible to calculate thermodynamic variables at higher and lower densities, and in three dimensions by using series expansions. When the lattice is only twice as fine, the core of each particle occupying two sites in two dimensions, the problem is so difficult that analytical solution has not yet been possible. It is therefore of practical interest to see how well the results for a continuous configuration space are approximated by those of discrete, coarse spaces.

The convergence to the continuum configuration space results is here investigated, by examining the properties of hard parallel lines, squares, and cubes as a function of mesh size. The convergence is found to be slow, even at quite low densities, so that a particle must occupy more than a few lattice sites for accurate results. This rules out analytical treatment. The only practical alternative way to study lattice gases with finer meshes is a numerical scheme using the Monte Carlo method. In any numerical scheme configuration space is a lattice, because the position of a particle can only be specified to an accuracy determined by the number of significant figures carried in the computer. This accuracy is typically one part in 10^8, so that the volume is spanned by an extremely fine lattice. However, it is an easy matter to decrease the number of significant figures by which a particle position is described. In this way lattice gases could be studied as a function of the number of sites covered per particle.

The Monte Carlo method has been extensively used to study lattice gases[2] but with emphasis on the dependence of the results on the number of particles, not on the lattice spacing. These studies illustrate some of the formal differences between lattice and real gases. For example, due to the lack of a dynamic analog of the lattice gas, the useful relation between the pressure and the radial distribution function given by the virial theorem in the continuum case does not hold on the lattice. However, somewhat more cumbersome alternative ways to calculate the pressure have been devised and used.[2] On the other hand, the mathematical treatment of the lattice gas resembles the treatment of the real situation in many ways. If the usual configuration space integration is replaced by a corresponding sum, as in numerical integration, the thermodynamic formulae, the Mayer cluster expansion formalism, and the Ornstein–Zernike relation can all be used without change. There is thus hope that the mathematical singularities at phase transitions will be the same for the lattice and real gases, so long as the lattice spacing is comparable to the linear dimension of the free volume. This criterion is satisfied at the gas–liquid phase transition, but not at the solid–fluid one. Thus there is evidence for a second-order phase transition for two- and three-dimensional lattice gases of hard particles,[3] while the continuum hard-circle and hard-sphere systems apparently have a first-order transition.[4] The hope that these solid–fluid transitions are related must be substantiated by making the mesh size finer.

2. ONE-DIMENSIONAL LATTICE GASES

The case of a one-dimensional lattice gas with an arbitrary mesh was worked out exactly by Lee and Yang,[5] complementing the corresponding continuum solution of Herzfeld and Goeppert-Mayer.[6] The one-dimensional example thus serves as a particularly good test case because, as is shown later, in two and three dimensions the behavior at both low and high densities is analogous. In the intermediate density region, the one-dimensional systems show no phase transition, but the qualitative deductions made at these densities can be applied to the higher-dimensional cases.

In the general one-dimensional hard lattice gas the one-dimensional "volume" corresponds to a line of L sites. N particles are placed on the line, and each particle covers s sites. The lattice is close-packed when the total number of sites, L, equals Ns. At lower densities, a lattice containing N particles leaves $L-Ns$ sites unoccupied. The configurational sum Q_Σ is merely the number of distinguishable ways N particles and $L-Ns$ unoccupied sites can be arranged:

$$Q_\Sigma(s)=\frac{[(L-Ns)+(N)]!}{[(L-Ns)!][(N)!]}. \tag{1}$$

The corresponding formula in the continuum case is

$$Q_f(s)=(L-Ns)^N/N! \tag{2}$$

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[1] T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), Chap. 7.

[2] D. A. Chesnut and Z. W. Salsburg, J. Chem. Phys. **38**, 2861 (1963).

[3] The "hard squares" model described by C. Domb [Nuovo Cimento Suppl. **9**, 9 (1958)] has recently been analyzed by M. E. Fisher and D. S. Gaunt (to be published). Fisher and Gaunt use Padé approximants for the 11-term low-density $P(z)$ series and the nine-term high-density $P(z^{-1})$ series; they find a second-order transition at about three-fourths the close-packed density. Their model forbids occupation of nearest-neighbor sites on a square lattice. The model we examine in Sec. 3 forbids not only nearest- but also second-nearest-neighbor site occupations in two dimensions, $s=2$.

[4] B. J. Alder and T. E. Wainwright, J. Chem. Phys. **33**, 1439 (1960); Phys. Rev. **127**, 359 (1962).

[5] T. D. Lee and C. N Yang, Phys. Rev. **87**, 417 (1952).

