Exact Solution of a Directed-Site Animals-Enumeration Problem in Three Dimensions

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An exact equivalence is established between the directed-site animals-enumeration (DSAE) problem in d dimensions and a crystal-growth model defined on the same lattice. In special cases, the latter reduces to the calculation of the free energy of a $(d-1)$-dimensional lattice gas with extended hard cores. The author solves a DSAE problem with $d=3$ exactly by using its equivalence to the hard-hexagon problem, and shows that the exponent $\theta=\frac{5}{6}$. A new and simpler solution to the DSAE problem on the square and triangular lattices is given.

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The directed-site animals-enumeriation (DSAE) problem is an elegant combinatorial formulation of a problem with applications in many different fields, and has been discussed in several papers recently.[1] In one dimension the problem is trivial. The $d=2$ problem can be solved exactly with use of its equivalence to a lattice-gas model studied earlier by Verhagen.[2] In this Letter, I solve exactly a three-dimensional DSAE problem on a simple-cubic lattice with nearest-neighbor (nn) and next-nearest-neighbor (nnn) connections by showing its equivalence to the hard-hexagon gas model solved recently by Baxter.[3] I show that the exponent θ and the "correction-to-scaling" exponent Ω are both $\frac{5}{6}$ in this case.

I establish a more general equivalence between the d-dimensional DSAE problem and the calculation of average density in a crystal-growth model (CGM) defined on the same lattice. In special cases (if the conditional probabilities of the CGM satisfy the detailed balance condition), the calculation of average density in the CGM reduces to that for a $(d-1)$-dimensional lattice gas with hard-core interactions. Using these equivalences, I also obtain a new and simpler solution to the DSAE problem on the square and triangular lattices.

Consider a d-dimensional lattice in which all bonds are directed, and there are no directed loops (Fig. 1). A site j will be said to be a successor of site i iff there exists a bond from i to j. For a set of sites C, the set of successor sites will be denoted by $S(C)$. The set of sites at least one of whose successors is in C will be denoted by $S^{-1}(C)$. A directed animal $\mathcal{A}$ with a source C is a configuration of occupied sites such that all the source sites are in $\mathcal{A}$, and a site $i\in C$ is in $\mathcal{A}$ only if at least one of the sites in $S^{-1}(i)$ is also in $\mathcal{A}$. This is the directed animals constraint. The number of sites in $\mathcal{A}$ will be denoted by $|\mathcal{A}|$.

We define[4] an integer-valued time coordinate $t(i)$ for each site i of the lattice, such that for any two sites i and j, if $j\in S(i)$, then $t(j)\geqslant t(i)+1$. It follows that allowed configurations of occupied sites at the surface $t=T$ depend only on the configuration of occupied sites at earlier times $t\leqslant T-1$. Consider first, for simplicity, the case when they depend only on the configuration at the surface $t=T-1$ [Figs. 1(a) and 1(b)]. Let C be a set of occupied sites on a constant-t hypersurface. We define the generating functions

$$A_C(x)=\sum_{n=1}^{\infty}x^n A_C(n), \tag{1}$$

where $A_C(n)$ is the number of distinct animals

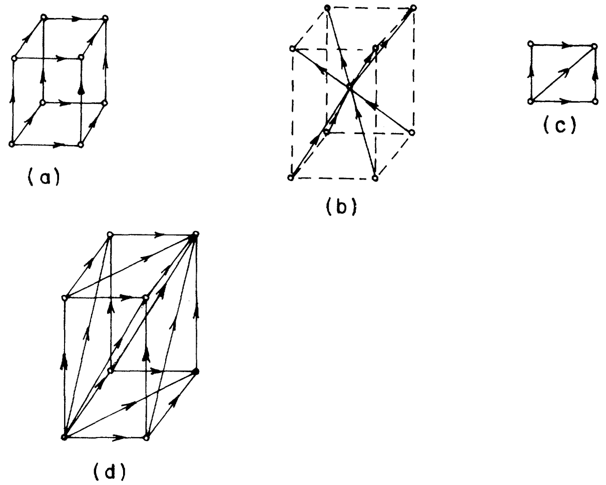

FIG. 1. Unit cells of the directed lattices discussed in text. (a) The d-dimensional simple-hypercubical lattice for $d=3$. (b) The body-centered hypercubical lattice for $d=3$. (c) The triangular lattice. (d) The simple-cubic lattice with nearest-neighbor and next-nearest neighbor bonds. Bonds from the site (0,0,0) have end points at (0,0,1), (1,0,0), (0,1,0), (1,1,0), (1,0,1), and (0,1,1).

with size n having source C.

