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An Algorithm To Calculate Exactly The Expectation And Variance Of The Average Atmosphere In Self Avoiding Walks

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In a recent development reported that our calculations on reacting polyethylene gas, indicated that reacting Polyethylene grows as a rigid coil and collapses to a globular state after the reaction is complete. The program used in the calculation of the radial dimensions of growing polyethylene was a modification continuous configurational Boltzmann Biased direct MonteCarlo sampling method developed earlier by Jiro Sadanobu and William A. Goddard III. The method used in the above case was almost identical, except the Boltzmann Bias factor was not taken into account, i.e., the radial dimensions of each Polyethylene chain were not divided by the Bias factor and the sum of the radial dimensions for the sample taken was not divided by the sum of the Bias factors. In other words calculations on the radial dimension of growing Polyethylene were exactly analogous to calculations on growing self avoiding walks that had been carried out earlier. To explain the phenomenon observed in that paper, that is the absence of polymer collapse in the growing polyethylene chain, the authors had reported exact values of the expectation and standard deviation of the average atmosphere of self avoiding walks and growing self avoiding walks which were defined in that paper.
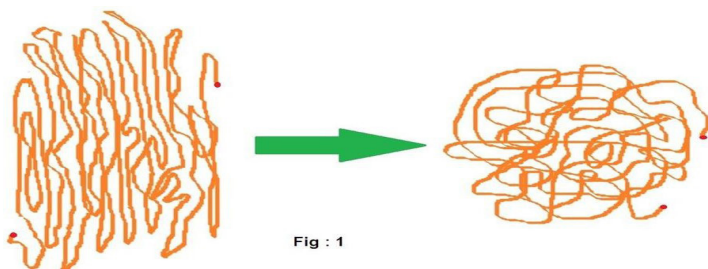

Fig : 1

Figure 1. The change in a growing Polyethylene molecule on completion of the reaction. We define the average atmosphere of self avoiding walk as the number of vacant (unoccupied) sites available for growth at each stage ($i = 0 \ to \ n - 1$, $i \ being \ the \ label \ of \ each \ vertex \ of \ the \ wa$) of an n step self avoiding walk divided by the number of steps n. We now report an algorithm that uses the back tracking paradigm to calculate exactly the expectation and variance of the average atmosphere of self avoiding walks of n steps, for square, cubic, hexagonal, etc. lattices.

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This algorithm can be generalized to the treatment of other theories in polymer chemistry such as (i) The Flory Huggins and Flory Krigbaum theories of the thermodynamics of polymer solution (ii) The theory of sol gel transition in multifunctional polymerisation.

The theory behind the algorithm can be generalised to calculating the average atmosphere on

$k \ regular$ graphs, which can then be used in the analysis of networks.

Fig : 2

$r^2 = 20 \ r^2 = 20$

Uniform Probability = $\quad \frac{1}{}$[1]

Uniform Probability = $\quad \frac{1}{}$[1]

Average Atmosphere = 31   Average Atmosphere = 27

GSAW Probability = $\quad \frac{1}{}$[1]

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Figure 2. Two self-avoiding walks with the same mean square end to end distance but different probabilities under the growing self-avoiding walk model and equal probabilities under the uniform probability model. (Note the average atmospheres for both walks are different.)

Biography

Taniya Rose Abraham Currently working on a DST project under guidance of Dr.manikandan paranjothy , Assistant Professor (Chemistry) ,IITJ.She participate in International conference on Current Trends in Material Science , organized

by AMMRC , MG University, Kerala and on Nov 15 , 2013.