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LETTER TO THE EDITOR

An algorithm for enumerating rigid clusters

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Abstract. A more efficient algorithm for enumerating rigid clusters is presented. Using this algorithm we have extended the series of site-rigid animals enumerated by Prunet and Blanc by five more terms and we have also calculated, for the first time, the exponent governing the growth of the radius of gyration for rigid animals.

In the study of critical phenomena, the series expansion technique has proven to be a powerful tool for calculating the critical exponent. The cluster enumeration is very time consuming when a longer series is needed. The computer time needed for cluster enumeration grows exponentially with cluster size. A Monte Carlo cluster enumeration [1] method has been proposed to enumerate clusters. The computer time grows linearly with cluster size. As a trade off, this method cannot enumerate clusters exactly, but only within a few percent (say) in a controlled way. Very often, we want to enumerate clusters which have some restrictions, e.g. clusters with no free ends, or rigid clusters, etc. It is possible to enumerate these clusters more efficiently. In this letter, we present an algorithm for enumerating rigid clusters on a site-diluted triangular lattice for the central force model [2]. In this model, the bonds between nearest-neighbour sites are present with spring constant k provided that the sites are present; a site is present with probability p and absent with probability $1-p$. A rigid cluster can be defined as having only translational and rotational degrees of freedom. Hence a rigid cluster in two dimensions has three zero-frequency modes.

There are two ways to generate rigid clusters.

(i) Generate [3] all one-loop clusters which are the exterior boundary of the rigid cluster. Then a rigid cluster is obtained by filling up all the possible interior bonds. This is particularly suitable for the bond-rigid animals.

(ii) Use [4] Martin's backtracking technique [5] to generate all clusters (lattice animal) and test their rigidity. Note that it is very time consuming to generate the lattice animal.

In this letter, we present a partial enumeration method in which some non-rigid clusters (e.g. the clusters with free ends) have been excluded. Then it is much easier to test the rigidity of the rest of clusters because the number of these clusters is much less than that of the lattice animal (see table 1). Our algorithm uses the backtracking technique based on the FORTRAN program given by Redner [6]. As described in detail in [6], all clusters are built successively according to Martin's algorithm. Once a cluster of maximum size $n_{\max}$ is constructed, then the cluster sites are removed intermittently, in the reverse order that they were added, so that the enumeration proceeds to completion. If the nth cluster site is attached to the jth site, then the jth site is called

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the root site. Once a jth-order site is removed, its location becomes j-prohibited, which means that additional sites cannot be added to this prohibited site until it is 'freed' at a later stage in the enumeration. Beginning with a single occupied site, the program adds sites to it. More generally, the program adds new sites to the available sites which are nearest neighbours of the current root. When no site can be attached to the jth root, the order j is incremented and the program then attempts to add another site to the cluster. If, however, the jth root or a lower-order root makes the cluster non-rigid, e.g. the jth root is a singly connected site, we do not need to enumerate the rest of clusters by adding a site on the $(j+1)$th or higher-order root. We can simply 'free' the nth prohibited site and proceed from there. Specifically, after line 20 in the program of [6] we check whether a root of order j or less makes the cluster non-rigid. (Note that we cannot test the non-local property.) If the cluster is non-rigid the control is transfered to line 22 instead of line 21. The clusters generated in this way are not necessarily rigid. We then test the rigidity of these clusters by calculating the number of zero-frequency modes.

We have tested this partial enumeration method on a Masscomp 5700 computer (about three times slower than a Vax 8650) to enumerate site-rigid clusters on a site-diluted triangular lattice for the central force model. For the rigid animal, we assume that

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

where $C(n)$ is the number of rigid clusters having n sites and θ_r is the corresponding critical exponent. The square radius of gyration with respect to the centre of the mass R_n^2 for a rigid cluster of n sites is defined as

$$R_n^2 = \frac{1}{n} \sum_i (\boldsymbol{r}_i - \boldsymbol{r}_c)^2 \tag{2}$$

and the mean-square radius of gyration with respect to the centre of mass, ρ_n, is

$$\rho_n = \frac{1}{C(n)} \sum_{\gamma_n} R_n^2(\gamma_n) \sim n^{2\nu_r} \tag{3}$$

where $\boldsymbol{r}_i$ is the position vector of site i, $\boldsymbol{r}_c$ is the vector of the centre of mass of the rigid cluster, γ_n denotes all rigid clusters having n sites, and ν_r is the correlation length exponent for the rigid animal.

For $n = 14$, using the program presented in [6], it takes about 87 minutes CPU time to count the lattice animal and about 6 hours CPU time to count the rigid animals. Using our new program, it takes 11 minutes to count the rigid animal and calculate the radius of gyration.

