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1984 J. Phys. A: Math. Gen. 17 L215

(http://iopscience.iop.org/0305-4470/17/4/011)

J. Phys. A: Math. Gen. **17** (1984) L215–L221. Printed in Great Britain

LETTER TO THE EDITOR

A direct real-space renormalisation calculation of the exponent gamma for self-avoiding walks

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Received 10 November 1983

Abstract. A real-space renormalisation group method of calculating the exponent γ for a single self-avoiding walk is presented. Application of the method on the square lattice yields $\gamma = 1.35 \pm 0.03$, in excellent agreement with the exact value of $\frac{43}{32}$.

Direct real-space renormalisation group methods for studying self-avoiding walks, in which the renormalisation is carried out by enumerating walk configurations that span (small) cells of the lattice, were first performed by Family (1981) in three dimensions an by de Queiroz and Chaves (1980) for two dimensions. (A detailed discussion and review is given by Stanley *et al* 1982.) These methods are similar to the successful cell renormalisation methods used in percolation (see e.g. Reynolds *et al* 1980, Stanley *et al* 1982.) However, in the self-avoiding walk case only one exponent—ν, describing the asymptotic behaviour of the mean square end-to-end distance of the walk—has to date been accessible. In this letter we illustrate a method of directly estimating the exponent γ by direct cell renormalisation of a *single* self-avoiding walk. This exponent describes the asymptotic behaviour of the number, c_N, of self-avoiding walks from a fixed origin, which varies as

$$c_N \approx A N^{\gamma-1} \mu^N, \qquad N \to \infty, \tag{1}$$

where μ is the connectivity constant of the walk on the lattice.

In a magnetic system, the exponent ν is related simply to the thermal field exponent while γ follows from the magnetic sclaing field. For percolation and the self-avoiding walk problem, the role of the thermal field is played by the percolation probability and the monomer fugacity, respectively. In percolation, the magnetic field is replaced by the ghost field (Stanley *et al* 1982), which is then renormalised along with the percolation probability within the cell calculation. Unfortunately, the analogue of the ghost field for the self-avoiding walk problem is unclear† and some alternative field must be introduced into a cell calculation if such a calculation is to yield the second scaling index of a self-avoiding walk. One possible field can be motivated by reference to a cross-over phenomenon occurring in magnetic systems.

† We are referring to the *single* walk problem. Des Cloizeaux (1975) (see also de Gennes 1979, Gujrati 1981) has shown that for a polymer *solution* the role of the magnetic field is played by the concentration.

0305-4470/84/040215+07$02.25

Consider a n-component spin system $\boldsymbol{s}=(s^1, s^2, \ldots, s^n)$ on a d-dimensional lattice Ω with Hamiltonian

$$H_0[\boldsymbol{s}]=K\sum_{\langle r,r'\rangle}\boldsymbol{s}_r\cdot\boldsymbol{s}_{r'}, \tag{2}$$

where the sum is over all near-neighbour bonds of the lattice. By the usual arguments (see e.g. the appendix of Daoud *et al* 1975, de Gennes 1979), the zero-field susceptibility of this model, in the limit $n\to 0$, is the chain generating function

$$C(K)=\sum_{N=0}^{\infty}c_N K^N \approx A(1-K/K_c)^{-\gamma}, \qquad K\to K_c^-. \tag{3}$$

The connective constant, appearing in (1),

$$\mu=1/K_c, \tag{4}$$

where K_c is the critical temperature (again for $n\to 0$) of the spin analogue.

In a renormalisation group calculation K_c (and hence μ) is determined by the fixed point of an appropriate recursion relation

$$K\to K'=R(K) \tag{5}$$

with

$$\nu=\ln b/\ln(R'(K_c)), \tag{6}$$

where b is the spatial rescaling factor of the transformationa and $R'(K)=\mathrm{d}R/\mathrm{d}K$. This is standard. The problem we address is estimating γ.

To do so, consider the *duplicated system*

$$H=H_0[\boldsymbol{s}]+H_0[\boldsymbol{t}]+\Delta\sum_r t_r^1 s_r^1, \tag{7}$$

where $\{\boldsymbol{t}\}$ are also n-component spins populating a lattice Ω' which is an identical copy of Ω and we have introduced a coupling Δ between the 1-components of the spins on equvalent sites on Ω and Ω'. The partition function of the duplicated system $Z(K,\Delta)$ can be written

$$Z(K,\Delta)=Z(K,0)\left\langle\exp\left(\Delta\sum_r t_r^1 s_r^1\right)\right\rangle_0, \tag{8}$$

where the expectation value is with regard to the decoupled Hamiltonian $H_0[\boldsymbol{s}]+H_0[\boldsymbol{t}]$. Hence, expanding the exponential and assuming $T>T_c$, the free energy per spin

$$\beta f(K,\Delta)=\beta f(K,0)-\tfrac{1}{4}\Delta^2\sum_r\langle s_0^1 s_r^1\rangle_0^2+\mathrm{O}(\Delta^4). \tag{9}$$

