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Self-avoiding walks which cross a square

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Abstract. We consider self-avoiding walks on the square lattice which are confined to lie in or on the boundary of a square with vertices at $(0,0)$, $(0,L)$, $(L,0)$ and (L,L). We ask for the number of such walks which begin at the origin and end at the vertex (L,L), especially in the large L limit. Similarly we ask for the mean number of steps in such walks as a function of L. At fixed L we also associate a fugacity with the number of steps of the walk and ask how the system behaves as a function of this fugacity. We provide some rigorous results, in particular proving that there is a phase transition at some particular value of the fugacity, and supplement these with the analysis of series data for the problem.

1. Introduction

There has been a good deal of recent interest in the theoretical treatment of several phase transitions which occur in long linear polymers in dilute solution. These include the collapse transition, in which the polymer can be modelled as a self-avoiding walk on a lattice, with attractive near-neighbour interactions between pairs of vertices which occupy adjacent lattice sites. If the attraction is weak the walk behaves as a random coil but, for sufficiently strong interactions, a collapse transition occurs to a ball with dimensions much less than those of the corresponding coil. This transition has been studied by a variety of different techniques [1-7]. A second kind of phase transition which has also received a good deal of attention is the rod-coil transition, associated with a change in the flexibility of the polymer [8-10].

In this paper we consider yet another self-avoiding walk problem which has an associated phase transition. Although the problem was first posed to us as a problem in communication theory (asking for the number of distinct self-avoiding walks which cross a square), we believe that its solution will help in the understanding of polymer phase transitions. We consider the square lattice (the integer points in R^2) and focus our attention on the square with vertices $(0,0)$, $(0,L)$, (L,L) and $(L,0)$. We ask for the number, $c(L)$, of self-avoiding walks which begin at the origin and end at the point (L,L), without ever leaving the square. In section 2 we show that this quantity grows as $\lambda^{L^2+o(L^2)}$.

We can associate a fugacity with the number of steps in the walk, so that for values of the fugacity much less than unity the dominant walks will be those which cross the square with only a small number of steps. One might expect that there will be a transition at some value of the fugacity from a regime in which walks with $O(L)$ steps dominate to one in which walks with $O(L^2)$ steps dominate. We investigate this question in section 3, and prove that such a phase transition exists.

In section 4 we derive exact values of $c_n(L)$, the number of walks with n steps which cross the $L \times L$ square, for small values of L, and analyse these data to form estimates of the large L behaviour and, in particular, of the location of the transition.

A similar problem has been treated by Hattori *et al* [11], for self-avoiding walks on the pre-Sierpinski gasket.

2. The number of walks and the mean number of edges

We consider an $L \times L$ square on the square lattice with one vertex the origin and the opposing vertex at (L, L). Suppose that $c_n(L)$ is the number of self-avoiding walks with n steps which are confined to lie in this square and which start at the origin and end at (L, L). Define

$$c(L) = \sum_n c_n(L). \tag{2.1}$$

Clearly the minimum value of n is given by $n_{\min} = 2L$. Similarly, the maximum value of n is given by $n_{\max} = L^2 + 2L$ if L is even and by $n_{\max} = L^2 + 2L - 1$ if L is odd. If we write c_n for the number of self-avoiding walks with n steps then, since $c_n(L) \leqslant c_n$, we have

$$c(L) \leqslant (L^2 + 2L - 2L + 1) \max[c_n : 2L \leqslant n \leqslant L^2 + 2L] = (L^2 + 1) c_{L^2+2L} \tag{2.2}$$

since $c_{n+1} \geqslant c_n$. Hence

$$\limsup_{L \to \infty} L^{-2} \log c(L) \leqslant \log \mu \tag{2.3}$$

where μ is the growth constant for self-avoiding walks [12] defined by

$$\lim_{n \to \infty} n^{-1} \log c_n = \log \mu \leqslant \log 3. \tag{2.4}$$

In order to prove the existence of a corresponding limit we first look for a suitable concatenation to derive a super-multiplicative inequality. We consider an $L \times L$ square and partially cover this with squares of side $M + 2$, as shown in figure 1. We write

$$L = p(M + 2) + q \tag{2.5}$$

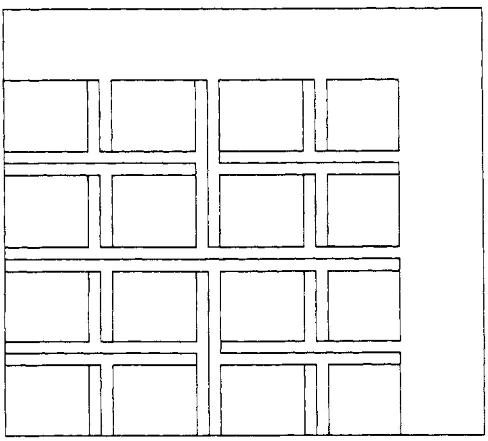

Figure 1. An $L \times L$ square contains p^2 squares of side $M \times M$ suitably concatenated. Each $M \times M$ square is independently crossed by a self-avoiding walk, confined to lie in this square.

