

BOOK REVIEW

The self-avoiding walk, by Neal Madras and Gordon Slade. Birkhäuser, Boston, 1993, xiv+425 pp., \$64.50. ISBN 3-7643-3589-0

Practically everyone is familiar with simple random walk (or the drunkard's walk) on the integer lattice in d -space, \mathbb{Z}^d , in which the walker moves at each step from a site in \mathbb{Z}^d to one of its $2d$ neighbors, picking each of the neighbors with the same probability $1/(2d)$. Denote the position of the walk after n steps by S_n , and let the walk start at the origin ($S_0 = \mathbf{0}$). When the chemists started investigating certain polymer molecules (such as rubber), it was suggested that these might be long chains of carbon atoms with small side arms and that the chain of carbon atoms might be modelled by a random walk. As chemists well knew, actual carbon atoms in 3-space do not sit on the lattice \mathbb{Z}^3 , but the angle between successive bonds is essentially 120° . So they used the so-called free flight model (described in [4, Chapter X] or [9, §§2.1–2.4]) with restrictions on the angles between successive bonds. Nowadays the chemical and physical literature, as well as the book by Madras and Slade, studies the self-avoiding walk problems on \mathbb{Z}^d . This first seems to have been suggested by Montrol [12]. If one prefers an angle of 120° between successive bonds, then one can study the problem on the “diamond structure”, that is, a lattice whose vertex set consists of the vertices of the tetrahedral lattice plus the centroids of the tetrahedra. It is, however, believed that for the questions of interest here the qualitative nature of the results is not changed by working on \mathbb{Z}^3 instead of the diamond structure. In fact, the universality hypothesis of statistical physics (see below) claims that even important quantitative aspects, to wit the critical exponents, are the same for walks on both lattices. Apparently one of the quantities which could be experimentally measured for polymers in solution was the radius of gyration, corresponding to $[\frac{1}{2(n+1)}E\{\sum_{i=0}^n \sum_{j=0}^n |S_i - S_j|^2\}]^{1/2}$ (where $||$ stands for the Euclidean norm and $E\{ \}$ denotes the expectation with respect to the random walk distribution or, equivalently, the average over the $(2d)^n$ possible random walk paths of n steps). This provided some measure of the diameter of the polymer molecule. For the sake of simplicity one usually studies the “mean square end to end distance” $E\{|S_n|^2\}$ (recall $S_0 = \mathbf{0}$) instead of (the square of the) radius of gyration. Of course, it is well known that for random walk $E\{|S_n|^2\} = n$, and the classical central limit theorem even gives us full information about the distribution of S_n/\sqrt{n} . The more refined invariance principle even tells us that the (random) function $t \rightarrow S_{[tn]}/\sqrt{n}$, $0 \leq t \leq 1$, behaves like the Wiener process. Roughly speaking, this says that the distribution of many functionals of the path $t \rightarrow S_{[tn]}/\sqrt{n}$ converge to the distribution of the same functional of the Wiener process; [2] is a standard reference for such theorems.

Kuhn [10] already pointed out that no two atoms could overlap, but no rigorous arguments were available to take this “excluded volume effect” into account. In Montroll’s lattice formulation [12] it was natural to model the fact that no two atoms could overlap by replacing $E\{|S_n|^2\}$ by

$$(1) \quad \langle |S_n|^2 \rangle = \frac{1}{c_n} \sum |S_n|^2,$$

where the sum runs over all self-avoiding walks of n steps and c_n denotes the number of such n -step walks. A self-avoiding walk of n steps is defined to be a path S_0, S_1, \dots, S_n with $S_i \neq S_j$ for $i \neq j$ (again we restrict ourselves here to $S_0 = \mathbf{0}$). The procedure to assign the same weight $1/c_n$ to all such walks in the average (1) and similar averages is motivated by the situation for unrestricted random walk, in which random walk measure assigns the same measure $(2d)^{-n}$ to each n -step walk.

The principal objects of study in the theory of self-avoiding walks have been the asymptotic behavior of c_n and $\langle |S_n|^2 \rangle$ and some related functions. This may seem a narrowly focused field of study, but these questions have turned out to be extremely challenging. The fact that the principal questions can be stated so simply gives them a special appeal (to some people). Moreover, the quantities c_n and $\langle |S_n|^2 \rangle$ exhibit behavior which is quite similar to that of certain functions in critical phenomena, such as magnetism. In fact, in a formal sense, as explained in Chapter 2 of this book, the self-avoiding walk model is a limit of a common spin model from statistical mechanics, the N -vector model. Despite the enormous physics literature very few rigorous results about behavior of functions near a critical point have been proven. Self-avoiding walks therefore provide a useful and appealing test problem to develop the theory of critical phenomena. From the probabilist’s point of view the appeal of the self-avoiding walk problems is that S_0, S_1, \dots, S_n is a natural example of a highly non-Markovian sequence; to say something about S_{k+1} , it is not enough to know S_k , nor even S_k, \dots, S_{k-j} for some fixed j , but one should know the full past, S_0, \dots, S_k . Because of this non-Markovian nature few of the existing tools of the trade apply, and also pure enumeration on a computer becomes extremely difficult.

