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Renormalization theory of self-avoiding walks which cross a square

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Abstract. The renormalization group theory is used to calculate the critical behaviour of self-avoiding walks which cross a square. This problem, which has been proposed recently, is especially well suited for a renormalization group analysis. The fixed-endpoint, diagonal-span trademark of the square-crossing walks leads naturally to a well defined renormalization scheme. Unlike other finite-lattice renormalization schemes for self-avoiding walks, this square-crossing renormalization is exact in the sense that the finite lattice (square) is uniquely defined, the spanning rule is unambiguous, and the end-to-end correlations are exactly preserved. The results for the critical point are in excellent agreement with series analysis estimates and support a conjecture on its exact value.

1. Introduction

Recently, Whittington and Guttmann [1] have proposed a new kind of self-avoiding walk problem and proved some rigorous statistical results. They consider self-avoiding walks on the square lattice which are confined to the interior or the boundary of a square with vertices at $(0,0)$, $(L,0)$, $(0,L)$ and (L,L). In particular, they focus on the class of self-avoiding walks which begin at the point $(0,0)$ and end at the point (L,L). Their two primary results are that the number of these self-avoiding walks which cross the square scales (for large L) like a constant to the power L^2, and a proof of the existence of a phase transition when a fugacity is associated with each step of the walk. Although their study does not identify the exact location of the phase transition point (critical fugacity), they do provide a numerical estimate based on series analysis of the exact (small L) statistics.

In this paper, the real space renormalization group theory is used to calculate the critical point and a critical exponent of the square-crossing self-avoiding walk problem. This problem is an excellent candidate for the renormalization group theory. The results of this theory for the critical point are in excellent agreement with the estimates of Whittington and Guttmann [1] and support their conjecture on its exact value. In section 2, the renormalization group theory is formulated. In section 3, the results are presented. Section 4 is a discussion.

2. Renormalization

This self-avoiding walk problem is ideally suited for a renormalization group analysis. First of all, the constraint that forces all the walks to span the $L\times L$ lattice between the two fixed points (0, 0) and (L, L) captures the essence of preserving the correlations (end-to-end distance) in the renormalization group formulation. Secondly, the set of lattice walk problems defined by the different values of L is precisely the set of lattice walk problems that are related by a renormalization (scale) transformation. In other words, studying the self-avoiding walk statistics as a function of the square size L is equivalent to studying the system at different length scales via a renormalization map. The connection between two lattice walk problems with differing L will uniquely determine the renormalization map.

To define the renormalization, we consider the statistical mechanics of this lattice statistics problem. Where possible, we use the same notation as Whittington and Guttmann [1]. The lattice is an $L \times L$ square lattice with one vertex at (0, 0) and the diagonally opposed vertex at (L, L). Self-avoiding walks are embedded on this finite lattice with the constraint that they must begin at (0, 0) and end at (L, L). A fugacity x is associated with each step of the walk. The grand partition function (generating function) $C_L(x)$ is defined by

$$C_L(x) = \sum_n c_n(L) x^n \tag{2.1}$$

where the partition function $c_n(L)$ is the number of self-avoiding walks with n steps that cross this square of side L. This partition function can be interpreted as the correlation function between the endpoints of the walk separated by a distance $\sqrt{2}\, L$. It should also be noted that the summation over n goes from a minimum value of $2L$ to a maximum value of L^2+2L if L is even and L^2+2L-1 if L is odd.

It has been proven [1] that this grand partition function is non-analytic in the large L thermodynamic limit at some singular point x_0 in the range

$$\mu^{-1} \leqslant x_0 \leqslant \mu_{\mathrm{H}}^{-1}. \tag{2.2}$$

The lower bound is determined by μ, which is the connective (growth) constant for unconstrained self-avoiding walks on the square lattice. The best numerical estimate of μ is 2.6381 [2]. The upper bound depends on μ_{H}, which is the connective constant for Hamiltonian polygons on the square lattice. Whittington and Guttmann [1] have analysed exact series data for $L \leqslant 6$ and estimate that x_0 is between 0.3 and 0.4. From their rigorous result that $x_0 \geqslant \mu^{-1} = 0.379$, they conclude that x_0 is between 0.379 and 0.4. They conjecture that the phase transition occurs exactly at a critical point $x_0 = \mu^{-1} = 0.379$.