with $0 \leqslant q < M+2$. Each of the p^2 $M \times M$ squares can be crossed independently in $c(M)$ ways so we have

$$c(L) \geqslant c(M)^{p^2}. \tag{2.6}$$

We write

$$\limsup_{L\to\infty} L^{-2} \log c(L) = \log \lambda. \tag{2.7}$$

For all $\varepsilon > 0$ there exists an infinite set of integers $\mathscr{S}(\varepsilon)$ such that for all $L \in \mathscr{S}(\varepsilon)$

$$\log \lambda - \frac{\varepsilon}{2} \leqslant L^{-2} \log c(L) \leqslant \log \lambda. \tag{2.8}$$

Now choose $M \in \mathscr{S}(\varepsilon)$ sufficiently large that

$$\left(\frac{M}{M+2}\right)^2 \left(\log \lambda - \frac{\varepsilon}{2}\right) \geqslant \log \lambda - \varepsilon. \tag{2.9}$$

Then

$$\frac{\log c(L)}{L^2} \geqslant \frac{p^2}{L^2} \log c(M) = \left(\frac{L-q}{L}\right)^2 \left(\frac{M}{M+2}\right)^2 \frac{\log c(M)}{M^2} \tag{2.10}$$

and

$$\liminf_{L\to\infty} \frac{\log c(L)}{L^2} \geqslant \left(\frac{M}{M+2}\right)^2 \left(\log \lambda - \frac{\varepsilon}{2}\right) \geqslant \log \lambda - \varepsilon. \tag{2.11}$$

Then letting $\varepsilon \to 0$ establishes that

$$\liminf_{L\to\infty} \frac{\log c(L)}{L^2} \geqslant \limsup_{L\to\infty} \frac{\log c(L)}{L^2} \tag{2.12}$$

so that the limit

$$\lim_{L\to\infty} \frac{\log c(L)}{L^2} = \log \lambda \tag{2.13}$$

exists.

We now consider a corresponding lower bound on $c(L)$. The idea is to notice that, at least for L even, walks with the maximum number of steps are *Hamiltonian* walks since they visit every vertex of the square. Since the number of Hamiltonian walks on the Manhattan lattice is known [13] one might hope to use this as a lower bound on $c(L)$. Unfortunately this result is for periodic boundary conditions while we are interested in walks which never leave the square. Instead we derive a lower bound on the number of Hamiltonian walks of this type by adapting an argument due to Gujirati [14]. We first cover a square of side $L_0 = L-1$ with disjoint rectangles of maximum size $(1 \times m)$. With fixed $m \geqslant 1$ we write

$$L_0 = (m+1)p + q \tag{2.14}$$

with $0 \leqslant q < m$. Each column of the square is covered with a stack of $p(1 \times m)$ rectangles, each pair separated by one lattice space, with finally a $(1 \times q)$ rectangle. The square is now covered with s of these stacks, separated by one lattice space, where $s = (L_0+1)/2$ if L_0 is odd and $s = L_0/2$ if L_0 is even. In each set of m rows the polygons can be connected to form a large polygon in m^{s-1} ways, and in the last row the polygons can be connected in q^{s-1} ways. Then each of the first p rows can be joined to its neighbour below in at least s ways. The resulting graphs are all polygons, and they are Hamiltonian if L_0 is odd. (For L_0 even, the vertices in the right-most column of the square are not covered by the polygon.) If $h^o(L_0)$ is the number of Hamiltonian polygons in the $L_0 \times L_0$ square we then obtain the following bound

$$h^o(L_0) \geq s^p m^{p(s-1)} \geq m^{[L_0^2/2(m+1)]}. \tag{2.15}$$

Hence

$$\log \mu_H = \lim_{L_0 \to \infty} L_0^{-2} \log h^o(L_0) \geq \frac{\log m}{2(m+1)}. \tag{2.16}$$