One expects the self-avoidance condition to make the walk more spread out. That is, one expects that $\langle |S_n|^2 \rangle > E\{|S_n|^2\} = n$. In fact, it is believed that

$$(2) \quad \langle |S_n|^2 \rangle \sim D_1 n^\nu \quad \text{if } d \neq 4,$$

for some constant D_1 and exponent ν . In dimension 4 the relation

$$(3) \quad \langle |S_n|^2 \rangle \sim D_1 n(\log n)^{1/4}$$

has been conjectured. A measure of the difficulty of the subject is that no rigorous proof exists for $d = 2, 3$ of $\langle |S_n|^2 \rangle \geq n^{1+\varepsilon}$ for some $\varepsilon > 0$ (which would say that self-avoiding walks are truly more spread out than unrestricted random walks), nor for $d = 2, 3, 4$ of $\langle |S_n|^2 \rangle \leq n^{2-\varepsilon}$ (note that trivially $|S_n| \leq n$). Hammersley and Morton [6] observed that

$$(4) \quad c_{n+m} \leq c_n c_m$$

and that this implies

$$(5) \quad (c_n)^{1/n} \rightarrow \mu \quad \text{and} \quad c_n \geq \mu^n$$

for some constant μ , the so-called *connective constant*. The submultiplicative property (4) has played a fundamental role in many of the asymptotic bounds for c_n which are explained in Chapter 3. A conjectured sharper form for (5) is

$$(6) \quad c_n \sim D_2 n^{\gamma-1} \mu^n$$

(again with logarithmic correction factors when $d = 4$). γ and ν are called *critical exponents*, and many more critical exponents have been introduced in statistical physics. Several of these are discussed by Madras and Slade. Not all these exponents are independent. It is believed on the basis of nonrigorous assumptions that they satisfy a number of so-called scaling relations. The universality hypothesis says that the values of these exponents depend only on the dimension and not on the detailed structure of the lattice. The exponents should have the same value for self-avoiding walks on the diamond structure as on \mathbb{Z}^3 , and similarly their values should be the same for the (planar) triangular and honeycomb lattices and for \mathbb{Z}^2 . The renormalization group was introduced in part to explain the universality hypothesis, but except for large d neither the existence of the critical exponents nor their universality has been proven. The connective constant will depend on the fine structure of the lattice, and for this reason it is usually regarded as more important to understand the critical exponents than to find the exact value of μ .

As with other effects due to interactions, it is reasonable to believe that the interactions become small when the dimension becomes high. More daringly, one assumes that there exists an *upper critical dimension* \bar{d} , such that for $d > \bar{d}$ the critical exponents are no longer dimension-dependent and, in fact, equal the exponents for some parallel model with minimal interactions. This so-called *mean field model* for self-avoiding walks is the unrestricted random walk. For self-avoiding walks the upper critical dimension was assumed to be 4. One reason why 4 plays a special role is that two independent simple random walks have a strictly positive probability never to intersect (except at their common starting point) if and only if $d \geq 5$. Thus it was believed that for $d \geq 5$,

$$(7) \quad c_n \sim D_3 \mu^n$$

and

$$(8) \quad \langle |S_n|^2 \rangle \sim D_4 n.$$

No rigorous progress on these relations was made until Brydges and Spencer [3]. By means of the so-called lace expansion, they proved the analogue of (8) for weakly self-avoiding walks (in which self-intersections are not ruled out, but the weight of a path is taken proportional to $(1 - \varepsilon)^{\text{number of self-intersections}}$; the authors actually stated that they could exclude large loops entirely from the walk). Slade [13–15] improved this method to obtain (7) and (8) for the truly self-avoiding walk in high d and even to prove a full invariance principle for $t \rightarrow S_{\lfloor tn \rfloor} / \sqrt{n}$, $0 \leq t \leq 1$. The lace expansion can be viewed as a form of the inclusion–exclusion principle from elementary combinatorics and can be used here to give an expansion for the “two-point function”

$$G_z(\mathbf{0}, x) := \sum_{n=0}^{\infty} z^n c_n(\mathbf{0}, x),$$

where $c_n(\mathbf{0}, x)$ denotes the number of n -step self-avoiding walks from $\mathbf{0}$ to x . This then leads to an estimate for small k of the Fourier transform

$$\widehat{G}_z(k) := \sum_{x \in \mathbb{Z}^d} e^{ik \cdot x} G_z(\mathbf{0}, x)$$

and its derivatives, a so-called infrared bound. It had been known for some time in analogy of results for spin models (see [1, 5] that such an infrared bound can be used to prove mean field behavior for large d . Hara and Slade [7, 8] recently proved (7) and (8) for $d \geq 5$ by further sharpening of the lace expansion. This shows that the upper critical dimension is not more than 4. Given the long history and difficulty of the subject, this was a major success. The lace expansion and the proof of (7) and (8) as well as the full invariance principle for high d form the centerpiece of the book under review (Chapters 5 and 6). For reasons of clarity and brevity the latest improvements of Hara and Slade to cover all $d \geq 5$ are not included. Also, some other models to which Hara and Slade successfully applied the lace expansion, such as percolation and lattice animals, are briefly discussed.

Chapter 9 of the book further gives a detailed treatment of many numerical and Monte Carlo methods which have been used to estimate critical exponents and the connective constant. This chapter explains what is rigorously known about these methods and proves, for instance, the result of Madras and Sokal [11] that one of the known methods of simulation typically samples only an exponentially small class of walks.

What can one expect for future work in this subject? There is general agreement that the most important and challenging problem is to prove power law behavior such as (2) and (6) for dimensions $\leq \bar{d}$; this is also the case for percolation and other critical phenomena. It may be overly pessimistic, but many people believe that the present methods are inadequate for this and that another breakthrough will be needed. One may also want to prove power laws and mean field behavior for large d for some alternative self-avoiding path models (some of these are briefly mentioned in Chapter 10; they do not give the same weight to all n -step self-avoiding paths).

In any case, the book by Madras and Slade gives an excellent introduction for graduate students and professional probabilists to recent rigorous advances in an important statistical physics model. This is the best place to find a self-contained exposition of the lace expansion. The book is devoted to rigorously proven results and does not attempt to give a full survey of the many nonrigorous physics and chemistry articles on self-avoiding walks. However, it does make an effort to explain some of the physicists' reasonings behind the various conjectures.

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