In this paper, the critical point x_0 is calculated using the renormalization group theory. The renormalization consists of a mapping of the self-avoiding walk system at microscopic length scale (lattice spacing) l to a system at length scale bl, where the scale factor $b > 1$. The mapping must preserve the macroscopic physics (statistics), and thus must leave the grand partition function invariant. We consider a finite lattice renormalization that maps an $L \times L$ square onto an $L' \times L'$ square where $L' < L$. This corresponds to a change in length scale from l to bl where $b = L/L'$. This kind of finite-lattice (cell-to-cell) renormalization scheme is known [3–5] to be very accurate for small b. It has been shown [4, 5] in other self-avoiding walk and lattice statistics problems that the cell-to-cell renormalization with $b = \frac{6}{5}$ is comparable in accuracy to that of a cell-to-bond renormalization with $b = 40$–80. The accuracy improves as b decreases and in the limit $b = 1$, the corresponding infinitesimal renormalization is exact [4–7]. Hence for accuracy, we choose $L' = L - 1$. Figure 1 illustrates this square-to-square renormalization for an $L = 5$ square. Under the renormalization, the class of

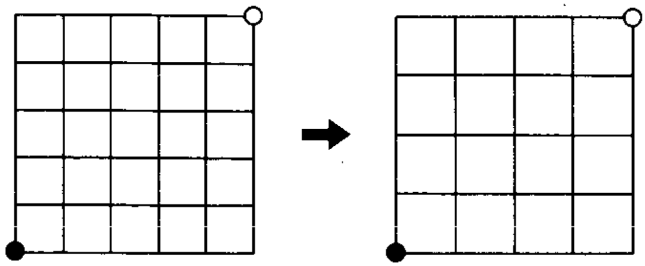

Figure 1. The finite-lattice renormalization from an $L = 5$ square to an $L' = 4$ square. The corresponding change in length scale (lattice spacing) is from l to bl where the scale factor $b = \frac{5}{4}$. The set of all self-avoiding walks which cross the 5×5 square are mapped (renormalized) onto the set which cross the 4×4 square. The beginning (●) and the ending (○) points of these diagonally spanning walks are shown on the lattices.

self-avoiding walks that cross the $L \times L$ square are mapped (renormalized) onto that class which cross the $L' \times L'$ square.

It is important to emphasize that this finite-lattice renormalization scheme for self-avoiding walks which cross a square is exact. The finite lattice is exactly determined by the square. The weight function or projection is characterized by a well defined and unambiguous spanning rule that emerges naturally from the trademark of this self-avoiding walk problem: a walk must span the lattice by beginning at $(0, 0)$ and ending at (L, L). The renormalization exactly preserves this fixed-endpoint diagonal span. These features are in contrast to other renormalization schemes for unconstrained self-avoiding walks which are not well defined or unique. These other schemes are plagued by ambiguities in the spanning rule which cannot uniquely specify where the walks should begin or end, by ambiguities in the intercell correlations, or by ambiguities in the cell cluster geometry [4].

Under the renormalization, the fugacity x is mapped onto a renormalized fugacity x' that is determined in the standard way [4, 5] by the preservation of the grand partition function:

$$C_L(x) = C_{L'}(x'). \tag{2.3}$$

This invariance relation implicitly determines x' as a function of x corresponding to the scale factor $b = L/L'$. We denote this renormalization map by

$$x' = f_b(x). \tag{2.4}$$

The fixed point x_0 of this map is determined by

$$x_0 = f_b(x_0) \tag{2.5}$$

or equivalently by the grand partition function relation

$$C_L(x_0) = C_{L'}(x_0). \tag{2.6}$$

This fixed point of the renormalization map is the critical point of the phase transition. Hence from equations (2.1) and (2.6), the critical point x_0 is determined by

$$\sum_n c_n(L) x_0^n = \sum_n c_n(L') x_0^n. \tag{2.7}$$

The renormalization theory can also be used to calculate the critical exponent associated with the average number of steps in the walk. The average number of steps in a self-avoiding walk with fugacity x on an $L \times L$ square is defined by

$$\langle n(x, L)\rangle = \frac{\Sigma_n n c_n(L) x^n}{\Sigma_n c_n(L) x^n}. \tag{2.8}$$

This quantity can be generated from the grand partition function (2.1) according to

$$\langle n(x, L)\rangle = \frac{\mathrm{d} \log C_L(x)}{\mathrm{d} \log x}. \tag{2.9}$$

