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## LETTER TO THE EDITOR

### Rigid animals in three dimensions

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**Abstract.** The number of rigid clusters  $C(n)$  is enumerated for the central force model on a site-diluted FCC lattice. The exponent  $\nu_r$  governing the growth of the radius of gyration of the rigid animal is also calculated. It is found that  $C(n) \sim n^{0.33} 3.0^n$  and  $\nu_r = 0.32 \pm 0.02$ .

The randomly diluted elastic network has been studied extensively over the past five years [1-6]. For the bond bending model [2], the rigidity threshold is the same as the percolation threshold and the bulk modulus exponent  $f$  is much larger than the conductivity exponent  $t$ . The relation  $f = 2\nu + t$  has been conjectured [6-9] ( $\nu$  is the correlation length exponent) which agrees very well with numerical estimates in two dimensions. The central force model [1], on the other hand, has a rigidity threshold much larger than the percolation threshold because there is only one elastic constant in this model. As a result, the rigidity of the central force model is non-local [5] in the sense that two sites may not be rigidly connected even though they are connected. It is currently believed that the central force model and the bond bending model belong to different universality classes. Due to the non-local property of the central force model, the number of rigid clusters is much less than the number of connected clusters. The rigid animal has been studied [10-12] on a triangular lattice, assuming that the number of rigid clusters  $C(n)$  and the mean-square radius of gyration with respect to the centre of mass  $\rho_n$  of the cluster having  $n$  sites obey the following scaling form:

$$C(n) \sim n^{-\theta_r} \lambda^n \quad (1)$$

$$\rho_n = \frac{1}{C(n)} \sum_{\gamma_n} R_n^2(\gamma_n) \sim n^{2\nu_r} \quad (2)$$

where

$$R_n^2 = \frac{1}{n} \sum_i (r_i - r_c)^2. \quad (3)$$

Here  $r_i$  is the position vector of site  $i$ ,  $r_c$  is the vector of the centre of mass of the rigid cluster,  $\gamma_n$  denotes all rigid clusters having  $n$  sites,  $\theta_r$  is a critical exponent, and  $\nu_r$  is the correlation length exponent for the rigid animal. The calculations of Prunet and Blanc [10] and Wang [11, 12] give  $\theta_{rs} = 0.57 \pm 0.02$ ,  $\nu_{rs} = 0.744 \pm 0.008$  for site dilution,

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and  $\theta_{rb} = 0.988 \pm 0.001$  for bond dilution. Note that the bond rigid animal and the site rigid animal belong to different universality classes. The same conclusion has been drawn [13] for the elastic property of the site and bond rigidity percolation for the central force model.

In this letter, we enumerate the site rigid animal and the radius of gyration up to  $p^{14}$  on a FCC lattice, which is a non-trivial task. Note that the enumeration of the lattice animal on the FCC lattice up to  $p^{10}$  already took about two hours of CPU time on an Apollo AD 4500 work station (which is a little slower than a VAX 8650). The computing time of the next order would be at least ten times as long than that of the previous order. Using a partial enumeration method [12] based on Martin's backtracking technique [14, 15], it took 46 hours of CPU time on the Apollo AD 4500 to complete the enumeration of the rigid animal and the radius of gyration. For a site cluster, there is a spring associated with any two nearest-neighbour sites. A cluster is considered to be rigid provided that the number of zero frequency modes  $N$  equals  $d(d+1)/2$ , corresponding to  $d$  translational and  $d(d-1)/2$  rotational degrees of freedom. For every cluster generated by the partial enumeration method, we first calculate the quantity  $id = 3 \times (ns) - (nb) - 6$ . If  $id > 0$ , then the cluster is non-rigid in three dimensions. Note that if  $id \leq 0$  it is not necessarily rigid.

The series  $\chi_1$  and  $\chi_2$  are defined as

$$\chi_1 = \sum_n C(n) K^n \sim (1 - \lambda K)^{\theta_r - 1} \quad (4)$$

$$\chi_2 = \sum_n C(n) n \rho_n K^n \sim \sum_n n^{-\theta_r + 1} \lambda^n n^{2\nu_r} K^n \sim (1 - \lambda K)^{\theta_r - 2\nu_r - 2} \quad (5)$$

where  $K$  is the fugacity and  $K_c = 1/\lambda$  is the critical value of  $K$ .

