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Statistics of confined chains. III: Hamiltonian paths

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Abstract. The entropy of self-avoiding walks embedded in a square lattice has been Monte Carlo estimated inside plane squares of various side sizes R. The length of the walks ranged from one to $R^2 - 1$ steps, the maximum allowed length, which corresponds to the so-called Hamiltonian paths. It was found that if Φ is the ratio of the occupied over the total number of available lattice sites inside the square, the number of configurations $Z(\Phi)$ scales to a good approximation as $[Y(\Phi)]^{R^2}$. The limiting $Y(\Phi)$ curve has then been estimated from the available data, and expressed as a fourth-degree polynomial in Φ. A table is given for $Z(1)$, that is Hamiltonian paths, comparing values obtained from the theoretical relationship given by Orland *et al*, from the exact enumeration data of Mayer *et al*, and from the Monte Carlo estimates of the present work.

1. Introduction

A Hamiltonian path (HP) is defined inside some bounded lattice as a path which fills all available lattice sites without ever crossing itself. If the two ends of the path are on adjacent lattice sites, the path is called a Hamiltonian circuit (HC). The number, $Z(N)$, of N-step HPs inside some bounded lattice is a long-standing problem in combinatorial analysis. As far back as 1947, Orr [1] gave the asymptotic estimate $Z(N) = A^N$, with the following estimated bounds for A: plane square lattice $1.30 < A < 1.50$, simple cubic lattice $1.55 < A < 2.22$. Flory [2], in 1953, using mean-field arguments, arrived at the general estimate $A = (q-1)/e$, where q is the coordination number of the lattice considered, and e the basis of Neperian logarithms. In 1963 Kasteleyn [3] gave the exact solution for the subclass of alternatively oriented HPs on the plane square lattice (the so-called Manhattan paths) which is $Z(N)_M = 1.338^N$, so that 1.338 was a new lower bound for A in that case. Some time later, Domb [4] pointed out that an upper bound for A in the case of the plane square lattice was provided by Lieb's exact solution for the entropy of two-dimensional ice [5], which yields $A < 1.59$. Other investigators who have addressed the problem are Gordon *et al* [6] and Gujrati and Goldstein [7]. Important progress was accomplished by Schmalz *et al* [8], who gave a precise asymptotic value of A for HCs in rectangles, using a transfer matrix method. Their result is $A = 1.472$, but according to these authors, asymptotically, many features of HPs should be the same as for HCs. A more general theory, applicable in principle to any dimensions, was devised in 1985 by Orland *et al* [9], who, using Ising-model-like calculations, arrived at the following simple law for HCs

$$A = q/e \tag{1}$$

which quite resembles the Flory law. Equation (1) yields $A = 1.4716$ for the plane square lattice and $A = 2.207$ for the simple cubic lattice.

More recently, exact enumeration (EE) data have been reported for $Z(N)$ by Mayer *et al* [10] up to the 7×7 square lattice, and by Shakhnovich *et al* [11] for the $3 \times 3 \times 3$ simple cubic lattice. The last paper on the subject we are aware of is that of Pande *et al* [12], who enumerate $Z(N)$ for cubic sublattices up to the $3 \times 4 \times 4$ parallelogram.

The purpose of the present paper is the presentation of the Monte Carlo (MC) estimates of $Z(N)$ inside $R \times S$ rectangles, a particular case of which are $R \times R$ squares. In this procedure, N, the number of steps of the self-avoiding walk, varies from 1 to $R \times S - 1$, the latter case corresponding to HPs. The basis of these MC estimates is provided by the Rosenbluth–Rosenbluth procedure [13] for generating self-avoiding walks.

The following relationship to estimate $Z(N)$ has been used [14]:

$$Z(N) = \mathrm{Z}_{\max}\langle w\rangle(1 - A_{\mathrm{RS}})K \tag{2}$$

where $\langle w\rangle$, the 'compactness parameter' [14] (called also the Rosenbluth–Rosenbluth factor [15]), is defined through

$$\langle w\rangle = (SZ_{\max})^{-1}\left\{\sum_{j=1}^{S}\prod_{i=1}^{4}(i)^{n_i^j}\right\}. \tag{3}$$

Here n_i^j is the number of instances where, in chain j of the MC sample, there were i possible directions to continue generating the walk ($1 \leqslant i \leqslant 3$, except for the first step in the chain, where i may take the value 4). A_{RS} is the attrition in reflecting statistics [14], that is the probability of failure of an initiated chain. This attrition originates in the fact that a growing chain may become trapped, so that further pursuing its generation procedure is not possible. Both $\langle w\rangle$ and A_{RS} are here computed by screening *one* step ahead for available directions. The case of screening several steps has been addressed by Meirovitch [16], but his calculations are irrelevant for present purposes. $Z_{\max}$ is here equal to $4 \times 3^{N-1}$. Finally K is the number of confined lattice sites.

