Rudimentary Concepts on Self Avoiding Walk

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Abstract: In this article we introduce the subject of Self Avoiding Walk and discuss some of the parameters that are associated with its study. Methods of simulating such a walk is also touched upon. A particle starting from the origin and taking one step at a time, randomly selects one of its 2d nearest neighbour and moves to that new location. This is known as a random walk, sometimes also referred to as a drunkard's walk. A self-avoiding walk (SAW) is a sequence of similar steps on a lattice under the restriction that the same point is not visited again.

Keywords: self-avoiding walk (SAW), Brownian motion, simulation

I. INTRODUCTION

Definition :A self-avoiding walk (SAW) of length N in the d-dimensional lattice Z^d starting at x, is defined as a path $\omega = (\omega_0, \omega_1, \ldots\ldots, \omega_n)$ with $\omega_j \in Z^d$, $\omega_0 = x$, $|\omega_j - \omega_{j-1}| = 1$, j = 1, 2, ..., n; and $\omega_i \neq \omega_j$ for $i \neq j$, $0 \le i < j \le n$. Let $|\omega| = N$ denote the length of ω. In other words, a SAW is a random walk path which does not visit the same site more than once.

Random walk theory has found wide ranging applications in Chemistry, Physics, modelling, and other Mathematical areas. The self-avoiding random walk is derived from the simple random walk (SRW). The SAW has been studied for nearly half a century and was developed initially in Physical Chemistry with the intention of modelling polymer chains when placed in a good solvent. Polymers have the unique characteristic that each chain cannot cross itself at any point. Thus, the SAW is a reasonable model of polymer chains since the chain cannot visit any site more than once.

Initially, the "best" mathematical model that could encode the polymer's unique properties was a random walk. The random walk approximation for polymers was proposed 60 years ago by a German chemist Kuhn who presented a model for which the mean squared end to end distance R^2 (which represents the polymer chain's length) grew as the squared root of the degree of polymerization N (i.e., $R \sim N^{1/2}$).

Years after this assumption was made it was proven incorrect by arguing that R (for polymers) grows faster than $N^{1/2}$. A new answer to the questions about this model was discovered by the Nobel laureate Flory who suggested that while the random walk tends to trap itself, the monomers try to bounce away from each other. (This is the so-called excluded volume constraint.) Thus he derived that at equilibrium $R \sim N^{3/(2+d)}$ where d = 1,2,3 is the dimension in which the polymer "lives". Ever since Flory presented his solution in terms of the SAW, physicists have been trying to verify his predictions, and mathematicians have been trying make his arguments rigorous. Significant non-rigorous progress was made by Edwards and de Gennes [1] but there are still dimensions d for which no exact solution has yet to be found.

II. MOTIVATION

In the study of self-avoiding walk, two important questions arose: How many possible paths were there for a self-avoiding walk? And, assuming each path was as likely as the other ones, what would be the distance on average from the origin to the point x? However, there was a third question that arose within the last two: What was the asymptotic behaviour of the self-avoiding walk as N (steps in a self-avoiding walk) tend to infinity? One would think that the simplest way to answer the questions would be by using computer simulations, but several works done in this field have shown that due to the exponential growth of the number of paths as N increased, obtaining results for large N was almost impossible; thus, the exact counting of the possible paths as mentioned by Madras and Slade [2] was only been done for $N \le 34$ in d = 2 and for $N \le 21$ in d = 3.

The above questions must be asked in each dimension d in order to generalize the results. The easiest case and therefore the one with a trivial answer was that for dimension d = 1. Indeed, a self-avoiding walk in one dimension had no other alternative but to move in the same initially chosen direction. Hence there existed only two paths for every value of N (recall that N is the number of steps in SAW), and therefore, the maximum distance for the origin is exactly N. In addition, it can be shown that higher dimensions ($d \ge 5$) provides a richer and more complex answer to the presented questions about SAW. Although it is also important to mention that the most interesting questions remain open for the low dimension(d = 2,3,4) cases.

