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LETTER TO THE EDITOR

Size of rings in two dimensions

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Abstract. We report enumeration results for the radius of gyration and caliper size distribution of self-avoiding unrooted polygons of up to 28 steps, on the square lattice. The (second moment) radius of gyration series is sufficiently smooth to allow verification of the theoretical prediction $\nu(\text{rings}) = \nu(\text{walks})$ to 0.2% accuracy.

It is generally believed that the size exponent, ν, for self-avoiding rings (polygons) is identical to that of self-avoiding walks. Indeed, in the $n \to 0$ limit of the n-vector model (de Gennes 1972, des Cloizeaux 1975), the *energy–energy* correlation function will describe distribution of vectors connecting all possible pairs of sites on the ring. Thus the mean squared radius of gyration of N-step rings,

$$\langle R_N^2 \rangle^{1/2} \sim N^{\nu}, \tag{1}$$

grows with exponent ν which is identical to that of the walks, end-to-end distance of which is distributed according to *spin–spin* correlation (in the $n \to 0$ limit).

An alternative argument is based on the renormalisation group ideas. Real space renormalisation along a chain involves a local transformation which should not be sensitive to the fact that the ends are joined somewhere (see Family (1982) and references therein). Obviously, this assertion must be taken with caution. One must prove that no significant longer-range interactions are generated along the chain: this has been established to first order in the $\varepsilon = 4 - d$ expansion by Lipkin *et al* (1981) and by Prentis (1982).

Numerical study of the size of self-avoiding rings was done mainly by Monte Carlo (MC) methods, for three-dimensional systems: see Baumgärtner (1982), Bishop and Michels (1985), and earlier work quoted by these authors. We are aware only of $d = 3$ series-enumeration studies, by Rapaport (1975), for the FCC lattice and by Wall and Hioe (1970) for the diamond lattice. Both the series analyses and most of the MC studies found an apparently larger exponent for rings than for walks (in $d = 3$) with the deviation, $\Delta\nu/\nu$, of at least 2% (up to 10% in some cases). However, Baumgärtner (1982) argued that the discrepancy is due to the low quality of the available data.

We report here study of the size of rings up to 28 bonds, *on the square lattice*. We concentrate on the $d = 2$ self-avoiding rings (unrooted N-step polygons) for several reasons. First, fluctuations are generally stronger in lower dimensions. Thus, there is a better chance of seeing deviation from ν(walks), if any. Secondly, for $d = 2$ walks, $\nu = \frac{3}{4}$ is known exactly (Nienhuis 1982). Lastly, we devised an enumeration method

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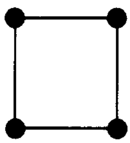
which is more efficient than techniques used in earlier direct enumerations (up to $N = 26$) of the number, p_N, of distinct rings (Sykes *et al* 1972, and references therein). Recently, Enting and Guttmann (1985) counted rings up to $N = 46$; however, it is not indicated if their technique can be used to measure ring sizes. Note that only rings of $N = 4, 6, 8, \ldots$ steps exist on the square lattice.

Our method is applicable *only* in $d = 2$ and, briefly, consists of generating all compact (no holes) site animals on the dual lattice. In two dimensions, these animals are in one-to-one correspondence with the rings on the original lattice. The results for $\langle R_N^2 \rangle$ are reported in table 1. The radius of gyration was calculated according to the *site* content (site coordinates). In table 2 we report the distribution of the number of rings according to their caliper size (projection) along a fixed square-lattice axis. Note that the bond length was measured, e.g. the 4-step ring



has length 1, despite the fact that two lattice rows are involved. The enumeration took about 160 h of CPU time on the RIDGE computer, of which about 100 h can be attributed to the calculation of $\langle R_{28}^2 \rangle$.

The $\langle R_N^2 \rangle$ series was analysed by standard ratio-type techniques. The sequence of approximants

$$\nu_N = \ln[\langle R_N^2 \rangle / \langle R_{N-2}^2 \rangle]/2 \ln (N/N-2), \tag{2}$$

is fitted to the form

$$\nu_N = \nu + \text{constant} \times N^{-\theta} + o(N^{-\theta}). \tag{3}$$

We will not lay out all the details of the analysis but describe the results. One finds that the values of θ near $\theta = 2$ provide the most stable fit. This value is an *apparent* convergence exponent since *asymptotically* the leading corrections to scaling decay slower provided they are the same as for walks (see an overview by Privman 1984).

Table 1. Mean-squared radius of gyration, $\langle R_N^2 \rangle$, for N-step polygons. The values listed are integers $p_N \langle R_N^2 \rangle N^2/2$, where p_N is the number of distinct (unrooted) polygons.

$N/2$	$p_N \langle R_N^2 \rangle N^2/2$	p_N
2	4	1
3	33	2
4	300	7
5	2582	28
6	21 436	124
7	173 414	588
8	1377 028	2938
9	10 774 890	15 268
10	83 313 372	81 826
11	637 932 666	449 572
12	4845 048 412	2521 270
13	36 545 191 560	14 385 376
14	274 032 229 984	83 290 424

Table 2. The number of N-step polygons having caliper size (projection) of D bonds along a fixed lattice axis.

