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LETTER TO THE EDITOR

Diffusivity and radius of random animals, percolation clusters and compact clusters

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Abstract. We define a cluster diffusivity D_s by introducing a random rearrangement between arbitrary cluster and perimeter sites such that the cluster remains connected. Monte Carlo simulation is used on the square and simple cubic lattices to determine the dependence of D_s and the radius of gyration R_s on s, the number of cluster sites. Three limiting cases are considered: random animals ($p = 0$), precolation clusters ($p = p_c$) and compact clusters ($p > p_c$). Our results for the exponent ρ of R_s are consistent with the best experimental and theoretical values. We develop an elementary scaling theory for the observed power law dependence of D_s in terms of different mechanisms dominant for small and large clusters. A position space renormalisation group calculation in two dimensions yields corrections to the elementary theory for random animals and percolation clusters; the predictions are consistent with the Monte Carlo results for D_s.

Although percolation has received much attention recently, little is known about time-dependent generalisations (Hammersley and Welsh 1980) of percolation related phenomena. We consider here a simple model for diffusion of an s-site percolation cluster. Our main interest is the Monte Carlo and renormalisation group calculation of the s-dependence of the cluster diffusion constant, a quantity of interest in phase separation kinetics (Binder and Kalos 1980). We also present new Monte Carlo results for the exponent ρ of the radius of gyration.

In site percolation each site on a lattice is randomly occupied with probability p and is unoccupied with probability $q = 1 - p$. A percolation cluster of size s is characterised by s sites connected by nearest-neighbour distances and by t unoccupied perimeter sites which terminate the cluster (Stauffer 1979). In order to obtain diffusion, we allow the interchange of an *arbitrary* cluster site and a perimeter site such that the cluster remains connected (see figure 1). For a given configuration the probability of an interchange or 'jump' is $q^{\Delta t}$ (Stauffer 1978), where Δt is the difference in the number of perimeter sites of the configuration produced by the jump. Since each jump leads to a displacement of the centre of mass of the cluster, we can define a cluster diffusion constant or 'cluster diffusivity' D_s by

$$\overline{(\Delta X_s)^2} = 2dD_s\tau, \tag{1}$$

where $\overline{(\Delta X_s)^2}$ is the mean square displacement of the centre of mass of an s-site cluster on a d-dimensional lattice. The time τ is chosen arbitrarily so that on the average every

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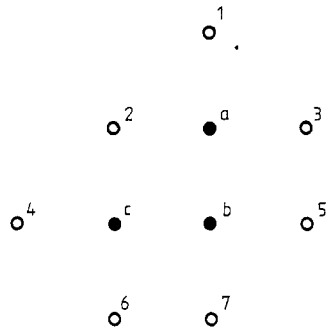

Figure 1. Example of a three-site cluster configuration with $t = 7$. According to the rules discussed above, site a cannot jump to perimeter sites 1 and 3; site b can jump only to site 2. The shift in the centre of mass due to the jump $c \to 1$ is $(\Delta R)^2 = \frac{5}{9}$.

cluster site is exchanged once in one unit of time, i.e. $\tau \sim 1/s$. The average in (1) is over all possible jumps of one cluster of fixed size s. We remark that although the time appears in (1), the calulation of D_s is essentially a rearrangement problem with no memory of prior interchanges.

Monte Carlo calculation of R_S. The rearrangement procedure described above can be used to generate all possible geometrically distinct configurations of an s-site cluster. This method is the basis of a 'dynamic' Monte Carlo (MC) calculation (Peters *et al* 1979) of R_s, the average radius of gyration of an s-site cluster. Hence it is straightforward to use the same method to generate MC results for the large-s behaviour of D_s.

Since the s-dependence of D_s depends in part on the s-dependence of R_s, we first discuss the new MC results for R_s. We define the exponent ρ in the usual way (Stauffer 1979),

$$R_s \sim s^{\rho} \qquad (s \to \infty). \tag{2}$$

Due to an improved algorithm (Franke 1980), our statistics are improved and more reliable than in earlier work (Peters *et al* 1979). We compare in table 1 the results (Holl 1980) for ρ in two and three dimensions with the corresponding best theoretical values. The maximum cluster sizes used in the MC calculations on the square and simple cubic

Table 1. Comparison of present MC results for the radius of gyration exponent ρ with best theoretical values.

