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J. Phys. A: Math. Gen. 27 (1994) 3683–3687. Printed in the UK

Random sequential adsorption on a 3 × ∞ lattice: an exact solution

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Received 26 November 1993

Abstract. The dynamics of a random sequential adsorption process on a quasi-one-dimensional lattice with three rows is solved exactly. The long-time behaviour of the coverage density is $\rho(t)=\frac{1}{3}-2\exp[-(\frac{2}{3}+t)]/9$. It is shown that the number of connected lattice animals increases like $n!^{2/3}$, indicating that most two-dimensional lattice animals are non-compact.

Random sequential adsorption (RSA) is an irreversible random deposition process. In its simplest form particles interacting via a short-range hard core repulsion are absorbed randomly, one at a time, into a d-dimensional space. The adsorbed particles obey the following conditions: (i) particles do not overlap; (ii) absorbed particles are permanently fixed in their spatial position. Thus at each step a new particle is either rejected from the volume, or it is added at random at an accessible point in the diminished volume formed by all previously adsorbed particles. The deposition process ceases when all unoccupied spaces are smaller than the size of an adsorbed particle. The system is then jammed in a non-equilibrium state, whose average density ρ_r is clearly expected to be smaller than the corresponding density of closest packing ρ_0. A variety of physical, chemical, biological and ecological irreversible processes are described by RSA models [1]. Furthermore, since the RSA phase is a non-equilibrium disordered phase for all values of ρ, it has been suggested as a phenomenological model for glasses and supercooled liquids [2].

Exact solutions for RSA models are available only for one-dimensional systems [3–6]. Recently, an exact solution was obtained for the RSA process with mutual nearest-neighbour (NN) exclusion on a quasi-one-dimensional lattice, consisting of a strip of two infinite rows ($2\times\infty$) [7, 8]. The filling process on this lattice exhibits some features typical of two-dimensional systems. In addition, the solution indicates that the number of lattice animals, consisting of n connected points, increases like $\sqrt{n!}$, in sharp contrast to the characteristic exponential dependence of the $d=1$ system. The dependence of these properties on the width of the strip is an interesting question. Therefore in this paper we extend the methods of [8] to obtain an exact solution for RSA on a lattice strip consisting of three infinite rows ($3\times\infty$).

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Let s_i be a two-state occupation variable defined as 1 in case site i is empty and 0 in case it is occupied. It has been shown [9] that the nth derivative of the ensemble average $\langle s_i\rangle$ with respect to $u=\exp(-t)$ at $u=1$ ($t=0$) is given by a sum of all possible combinations of n points connected lattice animals (provided the lattice is empty at $t=0$, more general initial conditions may be implemented as well). The connectivity range between lattice sites is determined by the range of the hard core repulsion. It is worthwhile to mention that time derivatives of $\langle s_i\rangle$ are redundant, since they are given by a sum of all combinations of n step paths, including paths that visit a point more than once. Therefore u is the natural time variable for RSA on lattices. As a result, macroscopic observables are given by expansions in powers of $(1-u)$, in particular the density is given by

$$\rho(t)=1-\langle s_i\rangle=\sum_{n=1}(-1)^{(n-1)}a_n(1-u)^n/n!. \tag{1}$$

The coefficients a_n are positive integers which are equal to the number of connected lattice animals containing n points, and their computation reduces to an enumeration problem.

The enumeration process of [9] simplifies considerably on quasi-one-dimensional lattices, since the number of boundary points at each step is independent of n. In the $d=1$ case with NN exclusion there is a single generating configuration resulting in the simple recursion relation $a_n=2a_{n-1}$. Similarly, the enumeration on the $2\times\infty$ strip with NN exclusion, described in [8], has three characteristic configurations, resulting in an exact solution of the problem. On the $3\times\infty$ strip of a square lattice, with mutual NN exclusion and periodic boundary conditions, the time evolution (enumeration process) has six characteristic generating configurations:

$$A_n(0,0,u)=\prod_{i=1} s_{1,i}s_{2,i}s_{3,i} \tag{2a}$$

$$A_n(j,k,u)=A_n(0,0,u)s_{1,0}\ldots s_{j,0}s_{1,n+1}\ldots s_{k,n+1}\qquad\text{with}\quad 0\leqslant j\leqslant k\leqslant 2. \tag{2b}$$