It should be noticed that equation (3) is also valid for free (non-confined) self-avoiding walks, by taking $K = 1$. This amounts to assuming that the walks being generated start permanently from the same lattice site.

Understandably, a walk, whether free or confined, sees its attrition increasing with increasing N. For HPs, where the confinement takes its uppermost value, A_{RS} tends rapidly to values close to one. For this reason, due to the computational times involved in obtaining significant MC samples, it is not possible at the present time using PCs to obtain convenient MC samples beyond the 9×9 square lattice. The situation is, however, improved if one considers not HPs, but chains somewhat shorter (that is chains which do not entirely fill the square). By this procedure it is possible to extrapolate, as indicated in figure 1, to obtain the value of Z for HPs.

2. Monte Carlo procedures and results

Self-avoiding walks of various lengths have been computer generated inside plane rectangles $R \times S$ and squares $R \times R$ on the square lattice according to the Rosenbluth–Rosenbluth procedure. The software used to this effect was an adaptation in two dimensions of the software we used in previous papers [14]. Screening for available directions proceeded one step ahead, so that equation (2) would be used as it is. Screening two (or more) steps ahead would reduce the attrition A_{RS}, and correspondingly the definition of the $\langle w\rangle$

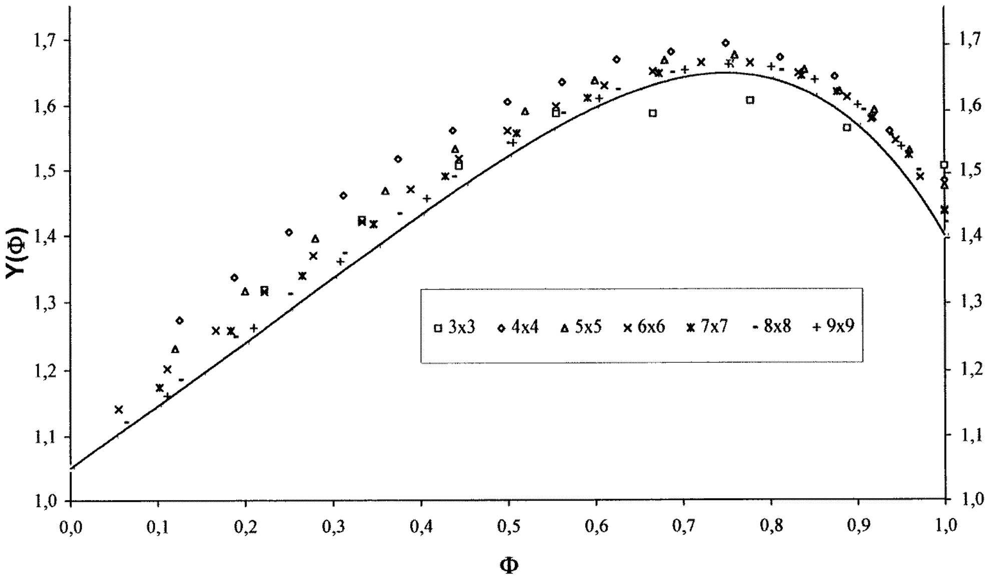

Figure 1. $Y(\Phi) = [Z(\Phi)]^{1/R^2}$ versus Φ, for $n \times n$ plane squares up to the 8×8 plane square. Here Φ is the ratio of the lattice sites occupied by the self-avoiding walk over the total number of available lattice sites, and $Z(\Phi)$ is the MC estimate for the number of configurations corresponding to each Φ value. Good scaling is observed, from which a limiting curve is drawn and then expressed as a fourth-degree polynomial in Φ (see text).

parameter in equation (3) will have to be changed. It was, however, empirically found that screening more than one step was not convenient with respect to computational efficiency. The standard value of the MC samples was 10^5 non-correlated configurations.

