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1991 J. Phys. A: Math. Gen. 24 L1221

(http://iopscience.iop.org/0305-4470/24/20/003)

J. Phys. A: Math. Gen. 24 (1991) L1221–L1228. Printed in the UK

LETTER TO THE EDITOR

Self-avoiding walks that cross a square

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Received 16 July 1991

Abstract. We consider self-avoiding walks that traverse an $L \times L$ square lattice. Whittington and Guttmann have proved the existence of a phase transition in the infinite-L limit at a critical value of the step fugacity. We make several finite-size scaling predictions for the critical region, using the relation between self-avoiding walks and the N-vector model of magnetism. Adsorbing as well as non-adsorbing boundaries are considered. The predictions are in good agreement with numerical data for $L \leqslant 9$.

Whittington and Guttmann [1] have recently studied some of the properties of the family of self-avoiding walks that cross a finite square lattice. The walks begin at $(0, 0)$ and end at (L, L) without leaving the square with corners at $(0, 0)$, $(0, L)$, $(L, 0)$, and (L, L). The generating function is defined by

$$C_L(x) = \sum_n c_n(L) x^n \tag{1}$$

where $c_n(L)$ is the number of such walks with n steps, and x is the step fugacity.

Whittington and Guttmann demonstrated rigorously that the total number of walks $C_L(1)$ increases exponentially with L^2 in the large-L limit, i.e.

$$\lim_{L\to\infty} L^{-2} \ln C_L(1) = \ln \lambda. \tag{2}$$

On the basis of numerical data for $L \leqslant 6$ they estimated $\lambda = 1.756 \pm 0.01$. They also proved that the quantity $\lim_{L\to\infty} L^{-2} \ln C_L(x)$ is a non-analytic function of x, i.e. there is a phase transition. Below and above the critical fugacity x^*, the average number of steps $\langle n \rangle_{L,x} = \partial \ln C_L(x)/\partial \ln x$ varies asymptotically as

$$\langle n \rangle_{L,x} \sim \begin{cases} L & x < x^* \\ L^2 & x > x^* \end{cases} \tag{3}$$

for large L. From numerical data and a rigorous bound they found that x^* is between 0.4 and the inverse connectivity [2]

$$\mu^{-1} = 0.379\,052\,28 \pm 0.000\,000\,14 \tag{4}$$

respectively, with a strong possibility that $x^* = \mu^{-1}$.

In this letter the transition is further explored using the equivalence [3] between self-avoiding walks and the N-vector model of magnetism in the limit $N \to 0$. Several predictions for the transition in the system of walks are obtained from finite-size scaling theory [4–6] for magnetic systems. The predictions are then compared with numerical data for $L \leqslant 9$.

0305-4470/91/201221+08\$03.50

According to [3] the generating function of the self-avoiding walks defined in equation (1) can be expressed as

$$C_L(x) = \lim_{N\to 0} N^{-1}\langle \boldsymbol{S}(0,0)\cdot\boldsymbol{S}(L,L)\rangle. \tag{5}$$

The quantity on the right denotes the correlation function of spins on opposite corners of a square of $(L+1)^2$ classical N-component spins, normalized so that $\boldsymbol{S}\cdot\boldsymbol{S}=N$, with nearest-neighbour interactions. Since $T\to T_c$ in the magnetic system corresponds to $x\to\mu^{-1}$ in the system of self-avoiding walks [3], the result $x^*=\mu^{-1}$, suggested as a strong possibility in [1], follows directly from this correspondence.

Table 1. Total number of walks $C_L(1)$ between opposite corners of the square and between the midpoints of opposite edges.