The time evolution of the generators is given by the close set of six n-independent coupled differential equations:

$$\mathrm{d}A(0,0)/\mathrm{d}u=6A(0,1) \tag{3a}$$

$$\mathrm{d}A(0,1)/\mathrm{d}u=2A(0,2)+3A(1,1)+u^2A(0,1) \tag{3b}$$

$$\mathrm{d}A(0,2)/\mathrm{d}u=A(0,0)+3A(1,2)+2uA(0,1) \tag{3c}$$

$$\mathrm{d}A(1,1)/\mathrm{d}u=4A(1,2)+2u^2A(1,1) \tag{3d}$$

$$\mathrm{d}A(1,2)/\mathrm{d}u=A(0,1)+2A(2,2)+2uA(1,1)+u^2A(1,2) \tag{3e}$$

$$\mathrm{d}A(2,2)/\mathrm{d}u=2A(0,2)+4uA(1,2) \tag{3f}$$

with the initial conditions $A(j,k,u=1)=1$ for all j and k.

Utilizing the C_3 symmetry of the set of equations, i.e. $u\to\exp(2\pi in/3)u$, $n=0,1,2$ under which the $A(j,k,u)$ transform covariantly, it is easy to see that the solution is

$$A(0,0)=u^4f(u) \tag{4a}$$

$$A(0,1)=(2u^3+u^6)f(u)/3 \tag{4b}$$

$$A(0,2)=(u^2+2u^5)f(u)/3 \tag{4c}$$

$$A(1,1)=(4u^2+4u^5+u^8)f(u)/9 \tag{4d}$$

$$A(1,2)=(2u+5u^4+2u^7)f(u)/9 \tag{4e}$$

$$A(2,2)=(1+4u^3+4u^6)f(u)/9 \tag{4f}$$

where $f(u)=\exp[2(u^3-1)/3]$. Each of the polynomials of equations (4) has a characteristic power, modulo 3, reflecting the C_3 symmetry of the problem. We recall that the set of three coupled differential equations on the $2\times\infty$ lattice possesses C_2 symmetry, resulting in a qualitatively similar solution with a common exponential factor $f(u)=\exp(u^2-1)$ [8].

The coverage density $\rho(u)$ is given by

$$\rho(u)=(1-u)-(1-u)^2-2\int_u^1 \mathrm{d}v\int_v^1 \mathrm{d}y\, A(1,1,y) + 2\int_u^1 \mathrm{d}v\int_v^1 \mathrm{d}y\int_y^1 \mathrm{d}x[A(0,0,x)+4A(1,2,x)]. \tag{5}$$

The long-time behaviour of the density is easily evaluated as a series in u:

$$\rho(u)=\tfrac{1}{3}-c_1u-c_2u^2-\mathrm{O}(u^3) \tag{6}$$

where

$$c_1=2f(0)/9=0.114\,092\,69\ldots$$

$$c_2=\left(\tfrac{1}{2}+f(0)\int_0^1 y\exp(2y^3/3)\,\mathrm{d}y\right)/9=0.093\,563\,227\,7\ldots.$$

The jamming density $\rho_r=\rho_0=\frac{1}{3}$. The source of this unusual equality and unusual low value of ρ_0 is the compatibility between the range of the interaction and the width of the lattice. It imposes abnormally strong correlations along columns, resulting in the occupation of one particle per column. At the $u=0$ limit every column is occupied with one particle, and $\rho_r=\frac{1}{3}$. It is worthwhile mentioning that ρ_r is well below the two-dimensional value $\rho_r(d=2)=0.364\,13$ (1) [9, 10]. In figure 1 the exact time evolution