		MC results	Best theoretical values	
$d = 2$	$p = 0$	0.65 ± 0.02	0.6408 ± 0.0003	Derrida and de Seze 1981
			0.647 ± 0.020	Family 1981
				0.61 Parisi and Sourlas 1981
	$p = p_c$	0.53 ± 0.01	$\frac{48}{91} \simeq 0.5275$	Pearson 1980 and Nienhius *et al* 1980
			0.52 ± 0.02	Family and Reynolds 1981
	$p > p_c$	0.495 ± 0.005	$\frac{1}{2}$ (exact)	
$d = 3$	$p = 0$	0.53 ± 0.02	$\frac{1}{2}$ (exact)	Parisi and Sourlas 1981
	$p = p_c$	0.39 ± 0.02	0.40 ± 0.01	Stauffer 1979
	$p > p_c$	0.330 ± 0.005	$\frac{1}{3}$ (exact)	

lattices are given in tables 2, 3 and 4. Renormalisation group arguments (Family and Coniglio 1980, Harris and Lubensky 1981) imply that ρ has three different values corresponding to $\rho(p=0)$, $\rho(p=p_c)$ and $\rho(p=1)$. That is, for $s \to \infty$, the behaviour of R_s is controlled for $p > p_c$ by the compact cluster ($p=1$) fixed point, and the behaviour of R_s for $p < p_c$ is determined by the random animal ($q=1$, $p=0$) fixed point. We see from table 1 that the MC values of ρ at $p=p_c$ for $d=2$ and 3 are now consistent with theory (Stauffer 1979, Pearson 1980, Nienhius *et al* 1980). For $p > p_c$ the MC results for ρ are close to the exact value $\rho = 1/d$.

Table 2. The cluster diffusivity component for compact clusters ($p=1$) in two and three dimensions obtained from the MC calculations. The interpretation of the MC values of y in terms of 'small,' 'intermediate' and 'large' clusters is made in terms of the crossover behaviour predicted by equations (5)–(7). The maximum cluster size used in the MC simulations is also shown.

		Exponent y					
	Maximum cluster size	Large clusters MC	Large clusters Equation (5)	Intermediate clusters MC	Intermediate clusters Equation (6)	Small clusters MC	Small clusters Equation (7)
2d	1400	—	0.0	0.45	0.5	0.9	1.0
3d	1500	0.33	0.33	—	0.67	0.95	1.0

Table 3. The cluster diffusivity exponent y for percolation clusters ($p=p_c$) in two and three dimensions obtained from the MC calculations. The interpretation of the MC values of y in terms of 'small' and 'large' clusters is made in terms of the crossover behaviour predicted by (5) and (6). The maximum cluster size used in the MC simulations is also given.

		Exponent y			
	Maximum cluster size	Large clusters MC	Large clusters Equation (5)	Small clusters MC	Small clusters Equation (6)
2d	400	0.4 (no crossover observed)	−0.06	0.4	0.55
3d	175	0.28	0.2	0.55	0.77

Table 4. Comparison of cluster diffusivity exponent y for random animals ($p=0$) in two and three dimensions obtained from the MC calculations and the predictions of (5) based on elementary scaling considerations. The maximum cluster size used in the MC simulations is also shown.

		Exponent y	
	Maximum cluster size	MC	Equation (5)
2d	150	0.27	−0.28
3d	125	0.37	0.0

Minor inconsistencies still exist between the MC and theoretical values of ρ for random animals. The value of ρ for random animals in d dimensions is related to the critical exponent for the magnetisation near the Lee–Yang edge singularity for the Ising model in d-2 dimensions (Parisi and Sourlas 1981). This relation yields for $d = 3$ the exact value $\rho = \frac{1}{2}$ in comparison with the MC result $\rho = 0.53 \pm 0.02$. The same relation together with an ε-expansion and interpolation procedure (Parisi and Sourlas 1981) yields $\rho = 0.61$ for $d = 2$ in contrast to the MC result $\rho = 0.65 \pm 0.02$. However, the MC result is consistent with a recent transfer matrix and phenomenological renormalisation result of $\rho = 0.6408 \pm 0.0003$ (Derrida and de Seze 1981) and a position space renormalisation group calculation of $\rho = 0.647 \pm 0.020$ (Family 1981).