[6] K. F. Herzfeld and M. Goeppert-Mayer, J. Chem. Phys. **2**, 38 (1934).

From (1) and (2) the following inequalities for Q_{Σ} and $Q_{\int}$ are obtained:

$$Q_{\Sigma}(s-1) > Q_{\int}(s-1) > Q_{\Sigma}(s) > Q_{\int}(s). \qquad (3)$$

Equations (1) and (2) show that the lattice gas entropy, $k \ln Q_{\Sigma}$, exceeds the continuum gas entropy at any density. The pressure is obtained by the usual thermodynamic formula and the use of Stirling's approximation. For the lattice gas the pressure is given by

$$P_{\Sigma}/kT = (\partial \ln Q_{\Sigma}/\partial L)_{N,T} = \ln(1+f^{-1}), \qquad (4)$$

while the corresponding continuum expression is

$$P_{\int}/kT = f^{-1}, \qquad (5)$$

where f is the one-dimensional equivalent of the free volume (unoccupied volume per particle), $(L-Ns)/N$. Equations (4) and (5) show that the pressure inequalities are opposite in direction to the entropy inequalities:

$$P_{\Sigma}(s-1) < P_{\int}(s-1) < P_{\Sigma}(s) < P_{\int}(s). \qquad (6)$$

For a particular value of s it can be seen that the pressures from (4) and (5) are identical only when there is an infinite number of unoccupied sites per particle. In general the expression $P_{\Sigma}/P_{\int} = \ln(1+f^{-1})^{f}$ describes the error in the pressure as determined from the lattice model. Thus the difference in pressure for $f=50$ is 1% at any density. The pressure error can be traced to an edge effect, due to measuring a line of nonintegral length by counting the number of lattice sites which fit within it. For values of f sufficiently large for edge effects to have meaning, the error incurred averages half a unit; thus an error of one-half unit out of 50 means an accuracy of 1%. The length of the free volume is always overestimated by the lattice model, and consequently the lattice gas pressure is too low.

The mesh size necessary to obtain any particular accuracy depends only on the number of sites contained in the free volume f. Thus, to maintain the same accuracy (same number of unoccupied sites per particle) as density increases, it is necessary to make the mesh finer. For example, demanding 1% agreement in the pressure requires an s of 12 at 20% of close packing and an s as large as 450 at 90% of close-packing. When s is 2, the lattice gas equation of state is accurate within 1% only for densities less than $Ns/L = \frac{1}{26}$. This corresponds to a very dilute gas, and it is not surprising, as will be shown in the next section, that the virial coefficients according to the lattice gas model differ significantly from those of the continuum model when the lattice is coarse. At the other extreme, in the limit of close packing, the ratio of lattice pressure to continuum pressure approaches zero for any finite mesh size or finite s. This is because the limiting free volume vanishes and the mesh spacing must also in order that a given number of unoccupied lattice sites remain. A reasonable limit at which the lattice model becomes totally unrealistic is reached when there is an average of only one unoccupied site per particle to estimate the free volume ($f=1$). This occurs at a density of $\frac{2}{3}$ of close packing for particles covering two sites each; for the more common choice, particles covering one site, the model becomes unrealistic at a density half that of close packing, the point at which the two- and three-dimensional Ising model phase transitions (with attractive forces in addition to the core) are found.[1]

Inequalities (3) and (6) suggest that a functional relation can be found which brings the lattice and continuum results into agreement. A simple way of finding such a relation, which can later be applied in two and three dimensions, is to choose an effective diameter σ for the continuum particles, such that the continuum pressure is the same as the lattice pressure at all number densities:

$$\sigma = (L/N) - \{\ln[(L-Ns+N)/(L-Ns)]\}^{-1}. \qquad (7)$$

At low density σ reduces to $s-\frac{1}{2}$. This functional relation depends, of course, on the mesh size; as an illustration σ is plotted versus density for s equals 2 in Fig. 1. Notice that σ is always less than s, and that the simple low-density approximation, $\sigma = \frac{3}{2}$, holds within 2% up to half the close-packed density.