This expression, together with (2.3), provides the renormalization group equation that relates the average number of steps on two different squares of size L and L'. At the fixed point x_0, we find

$$\langle n(x_0, L)\rangle = \langle n(x_0, L')\rangle f_b^1(x_0) \tag{2.10}$$

where

$$f_b^1(x_0) = \left.\frac{\mathrm{d}f_b}{\mathrm{d}x}\right|_{x=x_0}. \tag{2.11}$$

If we define the critical exponent y by the scaling behaviour

$$\langle n(x_0 L)\rangle \sim L^y \qquad L \to \infty \tag{2.12}$$

then from (2.10), this exponent is determined by

$$y = \frac{\log f_b^1(x_0)}{\log b} \tag{2.13}$$

where $b = L/L'$. Thus the critical exponent y can be calculated from the renormalization map $f_b(x)$.

From finite-size scaling theory [5, 8] applied to ordinary (unconstrained) self-avoiding walks, the critical index $y = 1/\nu$, where ν is the standard (end-to-end distance) critical exponent for ordinary walks on the infinite lattice. For the square-crossing walk problem, this connection is also suggested by the fact that the end-to-end distance R of walks which cross an $L \times L$ square is

$$R = \sqrt{2}\, L. \tag{2.14}$$

From (2.12), this can be expressed as

$$R \sim \langle n(x_0, L)\rangle^{1/y}. \tag{2.15}$$

3. Results

We use equation (2.7) to calculate the critical point x_0 as a function of the scale factor $b = L/L'$. The series coefficients $c_n(L)$ were taken from Whittington and Guttmann [1] who have computed them exactly for $L \leq 6$, which corresponds to $n \leq 48$. The results are displayed in table 1 and graphed in figure 2. The critical point displays a surprisingly accurate and suggestive linear dependence on $1/b$. Extrapolation of the data to the exact limit $b = 1$ yields an estimate for the critical point of $x_0 = 0.373$. Also shown on the graph in figure 2 is the result of a square-to-bond renormalization. It is known [4]

Table 1. The critical point x_0 and the critical exponent y as a function of the scale factor b for a square-to-square renormalization.

b	x_0	y
$\frac{2}{1}$	0.5250	1.133
$\frac{3}{2}$	0.4741	1.178
$\frac{4}{3}$	0.4488	1.210
$\frac{5}{4}$	0.4336	1.235
$\frac{6}{5}$	0.4235	1.257

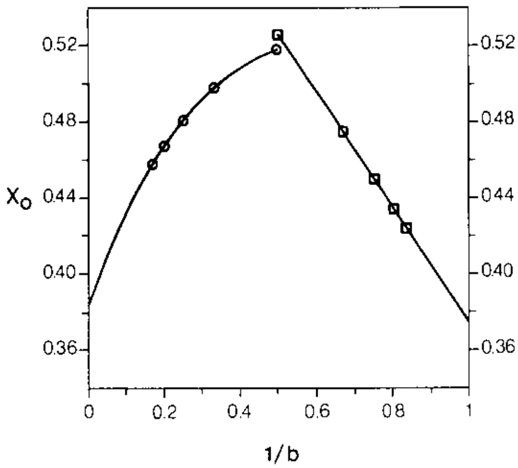

Figure 2. The critical point x_0 as a function of the inverse scale factor $1/b$ for a square-to-square (□) and a square-to-bond (○) renormalization. The best fit curves through the data points provide estimates for the exact critical point where they intersect the $1/b = 0$ axis and the $1/b = 1$ axis.

that this type of (cell-to-bond) renormalization scheme improves in accuracy as b increases and becomes exact in the limit $b = \infty$. We have performed this square-to-bond calculation in order to compliment the square-to-square renormalization which is exact in the opposite limit $b = 1$. A polynomial fit to the square-to-bond data yields the exact limit $b = \infty$ estimate for the critical point of $x_0 = 0.383$.

