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LETTER TO THE EDITOR

Selfavoiding walks on a crystal lattice; a new approach to the mean-square end-to-end length ρ_n

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Abstract. It is pointed out that the exponent γ (for which the mean-square end-to-end length of an n step walk $\simeq$ constant n^{γ}) is associated also with other *purely topological* properties of the lattice. It is therefore suggested that a better numerical estimate of γ may be possible, since the problem of the 'distance' between two sites of a network has been bypassed.

For a long time selfavoiding walks on a crystal lattice have provided a useful model of a chain polymer in dilute solution (several references are given in Martin and Watts 1971). The mean-square end-to-end length ρ_n of the set of all n step selfavoiding walks has been of particular interest as a measure of the typical size of a chain of n monomers; sometimes the mean moment of inertia has been proposed as an alternative. The idea of a mean length itself implies the existence of a *metric*, specified by embedding the lattice in a euclidean space of the relevant dimensionality d, and using the 'usual' cartesian distance.

Such an embedding is of course necessary before the model can be applied physically. However, it sometimes happens that important quantities of experimental interest depend *solely* on the topological structure of the lattice; in such a case, numerical extrapolation may reasonably be expected to yield more satisfactory results once the gratuitous metric is dispensed with.

For example, let us consider the exponent γ for which $\rho_n \simeq n^{\gamma}$ for large n. Suppose that $p_n(A)$ is that proportion ending at the site A of all n step selfavoiding walks starting from O. Define the *entropy* of this distribution by the purely combinatorial formula

$$S_n = -\sum_{\text{all } A} p_n(A) \ln p_n(A).$$

An exponent Γ is defined (when it exists) by

$$\exp S_n \simeq \text{constant } n^{\Gamma} \qquad \text{(for large } n\text{)}.$$

There is good numerical evidence for presuming that the distribution $p_n(A)$ acquires a 'limiting shape' as $n \to \infty$: if this is so, then it is simple to show that $\gamma = 2\Gamma/d$ for a d dimensional lattice. Consequently, we now have a purely combinatorial route to the exponent γ.

Table 1. Estimates of γ

n	γ_n for the sequence $\exp S_n$ (the nonmetric approach)	γ_n for the sequence ρ_n (the metric approach)
8	1·49761	1·48667
9	1·49828	1·48792
10	1·49922	1·48597
11	1·49855	1·48746
12	1·49852	1·48743
13	1·49816	1·48782

As an example of numerical behaviour, sequences of estimates for γ are given in table 1, using distributions already obtained for the triangular lattice by methods described elsewhere (Martin and Watts 1971). The estimates are given by

$$\gamma_n = \frac{(a_{n+1}-a_n)(a_n-a_{n-1})}{a_n{}^2-a_{n+1}a_{n-1}}$$

applied in turn to the sequences $a_n = \exp S_n$ and (for the sake of comparison) $a_n = \rho_n$. A conjecture favoured by many workers in this field is that $\gamma = 1{\cdot}5$ exactly; certainly the nonmetric approach to a numerical estimate of γ appears to support this conjecture rather more strongly.

A later paper will present the underlying concepts and other numerical results.

References

Martin J L and Watts M G 1971 *J. Phys.* A: *Gen. Phys.* **4** 456–63