Our interest is in the behaviour of $f(K,\Delta)$ for small Δ and K near $K_c=K_c(\Delta=0)$. Here we expect the singular part of f to scale as

$$\beta f_s(K,\Delta)\approx t^{d\nu}\tilde{Q}(\Delta/t^{\phi}) \tag{10}$$

with $t\approx K_c-K$. If we assume that $\langle s_0^1 s_r^1\rangle_0$ scales as

$$\langle s_0^1 s_r^1\rangle_0\approx D(r/\xi)/r^{d-2+\eta}, \qquad r\to\infty, \tag{11}$$

where $\xi\sim t^{-\nu}$ is the correlation length, substitution of (11) in (9) implies that

$$\beta f_s(K,\Delta)\approx At^{d\nu}+\Delta^2 Bt^{\nu d-2\gamma}\ldots, \qquad t\to 0, \tag{12}$$

where A and B are constants and $\gamma = (2-\eta)\nu$. This result is consistent with (10) if

$$\phi = \gamma. \tag{13}$$

If we extend the scaling formulation to include a magnetic field, it is then straightforward to show that the zero-field susceptibility of the duplicated model similarily scales as

$$\chi_n(K, \Delta) \approx t^{-\gamma} Q(\Delta/t^{\gamma}) \tag{14}$$

as $\Delta \to 0$ and $K \to K_c$.

To apply this result to our self-avoiding walk problem consider the expansion of χ as a double series in K and Δ, following the standard arguments (see e.g. the appendix of Dauod *et al* 1975). In the limit $n \to 0$, the only diagrams that contribute are self-avoiding walks, in which each step between points *in* Ω (or Ω') is assigned a fugacity K but steps *from* Ω to Ω' (and vice versa) carry fugacity Δ. Explicitly

$$\lim_{n\to 0} \chi_n(K, \Delta) = \sum_{N,N_1} c_{N,N_1} K^{N-N_1} \Delta^{N_1} \equiv C(K, \Delta), \tag{15}$$

where c_{N,N_1} is the number of N step walks with N_1 steps between the two copies. The cross-over scaling form (14) implies that

$$C(K, \Delta) \approx (K - K_c)^{-\gamma} Q(\Delta/(K-K_c)^{\gamma}), \qquad K \to K_c^-, \qquad \Delta \to 0, \tag{16}$$

where $K_c^{-1} = \mu$ is the connective constant of Ω.

Several remarks are in order. We have considered what may be called a 'layer' duplication since for $d = 2$, the Hamiltonian (7) corresponds to two layers Ω and Ω' linked by an inter-layer coupling Δ between equivalent sites. Alternative ways of coupling the two copies Ω and Ω' together can be defined. For example,

$$H = H_0[s] + H_0[t] + \Delta \sum_r s_r^1 \left(\sum_\delta t_{r+\delta}^1 \right), \tag{17}$$

where $r + \delta$ labels some set of sites in Ω'. Provided this set is suitably local, there is no effect on the preceding analysis except to modify the coefficient B appearing in (12). The most useful duplication of the type (17) is where Ω and Ω' are taken as isomorphic sub-lattices of some larger lattice. On the square lattice, for example, we can obtain a duplicated system if we regard K and Δ as the nearest and next-nearest neighbour interactions respectively; or in the context of a self-avoiding walk the fugacities associated with steps to next and next-neareast neighbour sites respectively.

The identification $\phi = \gamma > 1$ implies that Δ is a *relevant* perturbation at the fixed point of the decoupled system. In the (K, Δ) plane, we expect a flow topology as shown in figure 1, where both fixed points (K^*, Δ^*) and $(K_c, 0)$ have the *same* thermal exponent since the duplication process does not change the dimensionality or universality class of the problem. This is in contrast, to a similar cross-over (in fact described by the same exponent $\phi = \gamma$) occurring if an infinite number of copies of Ω are coupled by Δ as occurs, for example, for inter-layer coupling on the simple cubic lattice (see Liu and Stanley 1973). In this case the fixed points have different exponents. In this context, the scaling theory has been discussed by Liu and Stanley (1973). (See also Huse and Fisher (1982) who consider the general problem of coupling two Ising systems together.) The identification $\phi = \gamma$ for magnetic systems was first made by Abe (1970) and Suzuki (1971). The extension of their idea to self-avoiding walks does not seem to have been made previously, although Liu and Stanley (1973) proved

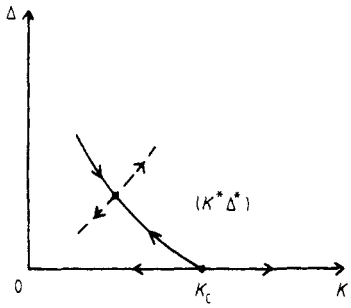

Figure 1. Flow diagram of renormalisation trajectories for a duplicated system.

that the derivatives $[\partial^r C(K,\Delta)/\partial\Delta^r]_{\Delta=0}$ diverge with exponent $(r+1)\gamma$ which is consistent with (and implied by) (16). The analogous cross-over in percolation has been discussed by Redner and Coniglio (1980) and exploited, in a similar way that we shall exploit for the self-avoiding walks, by Oliviera (1981).