Monte Carlo calculation and crossover behaviour of D_s. We present the MC results (Holl 1980) for D_s as a function of s in figures 2(a) and (b) for the square and simple cubic lattice respectively. Since D_s is not well defined at $p = 1$, we consider $p = 0.9$ (2d) and $p = 0.8$ (3d). We expect that D_s follows a power law dependence (Binder and Stauffer 1974)

$$D_s \sim s^{-y} \qquad (s \to \infty), \tag{3}$$

and that the exponent y depends on d and on the three limiting values of p. In the following we discuss an elementary scaling theory for the s-dependence of the different mechanisms contributing to D_s. The main results of this theory are that D_s exhibits crossover for $p \geqslant p_c$ as the cluster size is increased; no crossover is predicted at $p = 0$. These qualitative predictions are consistent with the analysis of the MC results for y shown in tables 2, 3 and 4 for $p > p_c$, $p = p_c$ and $p = 0$ respectively. For large clusters and $p \leqslant p_c$, the discrepancies between the MC values of y and the predictions of the elementary scaling theory are at least partially resolved by the renormalisation group calculations presented below.

Since the characteristic length of a cluster scales as R_s, we expect that the displacement in the cluster centre of mass due to one jump scales as R_s/s. The other property of interest is the average number of perimenter sites t_s, which for $p \geqslant p_c$ scales as (Stauffer 1979)

$$t_s = (q/p)s + \text{constant } s^{\sigma}. \tag{4}$$

Note that t_s consists of a *bulk* perimeter term $(q/p)s$ and an *excess* perimeter term $t_s' = t_s - (q/p)s$. The presence of bulk and excess perimeter sites implies that there are at least two different mechanisms for D_s. The dominant mechanism for large s corresponds to the exchange of a site with a bulk perimeter site and from (1) yields the behaviour

$$D_s \sim s(R_s/s)^2 = s^{2\rho-1}, \qquad y = 1 - 2\rho. \tag{5}$$

For smaller s we can have the exchange of a site with an excess perimeter site and hence

$$D_s \sim s^{\sigma}(R_s/s)^2 = s^{2\rho+\sigma-2}, \qquad y = 2 - \sigma - 2\rho. \tag{6}$$

For $p > p_c$, $\sigma = 1 - 1/d$ (Stauffer 1979), and the second term in (4) can be interpreted as a surface effect. Hence for $p > p_c$ we can distinguish *bulk* sites from *surface* sites, and we have two additional types of mechanisms involving surface rather than bulk sites. The exchange of a surface site with a bulk perimeter site leads to $D_s \sim s^{-1/d}s(R_s/s)^2 = s^{1-1/d}(R_s/s)^2$. This behaviour is the same as (6) with $\sigma = 1 - 1/d$. The exchange of a surface site with an excess perimeter site yields