The effect of adding a nearest-neighbor repulsive mound or attractive well to the one-dimensional hard-core model has been worked out both in the lattice[5] and in the continuum[6] case. In Fig. 2 $P_{\Sigma}/P_{\int}$ is plotted as a function of density for the nearest-neighbor potential $\phi(r<1)=\infty$, $\phi(1 \leq r < 2) = E$, $\phi(2 \leq r) = 0$; the curves labeled "mound" and "well" correspond to E/kT equals ln10 and $-$ln10, respectively. The purely hard-core case is also drawn for comparison. It can be observed that the pressure error for densities less than half of close packing is nearly independent of the sign or magnitude of E. The pressure differences at low density can therefore be attributed mainly to the repulsive core of the potential. At higher densities the pressure discrepancy depends more strongly upon the nature of the potential surrounding the hard core, being greatest for attractive forces. Again the pressure

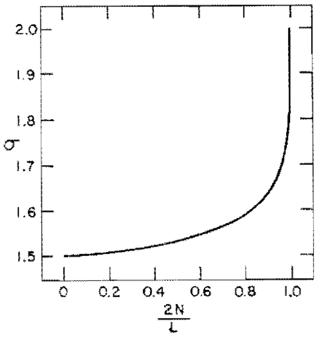

FIG. 1. Variation of the effective diameter of a particle in the continuum case. σ is chosen such that the lattice and continuum gas pressures are identical for one-dimensional hard lines in which the lattice gas particles cover two sites each.

from the lattice model is always less than that from the continuum model.

3. TWO- AND THREE-DIMENSIONAL HARD LATTICE GASES

The lattice gas on a square lattice in which each particle covers more than one site has not been worked out completely. The low-density properties can, however, be easily derived from the virial expansion of the pressure. This is because Mayer's cluster expansion can be specialized to a discrete configuration space, and, just as in the continuum case for squares and cubes, the Mayer $\mathfrak{f}$ function can be factored into a product of one-dimensional $\mathfrak{f}$ functions.[7,8] Thus, the lattice gas star sums factor into products of one-dimensional star sums. These one-dimensional star sums for the case in which each particle covers two sites have been worked out in detail and are listed in the Appendix through the seven point stars. From these it is possible to evaluate the first seven virial coefficients in one, two, and three dimensions (particles covering 2, 4, and 8 sites, respectively). These are listed in Table I. In one dimension the general nth virial coefficient B_n for a lattice gas is known from the expansion of the pressure [see Eq. (4)] as a power series in the number density,

$$P/kT=\sum B_n(N/L)^n; \qquad B_n=[s^n-(s-1)^n]/n. \quad (8)$$

The analogous value in the continuum case is $B_n=s^{n-1}$, corresponding to the limit of the lattice value as the number of sites each particle covers goes to infinity. The virial coefficients in one, two, and three dimensions for the continuum situation have been evaluated by integration of Mayer's star integrals,[7,8] and are listed in Table I for comparison with the lattice results. As was already inferred from the differences between the lattice and continuum one-dimensional equations of state at low densities, even the first few virial coefficients are significantly different in this case, in which the number of sites covered by each particle is so small. A comparison between the lattice and continuum versions of the two- and three-dimensional virial coefficients shows that in higher dimensions the discrepancy becomes even larger. Thus the radius of convergence of the lattice virial series can be, for coarse lattices, significantly different from that of the continuum series. This should serve primarily as a warning that the behavior observed at high density in the conventional treatment of a lattice gas may differ qualitatively, as well as quantitatively, from that of its continuum analog.

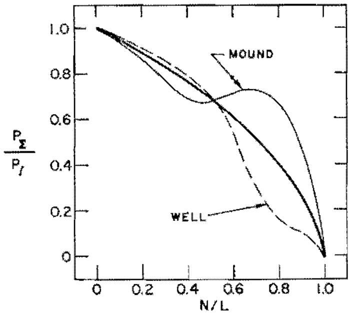

FIG. 2. The ratio of the one-dimensional lattice gas pressure to the continuum gas pressure as a function of density, when repulsive or attractive potentials are present. The heavy curve corresponds to the purely hard-core case.

TABLE I. Virial coefficients for hard lines, squares, and cubes in units of particle volume. The particles on the lattice cover 2^D sites in D dimensions and the particles in the continuum case have a volume in D dimensions of σ^D.

