OPEN PROBLEMS IN MATHEMATICAL CHEMISTRY

PROBLEM 2

A CONJECTURE ON THE CROSSING NUMBER OF LOOPS OF POLYMER CHAINS EMBEDDED IN A CUBIC LATTICE

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Most fundamental conformational properties of polymer chains can be studied using the model of self-avoiding polygons on the three-dimensional simple cubic lattice [1,2]. If the chain forms a loop it may be knotted [3–5]. An important property of such loops is their crossing number, which is defined as the minimum number of crossings occurring in regular projections of the knot, i.e. when no two crossings are projected on top of one another. The length L of the loop is defined as the number of occupied lattice points.

It is conjectured that $L^{4/3}$ is an upper bound for the crossing number of any knotted loop of length L embedded in a simple cubic lattice.

References

[1] C. Ernst and D.W. Sumners, Math. Proc. Camb. Phil. Soc. 102(1987)303.
[2] D.W. Sumners and S.G. Whittington, J. Phys. A21(1988)1689.
[3] D.W. Sumners, J. Math. Chem. 1(1987)1.
[4] D.W. Sumners, in: *Geometry and Topology, Manifolds, Varieties and Knots*, ed. C.M. McCrory and T. Shifrin (Marcel Dekker, New York, 1987).
[5] C. Soteros and S.G. Whittington, in preparation.

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 our series will be published in future issues of the Journal of Mathematical Chemistry.