Let us now illustrate how the preceding scaling ideas and results can be implimented and exploited in a cell calculation on a single self-avoiding walk. We shall report results for both 'layer' and 'sub-lattice' duplications, although, for sake of clarity, we focus attention on the sub-lattice procedure.

For a detailed description of the cell method of renormalising a self-avoiding walk we refer to Stanley *et al* (1982). The only extension necessary is the inclusion of the second (duplicated) lattice. The resulting simplest cell constructions for the square lattice using both layer and sub-lattice duplication are shown in figure 2. Under renormalisation, these cells lead to renormalised couplings K' and Δ' corresponding to the reduced cells as shown. For this transformation, $b=2$. Clearly, K' and Δ' are (complicated) functions of K and Δ. However, we only require the recursion relations for small Δ.

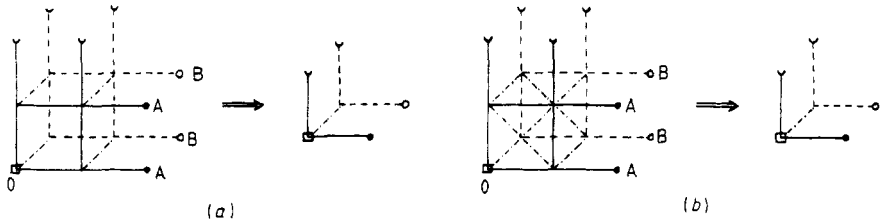

Figure 2. Simplest cells for (*a*) layer duplication, (*b*) sub-lattice duplication. Bonds (——) or (– – – –) have fugacity K, while inter-copy bonds (– · – · – · –) have fucacity Δ.

Inspection of figure 2 shows that, for small Δ, the recursion relations will have the form

$$K' = R(K) + O(\Delta^2) \qquad \Delta' = \Delta g(K) + O(\Delta^3) \tag{18a, b}$$

since any walk contributing to the renormalisation of the fugacity K in the *same* copy must make either no transition or an even number of transitions between the copies. Similarly, the renormalisation of Δ involves an odd number of inter-copy steps. For $\Delta=0$, (18*a*) is simply the recursion relation for walks on a single copy of the lattice,

while (18*b*) shows that the resulting linear transform near $(K_c, 0)$ is diagonal with two eigenvalues

$$\Lambda_T = R'(K_c) = b^{1/\nu} \qquad \text{and} \qquad \Lambda_\Delta = g(K_c) = b^{\gamma/\nu}. \tag{19}$$

From this we obtain

$$\nu^{-1} = \ln \Lambda_T / \ln b \tag{20}$$

and

$$\gamma = \nu(\ln \Lambda_\Delta / \ln b), \tag{21}$$

where b is the spatial rescaling factor.

In practice the functions $R(K)$ and $g(K)$ appearing in (18) are constructed by enumerating walks that appropriately span the cell. To illustrate the method we consider the cell of figure 2(*b*) and use the 'corner-rule' of Stanley *et al* (1982) in which the walk is assumed to enter the cell at the corner indicated by '0'. The walk will then contribute to K' if it reaches either of the sites A and to Δ' if it reaches either of the sites B. Hence we obtain

$$R(K) = K^2 + 2K^3 + K^4$$

$$g(K) = (K^2 + 2K^3 + K^4)(1 + 3K + 4K^2 + 3K^3) + (K + K^2 + K^4)(K + 4K^2 + K^3) \tag{22}$$

from which we find

$$K_c = 0.466, \qquad \nu = 0.715 \qquad \text{and} \qquad \gamma = 1.483. \tag{23}$$

These estimates are improved by considering larger cells and different values of b. Rational values of b can be realised by renormalising a cell of s_1 sites to a cell of $s_2 = s_1/b$ sites (see Stanley *et al* 1982). The results of these calculations, carried out by enumerating the required walks on a computer, are given in table 1. In all cases, the estimates of K_c and ν agree with these of earlier works (see e.g., Kremer 1983a, b). Apparently, the sub-lattice method overestimates γ while the layer method underestimates. These estimates of γ can be further refined by extrapolation to $b = 1$ (Stanley

Table 1. Results of direct renormalisation of a self-avoiding walk on the square lattice. Symbols refer to extrapolation shown in figure 3. (Detailed data on the enumeration can be obtained from the first author.)