$$D_s \sim s^{-1/d}s^{1-1/d}(R_s/s)^2 = s^{-1}, \qquad y = 1 \tag{7}$$

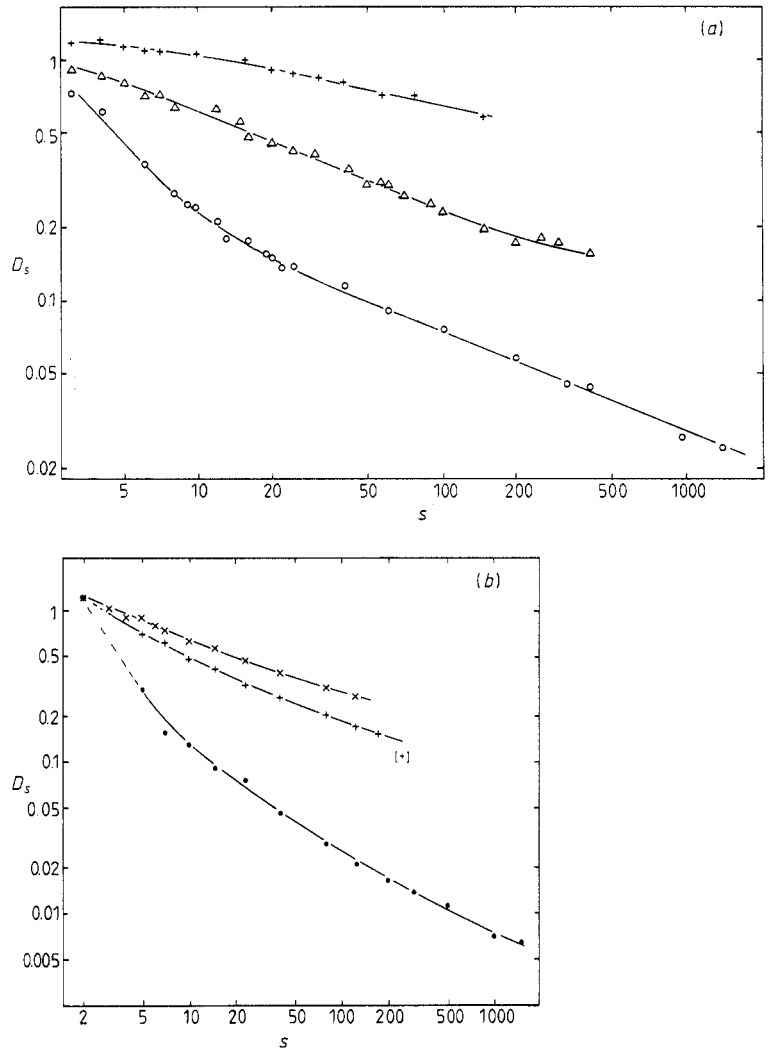

Figure 2. Log–log plot of the cluster diffusivity D_s against number of cluster sites s for different values of the site occupation probability. (*a*) Square lattice, 2D. +, $p = 0.0$; △, $p = p_c$; ○, $p = 0.9$. (*b*) Simple cubic lattice, 3D. ×, $p = 0.0$; +, $p = p_c$; ●, $p = 0.8$.

where in (7) we have used $\rho = 1/d$. The result of this analysis is that for $p > p_c$, D_s is expected to exhibit crossover between $y = 1$ (equation (7)) for small clusters to $y = 1 - 2d$ (equation (5)) for large clusters. An intermediate cluster size value of $y = 1 - 1/d$ is also predicted from (6). These predicted values of y are compared with the MC values in table 2 together with the maximum cluster size used in the MC simulations. There is reasonable agreement between theory and experiment, if at $d = 2$ we interpret the observed crossover behaviour of D_s to be from 'small' to 'intermediate' clusters.

Renormalisation group calculation of D_s. At $p = p_c$ scaling arguments (Stauffer 1979) yield $\sigma = 1/\beta\delta$. According to the extended den Nijs conjecture (Nienhuis *et al* 1980, Pearson 1980), $\beta\delta = \frac{91}{36}$ and hence $\sigma = 0.396$ for $d = 2$. For $d = 3$ scaling

arguments imply that $\sigma \simeq 0.45$ (Stauffer 1979). These values of σ imply that at $p = p_c$ the second term in (4) cannot be interpreted as a surface effect. Hence D_s should exhibit crossover between the power law dependence given by mechanisms (5) and (6). We use $\rho = 0.53$ for $d = 2$ and $\rho = 0.39$ for $d = 3$ together with the above values of σ obtain the predicted values of y shown in table 3 for $p = p_c$. It is seen that there is qualitative agreement between the predictions of the simple theory and the MC values for $d = 3$; no crossover is observed for $d = 2$, a result that can probably be attributed to finite cluster size effects (see table 3).

For random animals ($p = 0$), $t_s = As + B$ for $s \to \infty$ with A and B independent of s (Stauffer 1979, Duarte 1979). Hence all exchanges are possible and according to our elementary theory, D_s behaves as in (5) with no crossover behaviour predicted. We assume $\rho = 0.65$ for $d = 2$ and $\rho = 0.5$ for $d = 3$ to obtain the predicted values of y shown in table 4. Note the discrepancies between the predictions of (5) and the MC results.

The elementary scaling theory summarised in (5) for the dominant s-dependence of D_s for large clusters implicitly assumes that a finite fraction of the s cluster sites can jump a distance that scales as R_s. We remove this assumption and rewrite (5) in the more general form

$$D_s \sim s\Phi_s(R_s/s)^2, \tag{8}$$

where Φ_s is the probability that a site can jump a distance that *scales* as R_s. We assume that

$$\Phi_s \sim s^{-x}, \qquad s \to \infty, \tag{9}$$

and hence from (2), (3), (8) and (9) we have

$$y = 1 + x - 2\rho. \tag{10}$$

In order to identify Φ_s with the internal structure of a cluster, we classify all occupied sites into either articulation or non-articulation sites. We define a site to be an *articulation* site if upon its removal the cluster separates into two or more pieces. Our calculation of Φ_s for large s rests on the conjecture that Φ_s can be interpreted as the probability that a site in cluster of size s is a non-articulation site. The physical basis of this identification is that the jumps of the articulation sites are restricted to perimeter sites which reconnect the cluster. In contrast, the jumps of the non-articulation sites are not so restricted. The identification of Φ_s with the non-articulation site probability can be checked by a MC calculation.