	Lattice gas $B_n/(2^D)^{n-1}$			Continuum gas $B_n/(\sigma^D)^{n-1}$		
	Lines	Squares	Cubes	Lines	Squares	Cubes
B_2	0.750	1.125	1.688	1.000	2.000	4.000
B_3	0.583	1.021	1.786	1.000	3.000	9.000
B_4	0.469	0.832	1.349	1.000	3.667	11.333
B_5	0.388	0.641	0.731	1.000	3.722	3.160
B_6	0.328	0.480	0.168	1.000	3.025	−18.880
B_7	0.283	0.355	−0.229	1.000	1.651	−43.505

A qualitative argument that the behavior in the solid–fluid phase transition region may be altered in a coarse lattice gas is based on the observation that these transitions occur,[4,9] in two and three dimensions, at a density corresponding to a linear expansion of about 15% from close packing. It has already been shown that for $s=2$ there is less than one unoccupied site available to estimate the free volume at that density. If, as seems likely, the melting phenomenon involves a highly cooperative motion corresponding to small channels connecting small pockets in configuration space, the lattice will have to be fine enough to allow the system to sample the detailed shape of these regions. In the gas–liquid transition region the situation is not nearly so bad. That transition occurs at a linear expansion of about 60%, and the accessible regions in phase space are broader and more extensively connected than in the solid–fluid case. It is possible that the mathematical nature of the continuum gas–liquid singularity will be preserved with a lattice particle covering only two sites because the significant narrow regions in phase space, might be comparable to the mesh width.

More quantitative statements are difficult to make, particularly in the phase transition region. However, interestingly enough, the lattice gas provides bounds on the thermodynamic functions for the real gas. For

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[7] R. W. Zwanzig, J. Chem. Phys. **24**, 855 (1956).

[8] W. G. Hoover and A. G. De Rocco, J. Chem. Phys. **36**, 3141 (1962).

[9] W. W. Wood and J. D. Jacobson, J. Chem. Phys. **27**, 1207 (1957); B. J. Alder and T. E. Wainwright, *ibid.*, p. 1208.

example, it can easily be shown that for hard particles the inequalities (3) are also satisfied in two and three dimensions, so that the lattice gas entropy is also too large. The physical basis of the proof does not depend on the number of dimensions: evaluating the hypervolume of accessible phase space by counting the integral number of unit hypercubes whose centers, lattice phase points, lie within the hypervolume always overestimates the hypervolume near the edge of accessible phase space. On the other hand, leaving out all unit hypercubes which intersect the edge underestimates the extent of accessible phase space, and so the bounds are established.

Because the entropy inequalities hold in two and three dimensions it is tempting to speculate that the pressure inequalities (6) are equally valid, even though individual virial coefficients (Table I) do *not* satisfy corresponding inequalities. However, with the use of the virial coefficients it can be confirmed that the lattice pressure is too low at low density. In support of the surmise that this is also true at higher densities, the asymptotic form of the lattice gas pressure, as the density approaches close packing, is estimated in the simplest possible example, namely, squares covering four sites. In that example, the area at close-packing, V, will contain $V/4$ particles, and the number density, $\rho=N/V$, will be $\frac{1}{4}$. Near close packing we expect that the leading two terms in the lattice gas grand partition function, $\Xi=\sum Q_N z^N$, correspond to putting $V/4$ and $(V-1)/4$ particles on the lattice. Then

$$\Xi=Q_{V/4}z^{V/4}+Q_{(V-1)/4}z^{(V-1)/4}+\cdots,$$

where z is the activity. $Q_{V/4}$ is 1, because there is only one way in which to arrange $V/4$ nonoverlapping squares on V sites. $Q_{(V-1)/4}$ is proportional to V, because any one of V sites can be left vacant, and the proportionality constant k accounts for the number of ways the $(V-1)/4$ particles can then be arranged. Because this is still a very limited number of ways, k is of the order of unity. Thus near close packing the grand partition function is of the form

$$\Xi=z^{V/4}(1+kVz^{-\frac{1}{4}}+\cdots)=z^{V/4}\exp(kVz^{-\frac{1}{4}}+\cdots). \quad (9)$$

Then, from the usual thermodynamic relations, the equations $P/kT=\ln z^{\frac{1}{4}}+kz^{-\frac{1}{4}}$ and $\rho=\frac{1}{4}-kz^{-\frac{1}{4}}/4$ are obtained. The asymptotic expression for the pressure is

$$P/kT=\ln[1/(1-4\rho)]+O(\ln k)+O(1-4\rho). \quad (10)$$

In order to arrive at (10) a term with a single vacant site was included in the grand partition function. This seems a peculiar choice, because removal of a particle from any *finite* close-packed system would leave four such unoccupied sites. We cannot justify this choice rigorously, and only point out here why we believe it is plausible. As V becomes large (and we are actually interested in the limit that V approaches infinity) V passes through values that are multiples of 4, with remainders of 0, 1, 2, or 3. We expect that each of these kinds of V will contribute to the limit of Ξ, although it is difficult to weight the different sizes (as well as shapes) properly. Even the one-dimensional system illustrates a part of this complexity. In the simplest relevant case, $s=2$, it is necessary to include volumes with both odd and even numbers of sites (weighted equally) in Ξ to obtain a correct high-density expansion of the equation of state.