The series coefficients are listed in table 1, where  $c_n$  is the rigid animal and  $d_n$  is the radius of gyration multiplied by the number of sites  $n$ . We also listed the ordinary animals  $a_n$  and the number of clusters  $b_n$  generated by our method for comparison. We used the Padé approximant and the differential Padé approximant [16] to estimate the exponents  $\theta_r$  and  $\nu_r$ . To get an accurate value of  $\nu_r$ , we obtained another series [17]  $\chi_3 = \sum_n n \rho_n K^n \sim (1 - K)^{-\alpha}$ , which is the quotient of  $\chi_2$  and  $\chi_1$  expanded term by term, where  $\alpha = 2\nu_r + 2$ . Then the critical point for this series is exactly 1, from which

Table 1. The coefficients of the series for the FCC lattice.

$n$	$a_n$	$b_n$	$c_n$	$d_n$
1	1	1	1	0.00
2	6	6	6	3.00
3	50	15	8	8.00
4	475	20	2	3.00
5	4 881	114	0	0.00
6	52 835	371	1	3.00
7	593 382	2 467	8	34.29
8	6 849 415	18 048	28	159.00
9	80 757 819	121 405	80	570.67
10	968 400 940	756 734	268	2 346.63
11		4 528 943	887	9 310.84
12		27 153 877	2 855	35 280.62
13		163 421 791	9 070	130 530.60
14		971 979 472	28 516	473 690.40

we obtained the exponent  $\nu_r$ . Using this value, we analysed the series  $\chi_1$  and  $\chi_2$  and computed the critical point  $K_c$  and critical exponent  $\theta_r$ . We obtained  $\nu_r = 0.32 \pm 0.02$ , which can be compared with the correlation length exponent for the lattice animal  $\nu = 0.53 \pm 0.02$  [18] and  $\nu = 0.51$  [19]. Note that  $\nu$  is larger than  $\nu_r$  in three dimensions, in contrast to the situation in two dimensions where  $\nu$  is smaller than  $\nu_r$ . We also obtained  $\theta_r = -0.33 \pm 0.08$  and  $K_c = 0.33 \pm 0.01$ . The ratio method has been used to analyse the series and the results are consistent with the above analysis.

In summary, we have enumerated rigid animals on a FCC lattice and calculated the exponent of the radius of gyration for the site rigid animal which is found to be smaller than that of the lattice animal.

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## References

- [1] Feng S and Sen P N 1984 *Phys. Rev. Lett.* **52** 216
- [2] Kantor Y and Webman I 1984 *Phys. Rev. Lett.* **52** 1891
- [3] Lemieux M A, Breton P and Tremblay A M S 1985 *J. Physique Lett.* **46** L1
- [4] Wang J and Harris A B 1985 *Phys. Rev. Lett.* **55** 2459
- [5] Day A R, Tremblay R R and Tremblay A M S 1986 *Phys. Rev. Lett.* **56** 2501
- [6] Feng S, Sen P N, Halperin B I and Lobb C J 1984 *Phys. Rev. B* **30** 5386
- [7] Roux S 1986 *J. Phys. A: Math. Gen.* **19** L351
- [8] Sahimi M 1986 *J. Phys. C: Solid State Phys.* **19** L79
- [9] Harris A B and Lubensky T C 1986 unpublished
- [10] Prunet V and Blanc R 1986 *J. Phys. A: Math. Gen.* **19** L1197
- [11] Wang J 1988 *J. Phys. A: Math. Gen.* **21** L353
- [12] Wang J 1989 An algorithm for enumerating rigid animals *J. Phys. A: Math. Gen.* **22** in press
- [13] Arbabi S and Sahimi M 1988 *J. Phys. A: Math. Gen.* **21** L863
- [14] Martin J L 1972 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) p 97
- [15] Redner S 1982 *J. Stat. Phys.* **29** 309
- [16] Chen J-H and Fisher M E 1981 *J. Phys. A: Math. Gen.* **14** 2553
- [17] Meir Y 1987 *J. Phys. A: Math. Gen.* **20** L349
- [18] Gould H and Holl K 1981 *J. Phys. A: Math. Gen.* **14** L443
- [19] Family F 1983 *J. Phys. A: Math. Gen.* **16** L97