Number of sites in cell (one lattice)	b	K_c	ν	γ (layer duplication)	γ (sub-lattice duplication)
2×2	2	0.466	0.715 (●)	0.390	1.483 (+)
3×3	3	0.447	0.719	0.677	1.493
3×3	$\frac{3}{2}$	0.432	0.722 (●)	1.243 (×)	1.535 (+)
4×4	4	0.435	0.722	0.790	1.475
4×4	2	0.423	0.726	1.263	1.488
4×4	$\frac{4}{3}$	0.416	0.731 (●)	1.289 (×)	1.416 (+)
5×5	5	0.426	0.724	0.855	1.462
5×5	$\frac{5}{2}$	0.417	0.729 (●)	1.278 (○)	1.464 (□)
5×5	$\frac{5}{3}$	0.411	0.733 (●)	1.303 (○)	1.401 (□)
5×5	$\frac{5}{4}$	0.407	0.736 (●)	1.319 (○) (×)	1.379 (□) (+)

et al 1982). This extrapolation is shown in figure 3 and yields the estimate

$$\gamma = 1.35 \pm 0.03. \tag{24}$$

For comparison, we show a similar extrapolation of ν.

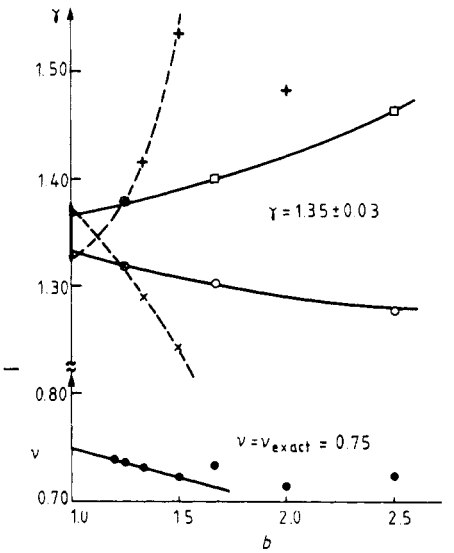

Figure 3. Extrapolation to $b = 1$ of estimates of γ and ν for $d = 2$ square lattice. Points marked (+) and (□) correspond to the sub-lattice method, while (○) and (×) refer to the layer procedure (see table 1).

The result in (24) compares favourably with direct series methods (see e.g. Guttmann 1983). On the basis of these calculations, γ for many years was believed to be $\frac{4}{3}$. Recently Nienhuis (1982) analytically investigated a special n-component spin system on the honeycomb lattice. In the limit $n \to 0$, he found

$$\gamma = \tfrac{43}{32} = 1.343\,75\ldots \tag{25}$$

Re-analysis of the series expansions (Guttmann 1983, Majid *et al* 1983) supports this value rather than $\frac{4}{3}$. We cannot, of course, distinguish between $\frac{4}{3}$ and $\frac{43}{32}$ but it is gratifying that the central value of our extrapolation is in such excellent agreement with (25).

In principle, the same method can be applied in three dimensions but here computing requirements limit the calculation to $2 \times 2 \times 2$ cells. In this case, the 'layer' duplication gives a completely wrong result, while the sub-lattice duplication yields $\gamma = 1.375$ compared to the 'accepted' value of $\frac{7}{6}$.

The method can also be modified to yield the 'surface' exponents γ_1 and $\gamma_{1,1}$, which describe the configuration of walks attached to a surface (Barber *et al* 1978). Here the duplicated lattices (now assumed to have a free surface) are coupled by an interaction Δ involving only spins in the surface. The scaling argument used for the bulk case can be carried through again with the conclusion that the relevant cross-over exponent is $\gamma_{1,1}$, which on the basis of directed enumeration, is expected to be (Barber *et al* 1978)

$$\gamma_{1,1} = -0.20 \pm 0.02 \qquad (d = 2).$$

The negative sign implies that the surface coupling between the lattices is now irrelevant. Unfortunately, the small cells used in the present study are too small, even for $d = 2$, to yield sensible estimates. Indeed, on the basis of this calculation one would conclude that $\gamma_{1,1} > 0$, although an appreciable decrease as $b \to 1$ is apparent.

Despite this failure, the method of duplicating the lattice and thereby calculating γ as a cross-over exponent is a useful addition to the armoury of renormalisation group techniques. One way of overcoming the small cell limitations would be to use Monte Carlo methods to sample larger cells as has been done for percolation (Reynolds *et al* 1980). Such a development, however, is beyond the scope of this paper.

Acknowledgments

This work was initiated while one of us (MNB) was a visitor at KFA-Jülich. He is grateful for the hospitality and support of KFA-Jülich during this time. The authors thank E Eisenriegler and W Kinzel for useful discussions.

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