The Markovian property of directed animals implies that the generating functions satisfy the recursion relations

$$A_C(x) = x^{|C|}[1 + \sum_D A_D(x)], \tag{2}$$

where the summation over D extends over all the proper subsets of $S(C)$. Note that the time coordinate of sites in D is greater by 1 than that of C. It is easy to generalize Eq. (2) to the case when the allowed configurations of occupied sites at $t = T$ depend on the configuration of sites at $t \leq T - 2$ also [Figs. 1(c) and 1(d)]. These recursion equations form the Bogoliubov-Born-Green-Kirkwood-Yvon heirarchy of equations for the DSAE problem. Iteration of these recursions is a fairly efficient way of generating animal numbers for various lattices.[5] In the following, we use these to establish the equivalence between DSAE and CGM.

The CGM is defined[6] as follows: We consider the same lattice as in the DSAE problem, and define a new "time coordinate" $\tau(i) = -t(i)$. In this model, at time $\tau = 0$, all sites with $\tau > 0$ are unoccupied and some of the sites with $\tau \leq 0$ are occupied. At time $\tau = T$, particles from an external reservoir come and occupy some of the sites on the surface $\tau = T$. The probability that a particular site i is occupied or stays unoccupied depends only on the configuration of sites in $S(i)$, and is independent of the occupancy of other sites. The state of sites on the surface $\tau = n$ does not change at any later time. The DSAE corresponds to a particularly simple choice of the conditional probability of occupation of i, given the occupancy of sites in $S(i)$: It is 0 if any of the sites in $S(i)$ is occupied; and it is p, if all sites in $S(i)$ are unoccupied.

Let $P(C)$ denote the probability that all sites in the set C lying on a constant-τ hypersurface are occupied. [I assume that τ is so large that $P(C)$ is independent of τ.] This is equal to $p^{|C|}$ multiplied by the probability that all sites in $S(C)$ are unoccupied. With use of the inclusion-exclusion principle

$$P(C) = p^{|C|}[1 + \sum_D (-1)^{|D|} P(D)], \tag{3}$$

where the summation over D extends over all the proper subsets of $S(C)$. Comparing with Eq. (2) we see that

$$A_C(x = -p) = (-1)^{|C|} P(C). \tag{4}$$

Thus the generating function of directed animals starting from a single point source is determined by the average density of occupied sites in the CGM problem. The equivalence is easily generalized to lattices with next-nearest-neighbor bonds, etc. [Fig. 1(c)].

The d-dimensional CGM may alternatively be viewed as describing the stochastic time development of a $(d-1)$-dimensional lattice gas. The $(d-1)$-dimensional lattice consists of r interpenetrating sublattices $L_1, L_2, \ldots, L_r$, each of which is isomorphic to a constant-τ hyperplane of the d-dimensional lattice ($r = 2$ or 3 in the cases discussed below). The configuration of occupied sites on the plane $\tau = mr + i$ of the CGM defines the configuration on the sublattice L_i at times $\tau = mr + i + j$, where m is any integer and $0 \leq j < r$. At times $\tau = mr + i$ $(1 \leq i \leq r)$ sublattice L_i undergoes a stochastic change of configuration of occupied sites while other sublattices are unchanged. As $\tau \to \infty$, the probability of different configurations of the lattice gas tends to an invariant limiting distribution. For arbitrary transition rates, the calculation of the invariant distribution is quite difficult. In the models studied below, the transition rates are particularly simple and correspond to commonly used Monte Carlo algorithms for studying the equilibrium properties of lattice gases with hard-core interactions. The invariant distribution is the equilibrium Boltzmann distribution corresponding to a lattice-gas Hamiltonian which can be written down by inspection. The Hamiltonian is of the form

$$H = +\infty \sum_{(ij)} n_i n_j - \ln(z) \sum_i n_i, \tag{5}$$

where the n_i's are the occupation numbers of the sites i, and the first sum is over all nn pairs. The calculation of equal-time correlation functions in the CGM then reduces to that of the equilibrium correlation functions in a $(d-1)$-dimensional lattice gas. I consider some illustrative examples below.

Example 1.—Consider DSAE on a d-dimensional body-centered hypercubical (d-bch) lattice. The sites are labeled by d integers $(n_1, n_2, \ldots, n_d)$, which are all odd or all even. There are 2^{d-1} bonds going outward from each site $(n_1, n_2, \ldots, n_d)$ to sites $(n_1 \pm 1, n_2 \pm 1, \ldots, n_{d-1} \pm 1, n_d + 1)$ [Fig. 1(b)]. It is easy to see that this case corresponds to successive relaxation to thermal equilibrium of the two sublattices of a lattice gas on a $(d-1)$-bch lattice having the Hamiltonian given by Eq. (4) with $z = p/(1-p)$.

If the animal-numbers generating function for a single point source on the d-bch lattice is $A_{d\text{-bch}}(x)$, we see from Eq. (4) that

$$A_{d\text{-bch}}(x) = -\rho_{(d-1)\text{-bch}}(z = -x/(1+x)), \qquad (6)$$

where $\rho_{(d-1)\text{-bch}}(z)$ is the density of the lattice gas on a $(d-1)$-bch lattice having nn exclusion (nne) and with activity z.