In view of the fact that (10) rests upon such intuitive ideas, it is worthwhile to obtain it in another way, also approximate, but unrelated to the foregoing arguments:

Consider the lattice gas equation of state from the viewpoint of the recent reformulation of the virial series.[10] It was shown that the nth virial coefficient can be expressed as

$$(-)^{(n,2)}\frac{1}{n}\int\prod_{i<j}^{n}\mathfrak{f}_{ij}d\mathbf{r}^{n-1}+\text{other terms},$$

where the "other terms" are numerous, and not necessarily small. Neglecting these terms, and using the fact that the lattice sum corresponding to the above integral is $(2^{\mu}-1)^2(-)^{n(n-1)/2}$ for hard squares of side length 2, yields $B_n=(4^n-2^{n+1}+1)/n$. Summing the virial series gives, in this approximation, an equation of state again of the form (10):

$$P/kT=\ln\{(1-2\rho)^2/[(1-\rho)(1-4\rho)]\}. \quad (11)$$

This approximate equation of state has also been arrived at (in a different way) by Temperley.[11] In support of the statement that the terms which have been kept are the dominant ones in this lattice gas virial series, some of the left-out terms mentioned above have been evaluated also, and found to make finite contributions to the pressure at the close-packed density.

The logarithmic dependence of the pressure on free volume shows that the lattice gas pressure is also too small at high densities, since in the continuum case the pressure depends inversely on the free volume; P/kT approaches $(2-8\rho)^{-1}$ near the close-packed situation just treated.[12] This establishes that, just as in the one-dimensional case, $P_{\Sigma}/P_{\int}$ approaches zero in the close-packed limit.

Besides the bounds just established it would be desirable to make the lattice gas results more quantitative without the prohibitive task of making the mesh finer. It was already pointed out that the chief difference between the lattice and continuum results came, in the lattice case, from an overestimate of the free volume. This overestimate was remedied in one dimension by introducing an effective diameter for the particles [see Eq. (7)]. The low density form of the effective diameter, $\sigma=s-\frac{1}{2}$, is exact for the second virial coeffi-

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[10] F. H. Ree and W. G. Hoover, J. Chem. Phys. **41**, 1635 (1964).

[11] H. N. V. Temperley, Proc. Phys. Soc. (London) **77**, 630 (1961).

[12] W. G. Hoover, J. Chem. Phys. **40**, 937 (1964).

TABLE II. One-dimensional star sums.