This bound is most effective when $m = 4$, giving $\lim_{L_0 \to \infty} L_0^{-2} \log h^o(L_0) \geq 0.1386\ldots$. To convert the polygon into a walk which crosses the square we first translate the $L_0 \times L_0$ square by one unit in the positive y direction. Then delete the edge $(0, 1)$-$(1, 1)$, add the edge $(0, 0)$-$(0, 1)$ and the edges $(1, 1)$-$(1, 0)$, $(1, 0)$-$(2, 0), \ldots, (L-1, 0)$-$(L, 0)$, $(L, 0)$-$(L, 1), \ldots, (L, L-1)$-(L, L). Each polygon gives a unique walk by this construction and we obtain the bound

$$\lim_{L \to \infty} L^{-2} \log c(L) \geq \lim_{L \to \infty} L^{-2} \log h^o(L) \geq 0.1386\ldots. \tag{2.17}$$

We are also interested in the mean number of steps in walks which cross an $L \times L$ square. We define

$$\langle n \rangle = \frac{\Sigma_n n c_n(L)}{\Sigma_n c_n(L)} \tag{2.18}$$

and note that

$$c_n(L) \leq c_n = \mu^{n+o(n)}. \tag{2.19}$$

If $n = o(L^2)$ then $c_n(L) \leq \mu^{o(L^2)}$ so that all except exponentially few walks have of order L^2 steps. Hence the mean number of steps must also be of order L^2.

3. The influence of a step fugacity

In this section we fix L, the size of the square, but give a weight to each walk which crosses the square, where the weight depends on the number of steps. We define the generating function

$$C_L(x) = \sum_n c_n(L) x^n \tag{3.1}$$

where x is a 'step fugacity'.

For fixed $x \leq 1$, $C_L(x) \leq c(L)$ and for fixed $x > 1$

$$C_L(x) \leq c(L) x^{n_{\max}} \tag{3.2}$$

so that $L^{-2} \log C_L(x)$ is bounded above for all finite x. We write

$$\limsup_{L \to \infty} L^{-2} \log C_L(x) = \log \lambda(x). \tag{3.3}$$

To prove that the corresponding limit exists we use an argument which is a refinement of that used in section 2. Consider a $L\times L$ square and partially cover it with p^2 squares of side $M+2$, where p is given by (2.5). Label these squares with two indices i and j, $1\leq i, j\leq p$. Let the walk crossing the (i,j) square of sides $M\times M$ have n_{ij} edges. In order to concatenate these walks and join $(0,0)$ to (L,L), as in figure 1, we need an additional

$$m=2p(p-1)+2q+4 \tag{3.4}$$

edges. Since each square can be crossed independently

$$\prod_{i=1}^{p}\prod_{j=1}^{p} c_{n_{ij}}(M)\leq c_{m+n_{11}+\ldots+n_{pp}}(L). \tag{3.5}$$

Multiplying both sides by $x^{n_{11}+\ldots+n_{pp}}$ and summing over $n_{11}, n_{12}, \ldots, n_{pp}$ gives

$$C_M(x)^{p^2}\leq[n_{\max}(M)-n_{\min}(M)+1]^{p^2}x^{-m}C_L(x). \tag{3.6}$$

For any $\varepsilon>0$ there exists an infinite set of integers $\mathscr{S}(\varepsilon)$ such that

$$\log\lambda(\varepsilon)-\frac{\varepsilon}{2}\leq L^{-2}\log C_L(x)\leq\log\lambda(\varepsilon) \tag{3.7}$$

for all $L\in\mathscr{S}(\varepsilon)$. For any $M\in\mathscr{S}(\varepsilon)$, (3.6) and (3.7) imply that

$$\begin{aligned}\liminf_{L\to\infty}\frac{\log C_L(x)}{L^2}\\ &\geq\frac{\log C_M(x)}{(M+2)^2}-\frac{\log(M^2+1)}{(M+2)^2}-\frac{2|\log x|}{(M+2)^2}\\ &\geq\left(\frac{M}{M+2}\right)^2\left(\log\lambda(x)-\frac{\varepsilon}{2}\right)-\frac{\log(M^2+1)}{(M+2)^2}-\frac{2|\log x|}{(M+2)^2}.\end{aligned} \tag{3.8}$$