Specializing to the case $d = 3$, we see that the DSAE problem on the 3-bch lattice corresponds to a "hard-squares" problem on the 2-bch (square) lattice. The exact solution to this problem is not yet known. Baxter, Enting, and Tsang[7] have evaluated the first 42 terms in the Taylor expansion of $\rho_{2\text{-bch}}(z)$ in powers of z. With use of Eq. (6), these determine the animal numbers on the 3-bch lattice up to size 42.

Setting $d = 2$, we get the equivalence of DSAE on the 2-bch (square) lattice to a nne lattice gas on a linear chain. It is easy to see that the density of the gas as a function of its activity z is given by

$$\rho_1(z) = \tfrac{1}{2} - (\tfrac{1}{4} + z)^{-1/2}. \qquad (7)$$

Substituting $z = -x/(1+x)$, we get the generating function for square-lattice animals[2]

$$A(x) = [\{(1+z)/(1-3z)\}^{1/2} - 1]/2. \qquad (8)$$

The generating functions for animals corresponding to a general source C are given in terms of the n-point functions of the one-dimensional gas, and are easily determined. We thus rederive the results of Hakim and Nadal[1] in a more transparent way.

Example 2.—The DSAE problem on the triangular lattice [Fig. 1(c)] also corresponds to a one-dimensional nne lattice gas. The only difference here is that an occupied site at time T must become vacant at time $T+2$, while a vacant site with vacant neighbors becomes occupied with a rate p. Hence, the activity of the lattice gas is $z = p$. Substitution of this relation into Eq. (7) gives the generating function for animal numbers on a triangular lattice.[2]

Example 3.—Consider a simple-cubic lattice with nn and nnn directed bonds. The bonds have a positive projection in the [111] direction. There are six bonds going out of each site [Fig. 1(d)]. it is easy to see that the corresponding two-dimensional stochastic process describes the cyclic relaxation to thermal equilibrium of the three sublattices of a nn-exclusion lattice gas on a triangular lattice. If $A_3(x)$ is the generating function of animals growing from a point source in this problem, we have from Eq. (4)

$$A_3(x) = -\rho_{\text{hh}}(z = -x/(1+x)),$$

where $\rho_{\text{hh}}(z)$ is the hard-hexagon density as a function of their activity z. With use of Baxter's expression for the free energy of the hexagon gas as a function of its activity, it can be shown that as x tends to $x_c = 2/(9+5\sqrt{5})$ from below, $\rho_{\text{hh}}(z)$ varies as

$$\rho_{\text{hh}}(z = -x/(1+x)) = -\epsilon^{-1/6}[a_0 + a_1\epsilon^{5/6}] + \text{less singular terms},$$

where $\epsilon = x_c - x$, and a_0 and a_1 are numerical constants. This implies that for large n, the animal numbers $A_3(n)$ vary as

$$A_3(n) = a_0\lambda^n n^{-\theta}[1 + b_0 n^{-\Omega} + O(1/n)],$$

where a_0, λ, and b_0 are some constants, and θ and Ω are critical exponents. In this case

$$\lambda = (9+5\sqrt{5})/2, \quad \theta = \Omega = \tfrac{5}{6}. \qquad (9)$$

To test the universality of the exponent θ, I analyzed the 42-term hard-square density series of Baxter *et al.* I used a seven-parameter sequential fit of the form

$$\ln A_n = a_0 n + a_1 - \theta\ln(n) + a_2 n^{-1} + a_3 n^{-2} + a_4 n^{-5/6} + a_5 n^{-11/6}.$$

The values of a_0 obtained for n lying between 28 and 42 using seven successive terms of the series agree with each other to the first eight significant digits. θ seems to converge to the value 0.83334 ±0.00003. The hard-square and the hard-hexagon gases correspond to two- and three-state Potts models, respectively, and are known to have different critical exponents for positive activities. The exponent for negative z, however, appears to be independent of the Potts index q. This value of θ agrees quite well with earlier numerical estimates,[8] 0.837±0.003. Finally, I note that because of relations between critical exponents, this implies that for four-dimensional undirected animals, $\theta = \frac{11}{6}$, and for two dimensions the Lee-Yang edge-singularity exponent is $\sigma = -\frac{1}{6}$.

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[1] See, for example, D. Dhar, M. K. Phani, and M. Barma, J. Phys. A 15, L279 (1982); H. E. Stanley, S. Redner, and Z. R. Yang, J. Phys. A 15, L569 (1982); J. L. Cardy, J. Phys. A 15, L593 (1982); F. Family, J. Phys.

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[4] This is always possible for acyclic directed graphs.

[5] The two-dimensional lattices were studied by Dhar *et al.* (Ref. 1). For the three-dimensional simple-cubic lattice, I was able to extend the animal series of Stanley *et al.* (Ref. 1) by two more terms using only about 3 h on a CYBER 170–730 machine. For completeness, the last two terms are listed here: $A_{16} = 11\,003\,117\,220$; $A_{17} = 56\,701\,633\,987$.

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