L	$(0,0)\to(L,L)$	$(0,L/2)\to(L,L/2)$	$(0,(L-1)/2)\to(L,(L+1)/2)$
1	2		2
2	12	9	
3	184		112
4	8 512	3 915	
5	1 262 816		574 068
6	575 780 564	247 484 661	
7	789 360 053 252		338 670 045 504
8	3 266 598 486 981 642	1 378 292 310 954 861	
9	41 044 208 702 632 496 804		17 160 258 555 040 648 616

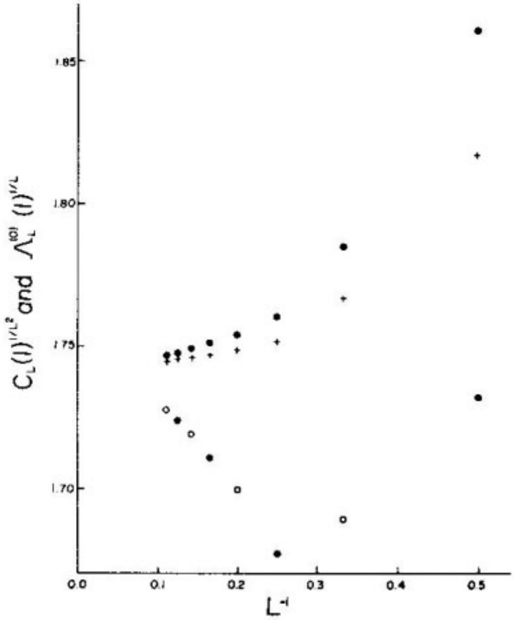

Figure 1. Dependence of $C_L(1)^{1/L^2}$ (circles) and $\Lambda_L^{(0)}(1)^{1/L}$ (crosses) on L^{-1}, with $L = 2, 3, \ldots, 9$. The upper and lower sequences of circles correspond to walks between opposite corners and the midpoints of opposite edges, respectively. The filled and empty points of the lower sequence correspond to even and odd L.

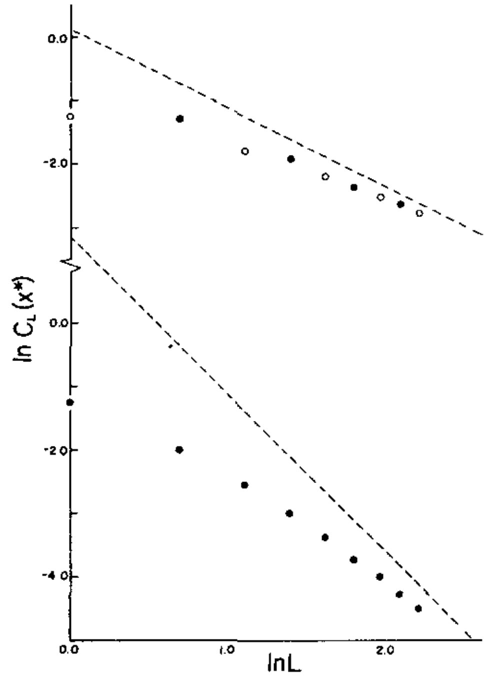

Figure 2. Dependence of ln $C_L(x^*)$ on ln L, with $L = 1, 2, \ldots, 9$, for walks between opposite corners (lower points) and walks between the midpoints of opposite edges (upper points). The filled and empty upper points correspond to even and odd L, respectively. The lower and upper broken lines have slopes $-\frac{5}{2}$ and $-\frac{5}{4}$.

Making a standard finite-size scaling ansatz [4–6] for the spin–spin correlation function in equation (5), we obtain the expression

$$C_L(x) = L^{-\eta_c} f[L^{1/\nu}(x^* - x)] \tag{6}$$

which is expected to hold in the critical region $L \gg 1$, $|x^* - x| \ll x^*$. Since there is no phase transition for finite L, the function f and its derivatives are assumed to exist. In equation (6), ν is the standard exponent that characterizes both the correlation length of the magnetic system and the radius of gyration of the polymer [3]. The quantity η_c is the corner exponent [7] of the magnetization. Equation (6) is not limited to the square geometry, but holds for any system with characteristic size L in general dimension d.

For $d = 2$ and for a 90° corner,

$$\nu = \tfrac{3}{4} \tag{7a}$$

$$\eta_c(\pi/2) = 2\eta_\parallel = \tfrac{5}{2}. \tag{7b}$$

The value for η_c follows from Cardy's [7] result $\eta_\parallel = \frac{5}{4}$ for the surface exponent that characterizes the decay of spin correlations parallel to the boundary in the semi-infinite geometry and the relation [7]

$$\eta_c(\theta) = \frac{\pi}{\theta}\eta_\parallel \tag{8}$$

for the corner exponent in a wedge with angle θ.

