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LETTER TO THE EDITOR

A new algorithm to enumerate the self-avoiding random walk

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Abstract. We present a new algorithm for enumerating the self-avoiding walk and extend the existing series of 19 terms by one more term on a triangular lattice. The leading correction-to-scaling exponent Δ_1 for the mean-square end-to-end distance of the self-avoiding walk is found to be less than one.

The subject of the self-avoiding walk (SAW) has been studied for a long time. Much work [1–7] has focused on calculating the exponent ν_{SAW} of the end-to-end distance of the SAW using series expansion techniques. Early work [1–4] used indirect methods. One of the works [2] used an indirect method to enumerate the self-avoiding rings on a lattice. The technique used in [2] is to determine the number of SAW of n steps, denoted by $b_n(x, y)$, to each point for two values of n, say r and s, and to form the sum:

$$B(r, s) = \sum_{x,y} b_r(x, y) b_s(x, y) \tag{1}$$

where x and y are the cartesian coordinates and the sum $B(r, s)$ includes all the rings corresponding to $r+s$ steps together with certain overlaps. The rings can be obtained by subtracting the overlaps in (1). These overlaps can be calculated by considering the symmetry and topology of SAW. Details can be found in [2]. The other indirect methods [1, 3, 4] are concerned with recurrence relations.

Recently, Grassberger [5] used a simple 'brute force' counting program to count all the SAW. This direct method turns out to be much faster than the indirect method described above. More recently, Rapaport [7] has extended the existing series for the SAW [6] on a triangular lattice (with 18 terms) to 19 terms. This calculation required about 219 hours of CPU time on an IBM 3081. It therefore might seem that the calculation of SAW on the triangular lattice has reached its limit. In this letter, however, we present a new algorithm where we have combined the two methods mentioned above. We first prepare a 'substrate' of all the s-step SAW b_s on the lattice, then perform the r-step SAW b_r on this 'substrate' and calculate the overlaps b_{op}. Thus the number of SAW of $r+s$ steps is $B_0(r, s) = b_r * b_s - b_{\text{op}}$. The end-to-end distance can be obtained similarly. Hence, the enumeration of the n-step SAW can be reduced to the enumeration of the overlaps of the r-step SAW on the 'substrate'.

To demonstrate the efficiency of the method, we have enumerated the SAW $c(n)$ and its mean-square end-to-end distance $c(n)\rho(n)$ on a triangular lattice for $n = 19$ and 20. These calculations took about 10 hours and 45 hours CPU time, respectively, on a Masscomp 5700, which is about six times slower than an IBM 3081. The next

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two terms would require about 20 times the amount of CPU time. Our result for the 19th term is the same as that found by Rapaport [7]. In the calculation we have considered the symmetry of the lattice [8] which reduced the computer time by about 40 percent. We also tested the method for the 17th term. The direct method took about 54 hours CPU time on the Masscomp 5700. Our method took about 37 minutes, 34 minutes, and 72 minutes for $B_0(12, 5)$, $B_0(13, 4)$, and $B_0(14, 3)$.

In table 1 we have listed all 20 coefficients of SAW on the triangular lattice for completeness, where the first 16 terms are from Grassberger [5], the 17th and 18th terms are from Majid *et al* [6] and Guttmann [9], the 19th term is from Rapaport [7], and the 20th term is from our method. Assume that

$$\rho_n \sim An^{2\nu_{\mathrm{SAW}}}(1+Bn^{-\Delta_1}+Cn^{-\Delta_2}+\ldots) \tag{2}$$

where Δ_1 and Δ_2 are the leading correction-to-scaling exponents and the dots denote the higher-order corrections. We define ν_{eff} as [10]

$$\nu_{\mathrm{eff}}=\frac{1}{2}\frac{\ln(\rho_{n+1}/\rho_n)}{\ln(1+1/n)}. \tag{3}$$

From (2) and (3), we obtain

$$\nu_{\mathrm{eff}}=\nu_{\mathrm{SAW}}-\tfrac{1}{2}B\Delta_1 n^{-\Delta_1}-\tfrac{1}{2}C\Delta_2 n^{-\Delta_2}. \tag{4}$$

We used (4) to fit the series and found that $\nu_{\mathrm{SAW}}=0.7508\pm0.010$, $\Delta_1=0.85\pm0.05$, and $\Delta_2\sim\Delta_1+1$. The value of ν_{SAW} is in good agreement with the presumably exact value, $\nu_{\mathrm{SAW}}(d=2)=\frac{3}{4}$ [11]. Our result also agrees with Adler [12], Djordjevic *et al* [10] and Privman [13] in that the leading correction-to-scaling exponent Δ_1 is less than one and does not agree with Rapaport [7], who obtains $\Delta_1=1$.

After this work was submitted, a paper by Guttmann [14] appeared. He calculated the number of 20-step SAW, which agrees with our result.

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

n	$c(n)$	$c(n)\rho(n)$
1	6	6
2	30	72
3	138	582
4	618	3 924
5	2 730	23 862
6	11 946	135 744
7	51 882	736 926
8	224 130	3 864 492
9	964 134	19 732 434
10	4 133 166	98 643 888
11	17 668 938	484 703 142
12	75 355 206	2 347 861 440
13	320 734 686	11 236 580 322
14	1 362 791 250	53 225 780 532
15	5 781 765 582	249 886 119 006
16	24 497 330 322	1 164 085 625 784
17	103 673 967 882	5 385 834 447 738
18	438 296 739 594	24 767 425 671 540
19	1 851 231 376 374	113 279 031 925 422
20	7 812 439 620 678	515 581 479 563 568

In summary, we have presented a new algorithm to enumerate the SAW and its end-to-end distance. We have extended the existing series of SAW on a triangular lattice by one more term. We found that Δ_1 is less than one.

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