We have extended the series of the site-rigid animal enumerated by Prunet and Blanc [4] to order p^{18} (five more terms). We also calculate the radius of gyration to the same order. These calculations took about 40 hours CPU time. Specifically, the series χ_2 we obtained is

$$\chi_2 = \sum_n C(n) n \rho_n K^n \sim \sum_n n^{-\theta_r+1} \lambda^n n^{2\nu_r} K^n \sim (1-\lambda K)^{\theta_r - 2\nu_r - 2} \tag{4}$$

and the series χ_1 is

$$\chi_1 = \sum_n C(n) K^n \sim (1-\lambda K)^{\theta_r - 1} \tag{5}$$

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

The series are listed in table 1, where c_n is the rigid animal and d_n is the radius of gyration multiplied by number of site n. We also list the ordinary animals [7] a_n and the number of clusters b_n generated by our method for comparison. We used the Padé approximant and differential Padé approximant [8] to extrapolate the exponents θ_r and ν_r. To analyse the series, we get another series [9] $\chi_3 = \Sigma_n n\rho_n K^n \sim (1-K)^{-\alpha}$ which is the term-by-term expansion of the quotient of χ_2 and χ_1, where $\alpha = 2\nu_r + 2$. Since the critical point for this series is exactly 1, we can obtain the exponent ν_r very accurately. Using this value, we can analyse the series χ_1 and χ_2 and locate the critical point K_c and critical exponent θ_r. Figure 1(*a*) is the pole-residue plot for series χ_3 from which we obtained $\nu_r = 0.744 \pm 0.008$, which is compared with the correlation length exponent for the lattice animal $\nu = 0.649 \pm 0.009$ [10] and $\nu = 0.6408 \pm 0.0003$ [11]. From figures 1(*b*) and 1(*c*) we obtained $\theta_r = 0.57 \pm 0.02$ and $K_c = 0.429 \pm 0.009$, which is consistent with previous estimates [3, 4]. We also used the ratio method to analyse the series and the results are consistent with the above analysis.

This method of generating clusters enables us to enumerate the clusters with no free ends on a square lattice up to p^{19} (which takes 40 hours CPU time). Harris [12] has mapped a number of problems (e.g. lattice animals, localisation and percolation) which need clusters with at most two free ends onto problems which need clusters with no free ends. Using the clusters we have, we could calculate the series for these problems with more terms.

In summary, we have presented a more efficient method for enumerating rigid animals and the clusters with no free ends. We have extended the series enumerated by Prunet and Blanc to five more terms and calculated the exponent of the radius of gyration for the site-rigid animal, which is found to be larger than that of the lattice animal.

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Table 1. The coefficients of the series on the triangular lattice.

n	a_n	b_n	c_n	d_n
1	1	1	1	0.00
2	3	0	3	1.50
3	11	2	2	2.00
4	44	3	3	6.00
5	186	8	6	20.40
6	814	17	14	72.00
7	3 652	64	31	228.86
8	16 689	243	69	693.75
9	77 359	801	151	1 998.68
10	362 671	2 763	335	5 673.90
11	1 716 033	9 763	747	15 819.98
12	8 182 213	34 361	1 671	43 439.32
13	39 267 086	120 218	3 749	117 722.02
14	189 492 795	423 380	8 487	317 347.34
15	918 837 374	1 502 179	19 432	853 275.81
16	4 474 080 844	5 347 909	44 882	2 290 983.25
17		19 069 574	104 220	6 101 195.00
18		68 185 668	242 804	16 127 592.00

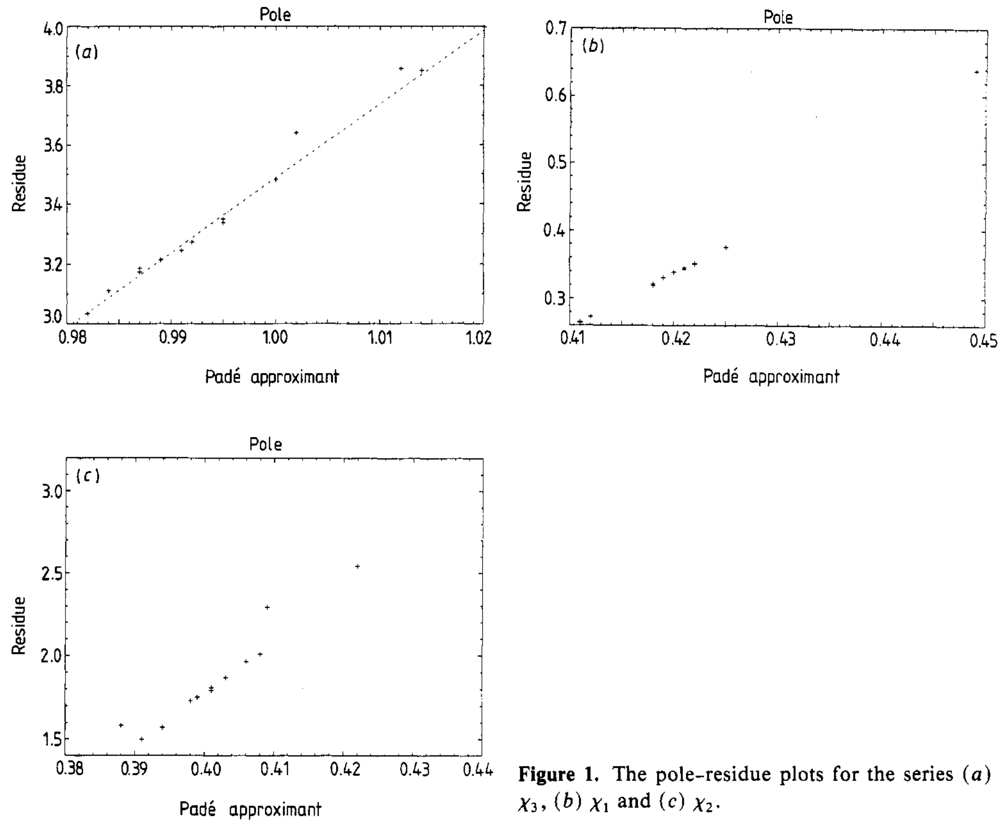

Figure 1. The pole-residue plots for the series (a) χ_3, (b) χ_1 and (c) χ_2.

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