OPEN PROBLEMS IN MATHEMATICAL CHEMISTRY

SOME PROPERTIES OF THE NUMBERS OF LATTICE ANIMALS AND LATTICE TREES

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A lattice animal is a connected subgraph of a lattice and a lattice tree is a lattice animal with no cycles. As an example, we consider the square lattice and ask for the numbers of lattice animals with n vertices (a_n) and of lattice trees with n vertices ($a_n(0)$). Two animals are considered distinct if one cannot be superimposed on the other by translation, with a similar definition for trees. For example, $a_1 = a_1(0) = 1$, $a_2 = a_2(0) = 2$, $a_3 = a_3(0) = 6$, $a_4 = 23$ and $a_4(0) = 22$.

Lattice animals and lattice trees have been considered as models of randomly branched polymers in dilute solution in good solvents. In this sense, they play the same role for branched polymers as do self-avoiding walks for linear polymers. The primary difference is that in the branched polymer case there is an averaging over the structure of the molecule as well as over the conformation.

These objects have been studied by numerical (e.g. [1]) and renormalization group (e.g. [2,3]) techniques, and it is believed that

$$a_n \sim A n^{-\theta} \lambda^n \tag{1}$$

and

$$a_n(0) \sim A_0 n^{-\theta_0} \lambda_0^n. \tag{2}$$

It is fairly easy to prove that $a_n = \lambda^{n+o(n)}$ and $a_n(0) = \lambda_0^{n+o(n)}$ [4,5], and (1) and (2) are natural conjectures in view of the relatonship of animals to critical phenomena problems such as percolation (see, for example, [6]). However, proving the existence of a critical exponent (i.e. that (1) and (2) are correct) seems to be extraordinarily difficult.

Note: Solutions to this and other problems published in this series should be addressed to Professor P.G. Mezey. It is anticipated that valid solutions to problems appearing in this series will be published in future issues of the Journal of Mathematical Chemistry.

There are also some well-known conjectures, based mainly on renormalization group arguments, about the values of θ and θ_0 (if they exist). It is believed that $\theta = \theta_0$ [2] and that $\theta_0 = 1$ in two dimensions and 3/2 in three dimensions [3]. It would be very worthwhile to supply combinatorial proofs of these results.

It is much easier to supply rigorous results on the growth constants. For instance, is it known [7] that $\lambda > \lambda_0$, although the exact values of λ and λ_0 are not known.

In an attempt to link θ and θ_0, a modification of this problem has been considered in which we ask for the number $a_n(c)$ of animals with n vertices and cyclomatic index c. It is easy to prove that

$$\lim_{n \to \infty} n^{-1} \log a_n(c) = \log \lambda_0 \tag{3}$$

for all c, so that the growth constant is independent of the cyclomatic index. In addition, if we assume that

$$a_n(c) \sim A_c n^{-\theta_c} \lambda_0^n, \tag{4}$$

then it can be shown [8] that

$$\theta_c = \theta_0 - c. \tag{5}$$

This proof is combinatorial.

The conjectures discussed above are well known in the statistical physics community. However, we describe them here in the hope that they will attract the attention of readers of the Journal of Mathematical Chemistry, and that this will result in the development of new approaches to these problems.

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