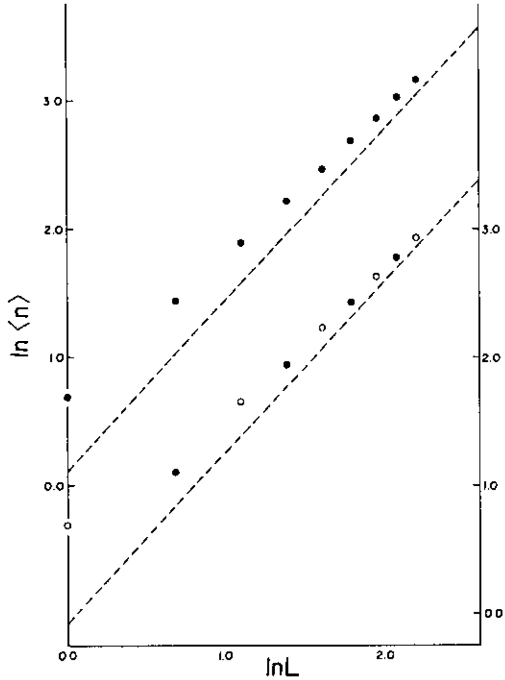

Figure 3. Dependence of $\ln \langle n\rangle_{x^*}$ on $\ln L$, with $L=1,2,\ldots,9$, for walks between opposite corners (upper points, left vertical axis) and walks between the midpoints of opposite edges (lower points, right vertical axis). The filled and empty lower points correspond to even and odd L, respectively. Both broken lines have slope $\frac{4}{3}$.

In addition to the walks $(0,0)$ to (L,L) between opposite corners of the square, we have considered walks between the midpoints of opposite edges, i.e. $(0, L/2)$ to $(L, L/2)$ for L even. For L odd we approximate the midpoints by $(0,(L-1)/2)$ and $(L,(L+1)/2)$. In both cases the functional form (6) applies. According to equation (8), for walks between the midpoints of opposite edges the appropriate corner exponent in (6) is $\eta_c(\pi)=\frac{5}{4}$ instead of $\eta_c(\pi/2)=\frac{5}{2}$.

From equation (6) and its first two derivatives with respect to x, one obtains the predictions

$$C_L(x^*)\sim L^{-\eta_c} \tag{9a}$$

$$\langle n\rangle_{L,x^*}=x\frac{\partial}{\partial x}\ln C_L(x^*)\sim L^{1/\nu} \tag{9b}$$

$$\langle(n-\langle n\rangle)^2\rangle_{L,x^*}=\left(x\frac{\partial}{\partial x}\right)^2\ln C_L(x^*)\sim L^{2/\nu} \tag{9c}$$

for large L, which complement the results (1), (2) of Whittington and Guttmann for $x<x^*$ and $x>x^*$. Equation (6) implies that the value $x_m(L)$ of x that maximizes $\langle(n-\langle n\rangle)^2\rangle_{L,x}$ for fixed $L\gg 1$ varies as

$$x_m(L)-x^*\sim L^{1/\nu}. \tag{10}$$

We have also considered adsorbing boundaries by assigning a surface fugacity x_s for each step along the boundary different from the bulk fugacity x for all other steps.