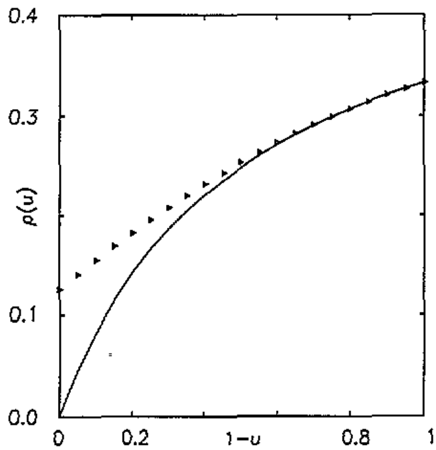

Figure 1. The exact time evolution of the coverage density $\rho(u)$ (continuous line) is shown as a function of $(1-u)$. The long-time approximation of equation (6) Δ bounds the exact values from above for all u.

is compared to the long-time approximation equation (6). The approximation bounds the exact values from above, and for $u<0.5$, i.e. $t>0.69$, the errors do not exceed 2%.

The expansion coefficients a_n of equation (1) are related to the coefficients $A_n(j, k)$ (the nth derivative of $A(j, k, u)$ at $u=1$) by

$$a_{n+3}=2A_n(0,0)+16A_n(1,2)+4[A_n(1,1)+n(2A_{n-1}(1,1)+(n-1)A_{n-2}(1,1))]. \qquad (7)$$

The n dependence of the coefficients is determined by the power of u in $f(u)$, resulting in an asymptotic increase of the forn $n!^{2/3}$; clearly, the a_ns have the same n dependence. Since the number of connected lattice animals on the $d=2$ square lattice is greater than their number on the $3\times\infty$ lattice, the result above is a lower bound for their number. This lower bound excludes the possibility that most of the lattice animals are compact with few interior vacancies and smooth perimeters. A growth process of compact lattice animals is determined by the number of sites on the perimeter, resulting in an $n!^{1/2}$ dependence.

Unfortunately, it is difficult to extend the present method to a $4\times\infty$ strip, since the time evolution (enumeration process) is determined by an infinite set of generators. The jump to infinity in the number of the generators results from the fact that the lattice width becomes bigger than the exclusion range of the NN hard core repulsion. Thus, lattice sites along the direction of the width of the lattice are no longer necessarily topologically equivalent. The enumeration process depends therefore on the details of the distribution of the occupations along this direction, resulting in an infinite number of generators. Nevertheless, one may construct an RSA process with an anisotropic exclusion, whose time evolution is given by a finite set of generators. Consider an RSA filling process on an $m\times\infty$ strip with NN exclusion along the infinite direction and $(m-1)$ neighbour exclusion along the width of the strip. The filling process of this artificial model obviously ends at a state that contains one particle at each column, resulting in $\rho_r=\rho_0=1/m$ $(m\geqslant 3)$. But the time evolution has some interesting features. It is described by a set of $m(m+1)/2$ coupled differential equations of the same form as equation (3). The solutions which possess a C_m symmetry are similar to the solutions equations (4), i.e. polynomials with a characteristic power modulo m, multiplied by a common exponent $f(u)=\exp(2(u^m-1)/m)$. In particular the $A(0,0)$ generalized generator is given by

$$A(0,0)=u^{2m-2}f(u) \qquad (8)$$

It is easily seen that the number of connected lattice animals increases asymptotically like $n!^{(m-1)/m}$. The set of n points connected lattice animals due to an NN isotropic exclusion is, for all n, a subset of the set of connected lattice animals of the artificial model whose interaction range in the lattice width direction exceeds the NN range. Therefore the value above is an upper bound to the number of connected lattice animals formed on an $m\times\infty$ lattice in the case of an NN interaction. Thus the number of connected lattice animals on the $d=2$ lattice is bound from below by $n!^{2/3}$ and by $n!$ from above. Numerical analysis of the coefficients $a_n(d=2)$ [9, 11] suggests that it is very likely that the exact behaviour is given by the upper bound.

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