We determine the exponents ρ and x by a position space renomalisation group (PSRG) approach, and introduce the generating function $\tilde{Z}(K, q, \tilde{h})$:

$$\tilde{Z}(K, q, \tilde{h}) = \sum_{st} g_{st} K^s q^t \tilde{h}^r. \tag{11}$$

K is the fugacity associated with an occupied site in the cluster (Family and Coniglio 1980), p is the site probability as before, $q = 1 - p$, and g_{st} is the number of geometrically distinct cluster configurations of s sites and perimeter t. The novel feature of (11) is the introduction of $\tilde{h}$ as a 'ghost' field which couples only to the r non-articulation (removable) sites of the cluster. The introduction of $\tilde{h}$ is similar in spirit to that of Shlifer *et al* (1979) in which the backbone problem is analysed by defining a ghost field which couples only to the backbone bonds.

The definition (11) of $\tilde{Z}$ and the identification of Φ_s with the non-articulation sites allows us to write

$$\Phi_s = \frac{\tilde{h}\partial\tilde{G}(K, q, \tilde{h})/\partial\tilde{h}|_{\tilde{h}=0}}{K\partial\tilde{G}(K, q, 0)/\partial K}, \tag{12}$$

where $\tilde{G} = \ln \tilde{Z}$. We follow standard RG arguments (Shlifer *et al* 1979) and assume that the singular part of $\tilde{G}$ is a generalised homogeneous function of $K - K^*$ and $\tilde{h} - \tilde{h}^*$ in the vicinity of the fixed point (K^*, h^*) and at $q = q^*$. The associated scaling powers $\tilde{y}_K$ and $\tilde{y}_h$ are defined near $(K^*, \tilde{h}^*)$ in terms of the renormalised quantities K' and $\tilde{h}'$ in the usual way. It is then easy to show from (12) that

$$x = d(\tilde{y}_K - \tilde{y}_h)/\tilde{y}_K\tilde{y}_h. \tag{13}$$

We know that in general $0 \leqslant x \leqslant 1$ and expect that $x(p = 0) > x(p = p_c) > x(p = 1) = 0$.

We use the cell to site renormalisation approach of Reynolds *et al* (1980) and Family and Coniglio (1980) to obtain recursion relations for K', q' and $\tilde{h}'$. At $\tilde{h} = 0$ the recursion relations for K' and q' reduce to the usual ones, and hence $\tilde{y}_K = y_K = 1/\rho = \ln b/\ln \lambda_K$, where b is the length rescaling factor in the transformation, and $\lambda_K = (\partial K'/\partial K)_{K=K^*, q=q^*, \tilde{h}=0}$. We define a cell to be occupied (Reynolds *et al* 1980) if and only if there is a spanning cluster which spans the cell in any direction (rule R_0) or in both directions (rule R_2).

In table 5 we show the results (Family 1981) of various small cell PSRG calculations of ρ for the square lattice. Although these results are consistent with the results of large cell PSRG calculations and other methods, we do not know *a priori* whether similar numerical accuracy for x can be obtained from small cell calculations. However our small cell results for x discussed below are consistent with the MC values of x inferred from (10).

We define a site in the cell to be a non-articulation site if upon its removal the remaining cluster spans the cell according to R_0 (rule A_0) or R_2 (rule A_2) and if the remaining cluster is not disconnected. The recursion relation for $\tilde{h}$ can be written in the form (Shlifer *et al* 1979)

$$K'\tilde{h}' = 1 - \langle(1 - \tilde{h})^{N_r(K, q^*)}\rangle, \tag{14}$$

where N_r is the number of non-articulation sites for a particular configuration and $\langle\cdots\rangle$ denotes the configurational average. For small $\tilde{h}$ (14) reduces to $K'\tilde{h}' = \tilde{h}\langle N_r(K, q^*)\rangle$. Since $\tilde{h}^* = 0$ we obtain

$$\tilde{y}_h = \ln \tilde{\lambda}_h/\ln b, \tag{15}$$

where

$$\tilde{\lambda}_h = \frac{\partial\tilde{h}'}{\partial\tilde{h}}\bigg|_{\substack{K=K^*, q=q^* \\ \tilde{h}=0}} = \frac{1}{K^*}\langle N_r(K^*, q^*)\rangle. \tag{16}$$