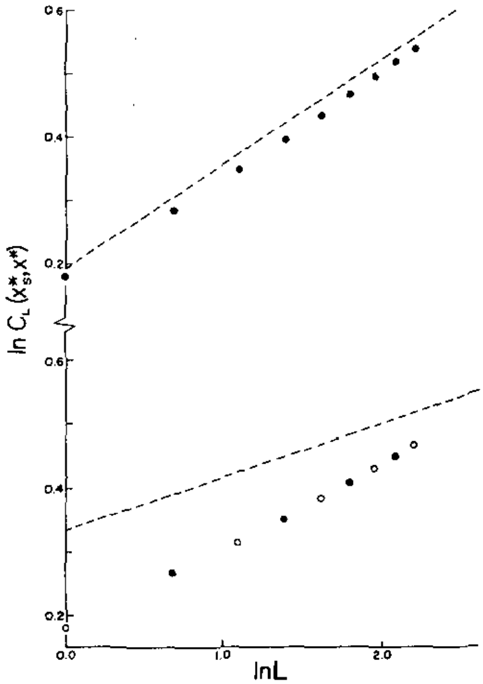

Figure 4. Dependence of $\ln C_L(x^*, x_s^*)$ on $\ln L$, with $L = 1, 2, \ldots, 9$, for walks between opposite corners (upper points) and walks between the midpoints of opposite edges (lower points). The filled and empty lower points correspond to even and odd L, respectively. The upper and lower broken lines have slopes $\frac{1}{6}$ and $\frac{1}{12}$.

In the half-space geometry a polymer adsorption transition [8-11], corresponding to the 'special' or 'multicritical' transition of semi-infinite magnetic systems with enhanced surface couplings [11, 12], takes place at the critical boundary and bulk fugacities x_s^* and x^*, respectively. For the square lattice $x^* = \mu^{-1}$ is given in equation (4). For x_s^* we use the estimate

$$x_s^* = 0.7738 \pm 0.0008 \tag{11}$$

of [9].

In the multicritical region $L \gg 1$, $|x_s^* - x_s| \ll x_s^*$, $|x^* - x| \ll x^*$, equation (6) is replaced by

$$C_L(x_s, x) = L^{-\eta_c^{sp}} g[L^{\phi^{sp}/\nu}(x_s^* - x_s), L^{1/\nu}(x^* - x)] \tag{12}$$

The quantities ϕ^{sp} and η_c^{sp} are the crossover and corner exponents [8-12], respectively, of the special transition.

For $d = 2$ the exact value [9, 10] of ϕ^{sp} is $\frac{1}{2}$, and $\eta_\parallel^{sp} = -\frac{1}{12}$ has been conjectured [9] on the basis of numerical data and conformal invariance. Thus (see equation (8)) we use the values

$$\phi^{sp} = \tfrac{1}{2} \tag{13a}$$

$$\eta_c^{sp}(\pi/2) = 2\eta_c^{sp}(\pi) = -\tfrac{1}{6} \tag{13b}$$

in making theoretical predictions for $d = 2$.

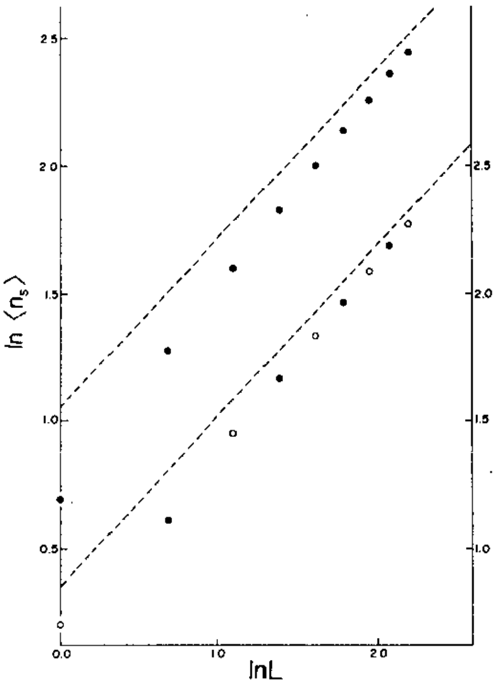

Figure 5. Dependence of $\ln\langle n_s\rangle_{x^*,x_s^*}$ on $\ln L$, with $L=1, 2, \ldots, 9$, for walks between opposite corners (upper points, left vertical axis) and walks between the midpoints of opposite edges (lower points, right vertical axis). The filled and empty lower points correspond to even and odd L, respectively. Both broken lines have slope $\frac{2}{3}$.

