

# Topological constraints in soft matter: the dynamics of dense rings as diffusion on a random graph.

Complexity Mini project offered by Dr M S Turner

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Random walks that close on themselves to form rings have a number of unusual properties. If these rings are all required to be unknotted, either with themselves or with any neighbours, the space of accessible configurations is much reduced, see Fig 1. Such systems can be realised as ring polymers and can either be chemically synthesised or isolated from the closed rings of DNA, called *plasmids*, commonly found in bacteria. Our formal understanding of the properties of linear polymers (with two ends) is relatively well developed [1]. No such corresponding results exist for rings, although there are some very crude scaling arguments that suggest that, when the rings are highly overlapping the rings are somewhat more compact than for linear polymers [2]. It has been conjectured that the configuration of the ring then resembles a tree-like random graph, with each edge containing an “outward” and “returning” section of polymer. Such a structure can then freely access its large configurational space without the risk of violating any (non-local) topological constraints involving its neighbours.

This mini-project will involve a computational study of the dynamics of these ring polymers.



Figure 1: A collection of overlapping rubber bands - a crude model for entangled rings/ring polymers.

Here we will assume that the rings adopt the configuration of a random graph, as described above, and then analyse the dynamics of this graph via diffusion *on* the graph, together with the random creation and annihilation of ends [3]. This process is to be simulated numerically and some familiarity with computing is therefore necessary. The student will be expected to familiarise themselves with the literature for diffusion on random graphs and will then be expected to write their own code to implement a Monte Carlo algorithm to simulate this diffusive process. The stress remaining after an initial strain is then the fraction of the original graph structure that remains intact.

If time permits we will investigate the process by which one ring can “thread” through another. In this case the *threaded* ring cannot move completely freely until the *threading* ring retracts itself. Corresponding constraints can be introduced into the diffusion process. We propose that this system may then exhibit a percolation transition in which, above a critical ring size  $N_c$ , the network of mutually entangled rings can extend to the size of the system. We believe that this material would then

form a previously unrecognised state of matter, a *topological glass*. In this material the microscopic motion of the rings would be indistinguishable from the non-glassy state but the motion on longer length scales, e.g. that of the centre of mass of the rings, would be dramatically slowed. A complete analysis of this problem is certainly the basis of a PhD project.

## References

- [1] M. Doi and S. F. Edwards. *The Theory of Polymer Dynamics*. Oxford University Press, Oxford, UK, 1986.
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- [3] S. T. Milner and J. D. Newhall. Stress relaxation in entangled melts of unlinked ring polymers. *Phys. Rev. Lett.*, 105:208302, 2010.