We now take $M\in\mathscr{S}(\varepsilon)$ sufficiently large that this final expression is bounded below by $\log\lambda(x)-\varepsilon$, giving

$$\liminf_{L\to\infty} L^{-2}\log C_L(x)\geq\limsup_{L\to\infty} L^{-2}\log C_L(x)-\varepsilon \tag{3.9}$$

which, on letting $\varepsilon\to 0$, establishes the existence of the limit

$$\lim_{L\to\infty} L^{-2}\log C_L(x)=\log\lambda(x). \tag{3.10}$$

Clearly $C_L(1)=c(L)$ and, for $x\geq 1$,

$$\max[c_{n_{\max}}(L)x^{n_{\max}}, c(L)]\leq C_L(x)\leq c(L)x^{n_{\max}} \tag{3.11}$$

so that

$$\max[\log\mu_H+\log x, \log\lambda]\leq\log\lambda(x)\leq\log\lambda+\log x \tag{3.12}$$

which implies that

$$\lim_{x\to\infty}\frac{\log\lambda(x)}{\log x}=1. \tag{3.13}$$

For $x \leqslant 1$ we obtain a convenient upper bound by noting that every walk which crosses the square is 'doubly unfolded' and hence $c_n(L) \leqslant \mu^n$ (since such walks can be concatenated to yield a super-multiplicative inequality [15]). This gives

$$C_L(x) \leqslant \sum_{n=2L}^{n_{\max}} \mu^n x^n = (\mu x)^{2L}(1-(\mu x)^{n_{\max}-2L+1})/(1-\mu). \tag{3.14}$$

If $x > 1/\mu$ this implies that

$$\log \lambda(x) \leqslant \log \mu + \log x. \tag{3.15}$$

If $x \leqslant 1/\mu$ we have

$$\log \lambda(x) \leqslant 0 \tag{3.16}$$

and this, together with the bound

$$C_L(x) \geqslant c_{2L}(L)x^{2L} \tag{3.17}$$

implies that

$$\log \lambda(x) = 0 \tag{3.18}$$

for all $x \leqslant 1/\mu$. Hence $\log \lambda(x)$ is non-analytic. Since

$$C_L(x) \geqslant c_{n_{\max}}(L)x^{n_{\max}} \tag{3.19}$$

and so

$$\log \lambda(x) \geqslant \log \mu_{\mathrm{H}} + \log x \tag{3.20}$$

there must be a singular point x_0 in the range

$$\mu^{-1} \leqslant x_0 \leqslant \mu_{\mathrm{H}}^{-1}. \tag{3.21}$$

The results of this section are summarized in the sketch of the expected behaviour given in figure 2.

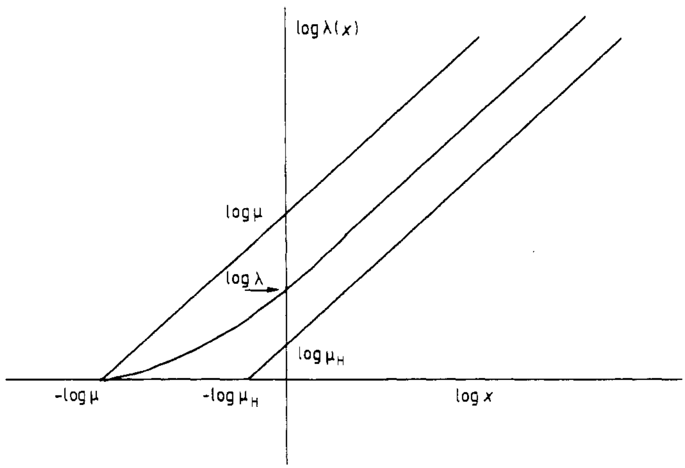

Figure 2. The expected behaviour of $\log \lambda(x)$ as a function of $\log x$.

4. Numerical results

We have derived exact values of $c_n(L)$ for $L \leq 6$ and the results are given in table 1. The rather small values of L which can be studied are a result of the λ^{L^2} behaviour. Summing over values of n we obtain $c(L)$ which, from section 2, behaves as $\lambda^{L^2+o(L^2)}$. We estimate that $\lambda = 1.756 \pm 0.01$.

We next consider the behaviour of the mean number of steps in a walk which crosses an $L \times L$ square. At fugacity x, the definition analogous to that given in (2.18) is

$$\langle n(x, L)\rangle = \frac{\Sigma_n nc_n(L)x^n}{\Sigma_n c_n(L)x^n} \tag{4.1}$$

and we expect that

$$\langle n(x, L)\rangle = A(x)L^2[1+o(1)] \tag{4.2}$$

for $x > x_0$. Plots of $\langle n(x, L)\rangle / L^2$ against L^{-1} show considerable curvature and we have estimated the amplitude $A(x)$ by quadratic fits to these curves in most cases. In figure 3 we show the x dependence of the amplitude estimates. It seems quite clear that the amplitude is going to zero as x decreases and will be zero for all x less than some x_0 which is between 0.3 and 0.4, but it is difficult to form a more precise estimate on the basis of the available data.