The upper critical dimension for the self-avoiding walk above which all critical exponents are dimensional independent is d = 4 due to the fact that the random walk paths tend to intersect below four dimensions, and have an opposite behaviour above it. As pointed out previously, there does not exist any rigorous proven results for the lower dimensional cases (d = 2,3,4). It became clear that in high dimensions, the SAW should be closer to the simple random walk (sometimes also referred to as the mean field model for the SAW), provided that a simple random walk is less likely to intersect itself in higher dimensions (for d> 4). Hence, using rigorous mathematical analysis and in some of the cases high-precision computer simulations, the following has been concluded:

For dimensions d > 4, the lace expansion has been used to prove the existence of answers and to solve the questions that were stated previously. Additionally, partial results for the case d = 4 have been obtained by applying logarithmic corrections. In contrast to dimensions four and above, the three dimensional case d = 3 remains mathematically unsolved. Finally, both rigorous and non-rigorous solutions for the two-dimensional case d = 2 (achieved and supported by numerical Monte Carlo simulations) have been found.

Frequently one rather considers the associated generating function

$$C(x) = \sum_{n \ge 0} c_n x^n$$

We take c_0 to be1, then $c_1 = 4$ as a one-step walk can be in any of 4 directions. Then $c_2 = 12$, $c_3 = 36$ and $c_4 = 100$. It is at the stage of 4-step SAWs that the self-avoiding constraint first manifests itself, and the problem becomes increasingly difficult thereafter. Accordingly, an enormous amount of effort has been expended over the last 50 years in developing efficient methods for counting SAW. For the square lattice, Jensen [3] has extended the known series to 79 step walks, for which he finds c_{79} = 10194710293557466193787900071923676. Methods for calculating these astonishing numbers are quite complicated [4, Chap. 7]. One of the few properties which has been proved by virtue of the sub-multiplicative inequality $c_{n+m} \le c_n c_m$, is that the number c_n grows exponentially. From this inequality it follows that

$$\mu = \lim_{n\to\infty} c_n^{\frac{1}{2}}$$

exists [2] and further that $c_n \ge \mu^n$. However even the value of this "growth constant" μ is difficult to calculate exactly. Only in 2010 was μ for one two-dimensional lattice, notably the honeycomb lattice, actually proved by Duminil-Copin and Smirnov [5] to be $\sqrt{2\sqrt{2}}$. For other lattices in two dimensions, and all lattices in higher dimensions, we only have numerical estimates. For example, for the square lattice the best current estimate is μ = 2.638158530323±2×10^{-12}, a result obtained based on extensive series of Jensen [3]. In fact it is believed that, for dimensionality d> 1 and $d \ne 4$,

$$c_n \sim \text{const.} \times \mu^n n^g.$$

The critical exponent *g* is believed to depend on the dimension, but not on the details of the lattice. In particular, it is predicted to be a rational number, namely 11/32, in two dimensions. In three dimensions, the best estimate we have is g = 0.156957±0.000009 given by Clisby [6].

Despite these accurate estimates, the existence of this exponent for d< 5 has not been proven, let alone establish its value rigorously. For d> 4 the higher dimensionality means that the self-avoiding restriction is less confining than in lower dimensions, and indeed has no effect on the dominant asymptotic behaviour, with the result that the SAW behaves as a random walk. More precisely, Hara and Slade [7, 8] have proved that g = 0 in this case, and that the scaling limit is Brownian motion. In four dimensions the above expression for c_n must be modified by an additional multiplicative factor (log n)1/4, with g = 0. The appropriately rescaled walk is also expected to have Brownian motion as its scaling limit. These assertions for the four-dimensional case are believed to be true, but no proof exists. Bounds established 50 years ago by Hammersley and Welsh [9] have hardly been improved upon. They proved that, for SAW in dimensionality

$$\mu^n \le c_n \le \mu^n e^{k\sqrt{n}}.$$

The lower bound follows immediately from sub-additivity, while the upper bound depends on an unfolding of the walk. The number of possible unfoldings can be bounded by the number of partitions of the integer n, which has the exponential behaviour given above. Note that the existence of a critical exponent implies behaviour $\mu^n e^{k \log n}$, which is rather far fromthe upper bound. A year later, Kesten [10] slightly improved the upper bound to

$$c_n \le \mu^n e^{kn^{2/(d+2)} \log n}.$$

III. CONCLUSION

In this article we have only tried to introduce the subject with some basic results. The reader can then follow upon some standard texts and review articles that are listed at the end.

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