We calculate the critical exponent y from the renormalization map (eigenvalue of linearized map) according to equation (2.13). The results are displayed in table 1. Based on finite-size scaling [4, 5], the difference between the approximate critical exponent and its exact value should converge to zero according to $\ln b$ as b approaches 1 for the square-to-square renormalization (and according to $1/\ln b$ as b approaches ∞ for a square-to-bond renormalization). Thus, to estimate the exact critical exponent, we have extrapolated the data according to this finite-size scaling behaviour. The data is graphed in figure 3. The square-to-square renormalization yields an estimate for the critical exponent of 1.35. The square-to-bond estimate is 1.27. Based on alternative extrapolation methods, and indeed from a rough visual extrapolation of the data, one can estimate that the critical exponent must fall (conservatively) in the range between 1.27 and 1.45. For this reason, and since the square-to-square renormalization scheme

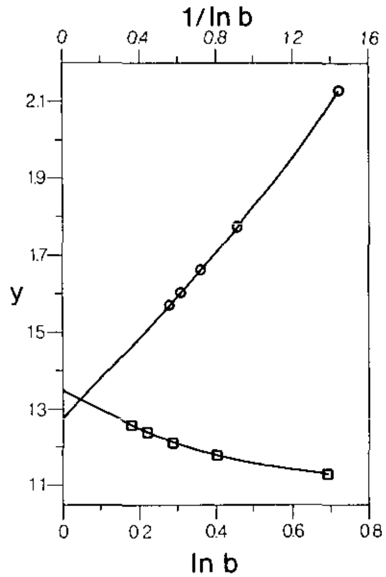

Figure 3. The critical exponent y as a function of ln b for a square-to-square (□) renormalization and 1/ln b for a square-to-bond (○) renormalization. The extrapolated points at $b = 1$ (square-to-square) and $b = \infty$ (square-to-bond) provide estimates for the exact critical exponent.

is known to be more accurate [5], the best estimate for the critical exponent is taken to be $y = 1.35$.

4. Discussion

The renormalization group theory has been used to calculate the critical point of self-avoiding walks which cross a square. In order to optimize our results, we have performed two kinds of renormalization that compliment one another. In the exact limit that the scale factor $b = 1$, a square-to-square renormalization calculation yields an estimate for the critical point of $x_0 = 0.373$. In the opposite exact limit $b = \infty$, a square-to-bond renormalization yields an estimate of $x_0 = 0.383$. These values are consistent with the series analysis results of Whittington and Guttmann [1] which predict that $0.3 < x_0 < 0.4$. Furthermore, our results support their conjecture that the exact value of $x_0 = 0.379$.

The renormalization theory has also been used to calculate the critical exponent associated with the average number of steps in the walks. We find a best estimate value for the critical exponent of $y = 1.35$. Away from the critical point, the average number of steps has been considered by Whittington and Guttmann [1]. For $x = 1$, they prove that $y = 2$. Furthermore, they observe that the critical point $x = x_0$ represents the transition from a regime ($x < x_0$) where walks of order L steps dominate ($y = 1$) to a regime ($x > x_0$) where walks of order L^2 steps dominate ($y = 2$). Our result for the exponent at the critical point is consistent with this interpretation of the phase transition in terms of the average number of steps in the walks.

Furthermore, our results for the critical point and the critical exponent are suggestive that this square-crossing self-avoiding walk problem is in the same universality class as the ordinary (unconstrained) self-avoiding walk problem. For the ordinary self-avoiding walk problem in two dimensions, the best estimate for the critical point x_0 is 0.379 06 [2], while the critical exponent ν is believed to be exactly $\frac{3}{4}$ [9]. If one identifies y with $1/\nu$, then the agreement between these critical descriptors and those obtained in this paper suggests universality. Clearly, a more complete phase diagram analysis is necessary to establish such universality.

This self-avoiding walk problem is interesting and relevant for two primary reasons. First of all, it is a simple realization of a self-avoiding walk system that exhibits a non-trivial phase transition. Hence, it can provide insight into polymer systems and critical phenomena in general. Secondly, it is a custom-designed model for use with the renormalization group theory. The model has built-in features which make it especially compatible with the ideas of renormalization. The most notable features are that it is defined on a sequence of finite lattices (squares) that can be related by a scale factor, and that all the walks must diagonally span each lattice between two fixed endpoints (which automatically preserves the endpoint correlations). Unlike other real-space renormalization schemes for self-avoiding walks, the renormalization of square-crossing walks is unambiguous (with regards to the connectivity rule, the endpoint correlations and the cell geometry) and exactly conforms to the basic ideas of the renormalization theory. Hence, in addition to providing insight into polymers and critical phenomena, this self-avoiding walk system can serve as a paradigm for, and can test the concepts of, real-space renormalization and finite-size scaling.

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