$N/2$	D	Number	$N/2$	D	Number
2	1	1	11	1	1
3	1	1	11	2	919
3	2	1	11	3	21 362
4	1	1	11	4	94 948
4	2	5	11	5	162 418
4	3	1	11	6	125 756
5	1	1	11	7	39 632
5	2	13	11	8	4390
5	3	13	11	9	145
5	4	1	11	10	1
6	1	1	12	1	1
6	2	27	12	2	1841
6	3	70	12	3	61 963
6	4	25	12	4	356 954
6	5	1	12	5	769 241
7	1	1	12	6	816 998
7	2	55	12	7	417 035
7	3	254	12	8	89 874
7	4	236	12	9	7181
7	5	41	12	10	181
7	6	1	12	11	1
8	1	1	13	1	1
8	2	113	13	2	3685
8	3	803	13	3	178 325
8	4	1352	13	4	1318 233
8	5	607	13	5	3472 899
8	6	61	13	6	4655 629
8	7	1	13	7	3363 957
9	1	1	13	8	1195 971
9	2	229	13	9	185 317
9	3	2443	13	10	11 137
9	4	6075	13	11	221
9	5	5123	13	12	1
9	6	1311	14	1	1
9	7	85	14	2	7371
9	8	1	14	3	510 460
10	1	1	14	4	4805 207
10	2	459	14	5	15 232 810
10	3	7282	14	6	24 573 941
10	4	24 589	14	7	22 898 120
10	5	31 412	14	8	11 835 447
10	6	15 461	14	9	3056 032
10	7	2508	14	10	354 223
10	8	113	14	11	16 546
10	9	1	14	12	265
			14	13	1

Indeed, a plot of ν_N against $1/N^2$, see figure 1, reveals a (very small) oscillation superimposed over the monotonic increase, which may be a reflection of an interplay of several power-law contributions to $\nu_N - \nu$. Although the single-correction term assumption is not really correct for $N \leq 28$, we cannot do a more sophisticated fit due

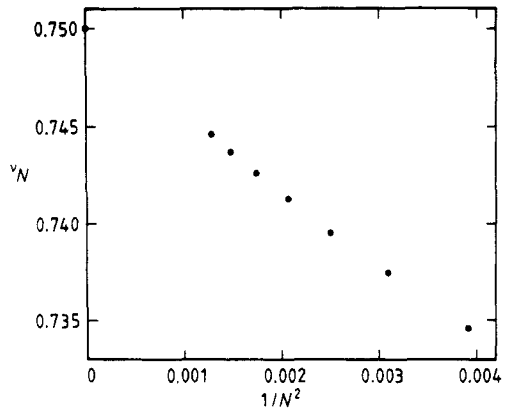


Figure 1. Plot of the estimates ν_N defined by relation (2), against $1/N^2$, for $N = 16, 18, \ldots, 28$. The value of $\nu(\text{walks}) = \frac{3}{4}$ is also marked.

to the shortness of the series. From figure 1 and our other analyses with varying θ, we propose

$$\nu(\text{rings}) = 0.750 \pm 0.0015. \tag{4}$$

This value is consistent with $\nu(\text{walks}) = \frac{3}{4}$.

From the data of table 2, one can also generate caliper diameter (D) moments. We studied $\langle D \rangle$ and $\langle D^2 \rangle$. These quantities provide generally less accurate estimates of ν due to proliferation of correction terms (see Privman *et al* 1984). A fit to the form (3) for both moments is most stable when θ is a few per cent below $\theta = 1$, and extrapolation suggests values clustering around $\nu(\text{rings}) \simeq 0.759$. If we *impose* $\theta = \nu$ as suggested by Privman *et al* (1984), for caliper moments, then values near $\nu(\text{rings}) \simeq 0.752$ are found. We believe that the deviation of the caliper diameter exponent estimates from (4) and $\nu(\text{walks})$ is due to that the asymptotic behaviour cannot be seen in the existing data, similarly to the $d = 3$ studies described above.

In summary, we presented the first (to our best knowledge) study of the size exponent, ν, for self-avoiding rings in two dimensions. We conclude that the theoretical expectation $\nu(\text{rings}) = \nu(\text{walks})$ holds to within 0.2% accuracy, see (4), based on the analysis of the radius of gyration series to order $N = 28$.

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References

Baumgärtner A 1982 *J. Chem. Phys.* **76** 4275
Bishop M and Michels J P J 1985 *J. Chem. Phys.* **82** 1059
de Gennes P G 1972 *Phys. Lett.* **38A** 339
des Cloizeaux J 1975 *J. Physique* **36** 281
Enting I G and Guttmann A J 1985 *J. Phys. A: Math. Gen.* **18** 1007

Family F 1982 *Phys. Lett.* **92A** 341
Lipkin M, Oono Y and Freed K F 1981 *Macromolecules* **14** 1270
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
Prentis J J 1982 *J. Chem. Phys.* **76** 1574
Privman V 1984 in *Kinetics of Aggregation and Gelation* ed F Family and D P Landau (Amsterdam: North-Holland) p 253
Privman V, Family F and Margolina A 1984 *J. Phys. A: Math. Gen.* **17** 2837
Rapaport D C 1975 *J. Phys. A: Math. Gen.* **8** 1328
Sykes M F, McKenzie D S, Watts M G and Martin J L 1972 *J. Phys. A: Math. Gen.* **5** 661
Wall F T and Hioe F T 1970 *J. Phys. Chem.* **74** 4416