Equation (12) and its derivatives with respect to x and x_s yield

$$C_L(x_s^*, x^*) \sim L^{-\eta_c^{sp}} \tag{14a}$$

$$\langle n\rangle_{L,x_s^*,x^*} \sim L^{1/\nu} \tag{14b}$$

$$\langle n_s\rangle_{L,x_s^*,x^*} \sim L^{\phi^{sp}/\nu}. \tag{14c}$$

We now compare some of the analytic predictions with numerical data. Whittington and Guttmann [1] tabulated the $c_n(L)$ in equation (1) for $L \leq 6$. We have calculated $C_L(x)$ and $C_L(x_s, x)$ numerically for $L \leq 9$ with the transfer-matrix approach [9, 13].

The results for the total number of walks $C_L(1)$ (see equation (1)) between opposite corners and between the midpoints of opposite edges of the $L\times L$ square are given in table 1. Figure 1 shows $C_L(1)^{1/L^2}$ as a function of L^{-1}. The quantity λ in equation (2) may be estimated by extrapolating to $L^{-1}=0$. The data are consistent with the same value of λ for walks between opposite corners and the midpoints of opposite edges. This seems reasonable. According to equation (3) the number of steps in an average walk is of order L^2. The walk wanders all over the square, and the limit in equation (2) is insensitive to the particular endpoints.

The same value of λ for both sets of endpoints is also consistent with the result

$$\lambda = \lim_{L\to\infty} \Lambda_L^{(0)}(1)^{1/L} \tag{15}$$

of the transfer-matrix analysis. Here $\Lambda_L^{(0)}(1)$ is the largest eigenvalue of the transfer matrix with $x_s = x = 1$. Numerical results for $\Lambda_L^{(0)}(1)^{1/L}$ are also shown in figure 1. From the three sequences in figure 1 we estimate

$$\lambda = 1.743 \pm 0.005. \tag{16}$$

According to equations (7)-(9), in the large-L limit $C_L(x^*)$ varies as $L^{-5/2}$ and $L^{-5/4}$ for walks between opposite corners and between the midpoints of opposite edges, respectively. For both classes of walks $\langle n \rangle_{L,x^*}$ varies as $L^{4/3}$. The numerical data, shown in figures 2 and 3, are in good agreement with these predictions.

According to equations (13) and (14), in the presence of critically adsorbing boundaries $C_L(x_s^*, x^*)$ varies as $L^{1/6}$ for walks between opposite corners and as $L^{1/12}$ for walks between the midpoints of opposite edges. For both classes of walks $\langle n_s \rangle_{L,x_s^*,x^*}$ varies as $L^{2/3}$. The numerical data shown, in figures 4 and 5, is again consistent with the predictions, although the convergence of $C_L(x_s^*, x^*)$ for walks between the midpoints of opposite edges (lower sequence of points in figure 4) is rather slow†. The upper curve lends convincing support to the conjecture $\eta_\parallel^{\mathrm{sp}} = -1/12$ of [9].

In summary our analytical and numerical results confirm the correspondence [3] between the transition in the system of self-avoiding walks, analysed rigorously by Whittington and Guttmann [1], and the second-order transition in the N-vector model of magnetism in the limit $N \to 0$. We have shown that the correspondence is a useful starting point for deriving finite-size scaling properties of the system of walks.

We thank A J Guttmann and S G Whittington for stimulating correspondence.

Note added in proof. Some additional related work has come to our attention. Edwards [14] has considered walks from the centre to the edges of a square containing L^2 sites of a square lattice. The boundaries of the square are rotated 45° with respect to the square lattice. The total number of such walks increases with L as in equation (2), and the value of λ is very close to (probably identical with) the value for our geometry. Duplantier and Saleur [15] also proposed equation (9*b*). Duplantier and David [16] have confirmed equation (8) for Hamiltonian walks on the Manhattan lattice.

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† In the large-L limit $C_L(x^*, x_s^*)$ grows more rapidly for walks between corners (as $L^{1/6}$) than for walks between the midpoints of edges (as $L^{1/12}$). In small squares with enhanced surface fugacity, walks originating at the midpoints of edges have a tendency to pass close to the corners. This suggests an effective exponent for small L larger than the asymptotic exponent $\frac{1}{12}$, as seen for the lower sequence of points in figure 4. This is a possible explanation for the slow convergence.

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