For compact clusters the recursion relations are $K' = K^{b^d}$ and $K'\tilde{h}' = K^{b^d}\tilde{h}$. Hence we obtain $y_K = \tilde{y}_h = d$ which yields $x = 0$ from (13). The result $x = 0$ implies that Φ_s is independent of s for compact clusters (see (9)). Hence in this case the dominant s-dependence of D_s is given correctly by the elementary scaling theory of (5). The results of our small cell calculations of $x(p = 0)$ and $x(p = p_c)$ according to rules A_0 and A_2 for $d = 2$ are summarised in table 5. The corresponding results for y derived from (10) are also shown. From table 5 we see that the magnitude of $x(p = p_c)$ is insenstive to

Table 5. Results of PSRG calculations on the square lattice for the radius of gyration exponent ρ and the non-articulation site probability exponent x for random animals and percolation clusters. The values of the exponent y of the cluster diffusivity are inferred from the relation $y = 1 + x - 2p$ (see (10)). The spanning rules R_0, R_2, A_0 and A_2 are explained in the text. For comparison the results of the MC calculations of ρ and y and the inferred values of x are aslso shown. The PSRG results for ρ are from Family (1981).

	Random animals				Percolation clusters			
	K^*	ρ	x	y	K^*	ρ	x	y
$b=2$, R_0, A_0	0.2056	0.8861	1.0	0.23	0.3820	0.7658	1.0	0.47
$b=2$, R_2, A_2	0.4728	0.6116	1.0	0.78	0.7676	0.5594	1.0	0.88
$b=2$, R_2, A_0	0.4728	0.6116	0.52	0.30	0.7676	0.5594	0.18	0.06
$b=3$, R_0, A_0	0.2405	0.8053	1.0	0.39	0.4726	0.6920	1.0	0.62
$b=3$, R_2, A_2	0.3819	0.6384	1.0	0.72	0.7325	0.5614	0.27	0.15
$b=3$, R_2, A_0	0.3819	0.6384	0.65	0.38	0.7325	0.5614	0.18	0.05
MC	—	0.65	0.57	0.27	—	0.53	0.5	0.4

our criteria for N_r, and we obtain $x(p = p_c) \sim 0.2$ and $y(p = p_c) \sim 0.1$, numerical values smaller than the corresponding MC values of x and y. Since rules A_0 and A_2 underestimate the number of non-articulation sites in a small cell, we expect the true value of x and hence of y to be less than our small cell results. For this reason we attribute the discrepancy between the value of $x(p = p_c)$ estimated by our small cell PSRG calculation and the MC calculation to finite cluster size effects in the latter analysis. For $p = 0$ we find that the magnitude of x does depend sensitively on the criteria for N_r, a result related to the fact that random animals are more stratified than percolation clusters. The less restrictive criterion A_0 yields $x(p = 0) \sim 0.6$. This value of x together with the corresponding PSRG result for ρ implies that $y(p = 0) \sim 0.4$ (see (10)). These results are consistent with the MC values of $x(p = 0)$ and $y(p = 0)$. Note that $x(p = 0) > x(p = p_c)$ as expected.

Discussion. One feature of our rearrangement procedure and hence the MC calculation of R_s and D_s should be noted. That is, our 'dynamical' method does not in general yield an exact equilibrium ensemble in which the probability of a configuration is $q^t / \Sigma_t g_{st} q^t$. To understand this problem consider the limit of random animals in which all possible geometrically distinct s-site clusters have equal weights. For $s = 3$ on a square lattice there are four clusters with $t = 7$ and two clusters with $t = 8$, i.e. the probability w of a $t = 8$ cluster is $\frac{1}{3}$ in the equilibrium ensemble. From this ensemble of six clusters the rearrangement procedure generates 64 possible configurations and yields $w = \frac{5}{16}$ For small s we can choose the relative weights of the different jumps so that the equilibrium ensemble is maintained. For example for $p = 0$ and $s = 3$ we obtain on a square lattice $D_3 = 1.1919$ for $w = \frac{1}{3}$ and $D_3 = 1.2292$ for $w = \frac{5}{16}$. (D_3 is dimensionless.) The consistency of our MC calculation of ρ with the theoretical values indicates that for large s, the difference between the ensemble average and the 'time' average vanishes.

In future work we plan to extend the MC calculations of D_s to larger clusters and to modify the rearrangement procedure so that the equilibrium ensemble is preserved for arbitrary s. A MC calculation of the probability distribution of jump distances would lead to a direct test of our assumption that this probability is related to the cluster non-articulation site probability. Since the small cell PSRG calculations of the latter

probability gave encouraging results, we plan to extend these calculations to larger cells and to three dimensions. Of more general interest is the study by MC and renormalisation group methods of more realistic diffusion processes and the establishment of 'dynamic' universality classes.

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