If one considers not only HPs, but also self-avoiding walks of any length inside some confining geometry, one can define Φ as being the ratio of occupied lattice sites by the walk, over the total number of available lattice sites, $\Phi = (N+1)/R \times S$. Thus, $\Phi = 1$ for a HP.

Let $Z(\Phi)$ be the MC estimated value, through equation (2), for the number of available configurations of an N-step confined self-avoiding walk. It was then empirically found for squares that a plot of

$$Y(\Phi) = [Z(\Phi)]^{1/R^2} \tag{4}$$

versus Φ, yielded regular curves, which tended to a limiting curve as the dimensions of the square were increased (figure 1).

This limit curve is analytically given through the following fourth-degree polynomial:

$$Y(\Phi) = 1.0500 + 1.0000\Phi - 0.5167\Phi^2 + 1.7333\Phi^3 - 1.8667\Phi^4. \tag{5}$$

Thus, equations (5) and (4) provide a MC estimate of the number of available configurations inside squares not too small, for walks of one step up to HPs. The procedure is similar for $R \times S$ rectangles.

In table 1 $Z(\Phi = 1)$ values for $R \times R$ squares obtained from exact enumeration data [10] are given, and for comparison values obtained using the Orland *et al* [9] relationship (1), and finally from MC estimates using equation (2). All data refer to non-oriented paths, so that to obtain the number of oriented paths, one has to multiply the above data by two. Let us notice that Z_{Orl} in column three of the table refers to HCs, a subclass of HPs.

Table 1. Comparison of $Z(\Phi = 1)$, that is the number of Hamiltonian paths inside $R \times R$ squares from exact enumeration data [10], from the Orland *et al* [9] theoretical relationship, and from the MC estimates of the present work. $Z_{\rm Orl}$ in the third column refers to Hamiltonian circuits (see text).

$n \times n$	$Z_{\rm EE}$	$Z_{\rm Orl}$ $(1.4715)^N$	$Z_{\rm MC}$
3×3	20	22	20
4×4	276	328	277
5×5	4324	10 623	4335
6×6	229 348	744 062	228 860
7×7	13 535 280	112 847 720	1.3582×10^7
8×8	—	3.7059×10^{10}	2.7791×10^9
9×9	—	2.6352×10^{13}	—

The main advantage of the MC procedure to evaluate the number of HPs here presented, lies in its flexibility and generality: the method is applicable to any dimensions, lattices, and boundary geometries. In contrast, for example, the Orland *et al* [9] theoretical procedure is sensitive to boundary conditions. It would, for instance, be severely in error for $R \times 2$ rectangles, where the number of HPs is given by the equation

$$Z(R \times 2, \Phi = 1) = R^2 - R + 2 \qquad (6)$$

and not by the exponential law of equation (1).

References

[1] Orr W J C 1947 *Trans. Faraday Soc.* **43** 12
[2] Flory P J 1953 *Principles of Polymer Chemistry* (Ithaca, NY: Cornell University Press)
[3] Kasteleyn P W 1963 *Physica* **29** 1329
[4] Domb C 1974 *Polymer* **15** 259
[5] Lieb E H 1967 *Phys. Rev. Lett.* **18** 692
[6] Gordon A, Kapadia P and Malakis A 1976 *J. Phys. A: Math. Gen.* **9** 751
[7] Gujrati P D and Goldstein M 1981 *J. Chem. Phys.* **74** 2596
[8] Schmalz T G, Hite G E and Klein D J 1984 *J. Phys. A: Math. Gen.* **17** 445
[9] Orland H, Itzykson C and de Dominicis C 1985 *J. Physique Lett.* **46** L353
[10] Mayer J-M, Guez C and Dayantis J 1990 *Phys. Rev.* B **42** 660
[11] Shakhnovich E and Gutin A 1990 *J. Chem. Phys.* **93** 5967
[12] Pande V S, Joerg C, Grosberg A U and Tanaka T 1994 *J. Phys. A: Math. Gen.* **27** 6231
[13] Rosenbluth M and Rosenbluth N 1955 *J. Chem. Phys.* **23** 356
[14] Jaeckel A and Dayantis J 1994 *J. Phys. A: Math. Gen.* **27** 2653
Jaeckel A and Dayantis J 1994 *J. Phys. A: Math. Gen.* **27** 7719
[15] Van Giessen A E and Szleifer I 1995 *J. Chem. Phys.* **102** 9069
[16] Meirovitch H 1985 *Phys. Rev.* A **32** 3709 and references therein