	Index	Absolute values of the sums
$n=2$	1	3
$n=3$	1	7
$n=4$	1–3	19, 17, 15
$n=5$	1–10	51, 45, 45, 43, 41, 39, 37, 35, 33, 31
$n=6$	1–18	141, 121, 121, 117, 111, 115, 109, 107, 107, 107, 103, 103, 101, 113, 103, 99, 99, 99,
	19–36	97, 97, 95, 97, 93, 91, 91, 87, 87, 95, 91, 91, 89, 87, 85, 85, 85, 83,
	37–54	83, 81, 81, 83, 81, 81, 79, 77, 77, 75, 75, 77, 75, 73, 71, 69, 69, 67,
	55–56	65, 63
$n=7$	1–18	393, 333, 325, 319, 309, 299, 293, 291, 287, 287, 289, 287, 287, 291, 281, 287, 279, 279,
	19–36	279, 275, 269, 271, 267, 261, 263, 309, 285, 275, 267, 265, 265, 263, 273, 263, 263, 261,
	37–54	265, 259, 259, 259, 255, 257, 259, 259, 257, 255, 255, 251, 253, 251, 249, 249, 257, 245,
	55–72	245, 247, 247, 243, 247, 243, 247, 245, 241, 241, 241, 239, 239, 237, 235, 237, 239, 233,
	73–90	227, 227, 223, 307, 269, 257, 249, 249, 249, 247, 247, 251, 243, 255, 239, 239, 239, 239,
	91–108	239, 239, 241, 237, 235, 239, 237, 233, 231, 231, 231, 233, 231, 231, 231, 229, 229, 231,
	109–126	231, 227, 227, 227, 227, 225, 225, 225, 225, 223, 227, 223, 229, 223, 221, 221, 221, 221,
	127–144	221, 219, 221, 219, 217, 219, 217, 221, 217, 217, 217, 219, 219, 215, 213, 213, 211, 211,
	145–162	211, 209, 209, 211, 209, 209, 209, 209, 213, 207, 203, 199, 199, 253, 233, 233, 227, 225,
	163–180	223, 223, 223, 225, 219, 219, 219, 215, 215, 215, 217, 215, 215, 215, 213, 215, 219, 211,
	181–198	211, 211, 213, 213, 209, 209, 209, 209, 207, 207, 211, 209, 207, 213, 207, 207, 207, 205,
	199–216	207, 203, 203, 205, 201, 203, 203, 203, 207, 201, 201, 201, 203, 199, 201, 199, 199, 199,
	217–234	199, 197, 197, 197, 199, 197, 197, 197, 201, 195, 197, 195, 195, 195, 193, 195, 193, 193,
	235–252	193, 195, 191, 191, 191, 189, 189, 189, 187, 187, 185, 185, 185, 183, 185, 183, 189, 217,
	253–270	211, 209, 207, 203, 203, 201, 199, 199, 199, 199, 199, 199, 195, 195, 201, 197, 195, 195,
	271–288	197, 193, 191, 191, 191, 191, 195, 189, 189, 189, 189, 189, 187, 187, 187, 189, 187, 187,
	289–306	187, 189, 187, 185, 185, 185, 185, 183, 183, 183, 183, 185, 183, 181, 183, 181, 181, 183,
	307–324	181, 181, 181, 179, 179, 179, 179, 177, 183, 177, 175, 175, 175, 175, 175, 173, 173, 173,
	325–342	173, 171, 171, 171, 169, 169, 171, 169, 199, 191, 193, 191, 187, 185, 183, 183, 183, 179,
	343–360	179, 179, 179, 177, 177, 177, 177, 177, 175, 175, 175, 177, 179, 175, 173, 171, 171, 171,
	361–378	171, 171, 169, 171, 169, 171, 171, 169, 167, 167, 167, 165, 165, 165, 165, 165, 165, 163,
	379–396	163, 163, 163, 163, 165, 163, 161, 159, 159, 159, 159, 157, 155, 175, 177, 171, 171, 169,
	397–414	169, 169, 167, 167, 165, 163, 165, 163, 165, 161, 161, 161, 159, 159, 157, 157, 157, 157,
	415–432	155, 155, 155, 153, 153, 153, 153, 153, 151, 153, 151, 151, 149, 149, 149, 163, 161, 159,
	433–450	159, 155, 153, 153, 151, 149, 149, 149, 147, 147, 147, 147, 145, 145, 143, 143, 143, 157,
	451–468	147, 145, 145, 143, 141, 141, 139, 139, 137, 141, 139, 137, 135, 133, 133, 131, 129, 127.

cient not only in one dimension, but in two and three dimensions as well, for the hard-core interparticle potentials considered here. Furthermore, the third virial coefficient is also much improved by the same choice of σ. For $s=2$, $B_3(\text{lattice})/B_3(\text{continuum})=1.04$, 1.08, and 1.12, as opposed to the uncorrected values of 0.58, 0.34, and 0.20 in one, two, and three dimensions, respectively. Indeed the scaling correction given by (7) is quite accurate for lattice gas densities up to $\frac{1}{2}$ of close packing not only in one dimension, but in three dimensions as well. The value of σ corresponding to $s=2$ at $\frac{1}{2}$ close-packing is $2-1/\ln(1.5)=1.5337$, so that in three dimensions the equation of state evaluated from the virial series gives for the lattice $PV/NkT=2.506$, and for the continuum $PV/NkT=2.481$ with this value of σ. The agreement between the lattice and continuum results is within 1%. This suggests that lattice gas results can be related to continuum results in general by some scaling such as the one demonstrated here. Other types of scaling might be obtained by considering that lattice gas results at a given density correspond to real gas results at a lower effective density. Thus, the Ising model phase transition at half the close-packed density may actually correspond to the experimentally observed gas–liquid transition, which occurs at a somewhat lower density.

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We thank Warren G. Cunningham for his help in coding the evaluation of the sums given in the Appendix.

APPENDIX

The one-dimensional star sums for hard particles on a lattice covering two sites each are listed in Table II. The numbers given are for the star sums contributing to B_2, B_3, B_4, B_5, B_6, and B_7. The ordering of the star sums is identical with that used in listing the star integrals in Ref. 8 for the continuum gas. There are 1, 1, 3, 10, 56, and 468 of these, respectively.