The mean number of steps plays the role of an energy and we might hope to form a better estimate of the location of the transition by studying the corresponding

Table 1. Values of $\frac{1}{2}c_n(L)$.

n	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$
2	1					
4		3				
6		2	10			
8		1	18	35		
10			24	112	126	
12			24	255	600	462
14			16	478	1 952	2 970
16				793	5 280	12 593
18				1112	12 914	44 042
20				1053	29 356	138 853
22				366	60 934	410 740
24				52	108 718	1 154 701
26					150 190	3 070 020
28					140 388	7 565 205
30					85 192	16 669 950
32					30 668	31 346 216
34					5 090	48 048 122
36						58 413 332
38						55 097 850
40						39 077 429
42						19 643 936
44						6 198 379
46						939 626
48						55 856

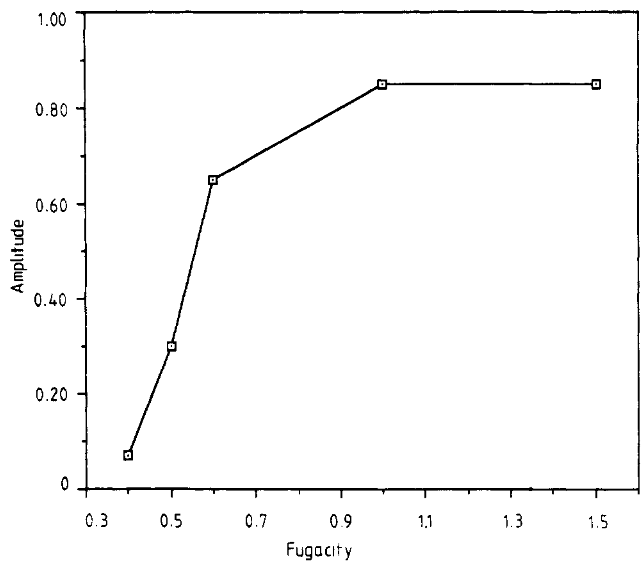

Figure 3. Estimate of the fugacity dependence of the amplitude for the mean number of edges in a walk crossing a square.

fluctuation quantity

$$V(x, L) = \frac{\sum_n n^2 c_n(L) x^n}{\sum_n c_n(L) x^n} - \langle n(x, L) \rangle^2 \tag{4.3}$$

which plays the role of a heat capacity. For each value of L this quantity has a single maximum and we have plotted the locations $x_{\max}(L)$ of these maxima against $1/L$ in figure 4. The curve shown there is a quadratic fit to the results. Again, it appears that the phase transition occurs between 0.3 and about 0.4, but it is difficult to give a precise

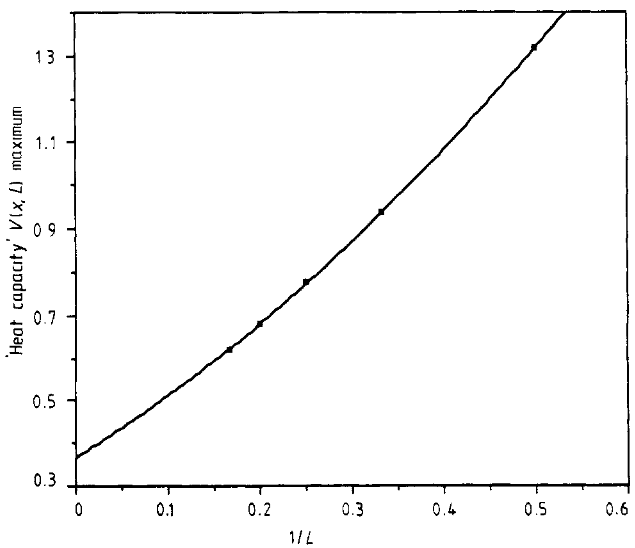

Figure 4. The location of the maximum in the $V(x, L)$ against x curves, as a function of L.

estimate. From the results of section 3 we know that $x_0 \geqslant \mu^{-1}$ and the best numerical estimate of μ is 2.6381 [16], so that $x_0 \geqslant 0.379\ldots$. Hence our results suggest that x_0 is between this value and about 0.4, with a strong possibility that the value is exactly μ^{-1}.

5. Discussion

The two primary results of this paper are the proof that the number of self-avoiding walks which cross a square of side L scales like a constant to the power L^2, and that, when a fugacity is associated with the number of steps in the walk, there is a phase transition in the problem. Hattori *et al* [11] have recently found a similar phase transition in the corresponding problem on a pre-Sierpinski gasket.

We have not identified the location of the transition (though we have suggested that it may occur at exactly $x_0 = \mu^{-1}$), nor have we investigated the associated critical exponents. Further study of these questions will, we believe, help in the understanding of phase transitions in polymer systems.

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