Chapter 5

Conclusions

5.1 Summary

In this thesis, the statistical physics of semiflexible polymers has been studied. A study on the elasticity of Red Blood Cell membranes has been discussed. The thesis concentrates on statistical physics of soft matter relevant to biological phenomena. Apart from the biological application, we are also motivated from the theoretical physics point of view. We have applied differential geometry and statistical mechanics to describe systems arising in soft matter physics.

In chapter 1, we have briefly introduced the essential features of different models of the polymer. We have described briefly the **Freely Jointed Chain (FJC)** model and the **Worm Like Chain Model (WLC)**. We have described the **WLC** model with pure bend following Samuel and Sinha [1]. The extension to include twist degrees of freedom to study the elastic properties of a torsionally constrained polymer has been studied following Mezard and Bouchiat [2]. We have briefly alluded to a similar piece of work by Moroz and Nelson [3].

In chapter 2 we present a statistical mechanical study of stiff polymers, motivated by experiments on actin filaments and the considerable current interest in polymer networks [4]. We have obtained simple, approximate analytical forms for the force-extension relations and compared these with numerical treatments. We have noted the important role of boundary conditions in determining force-extension relations. The theoretical predictions presented here can be tested against single molecule experiments on neurofilaments and cytoskeletal filaments like actin and microtubules. Our work is motivated by the buckling of the cytoskeleton of a cell under compression, a phenomenon of interest to biology. We then extend the above treatment to study the twist elasticity of stiff polymers in the paraxial approximation. We have obtained simple, approximate analytical forms for the writhe distribution at zero applied force. We have also derived simple analytical expressions for the torque-twist relation and discussed buckling of stiff polymers due to the applied torques. To the best of our knowledge, stiff filaments with torsional constraints have not been studied experimentally; we expect our work to initiate experimental efforts in this direction.

In chapter 3 we have described a theoretical treatment of DNA stretching and twisting experiments, in which we have discussed global topological subtleties of self avoiding ribbons and provided an underlying justification for the worm like rod chain (WLRC) model proposed by Bouchiat and Mezard [6]. Some theoretical points regarding the WLRC model are clarified: the "local writhe formula" and the use of an adjustable cutoff parameter to "regularise" the model. Our treatment brings out the precise relation between the worm like chain (WLC), the paraxial worm like chain (PWLC) and the WLRC models. We have described the phenomenon of "topological untwisting" and the resulting collapse of link sectors in the WLC model and note that this leads to a free energy profile *periodic* in the applied link. This periodicity disappears when one takes into account the topology of self avoidance or at large stretch forces (paraxial limit). We note that the difficult nonlocal notion of self avoidance can be replaced (in an approximation) by the simpler local notion of "south avoidance". This gives an explanation for the efficacy of the approach of Bouchiat and Mezard in explaining the "hat curves" using the WLRC model, which is a south avoiding model. We have proposed a new class of experiments to probe the continuous transition between the periodic and aperiodic behavior of the free energy.

In chapter 4 we have discussed the physics of an optically-driven micromotor of biological origin [7]. A single, live red blood cell, when placed in an optical trap folds into a rod-like shape. If the trapping laser beam is circularly polarized, the folded RBC rotates. A model based on geometric considerations, using the concept of buckling instabilities, captures the folding phenomenon; the rotation of the cell is rationalized using the Poincarè sphere. We predict that (i) at a critical power of the trapping laser beam the RBC shape undergoes large fluctuations and (ii) the torque is proportional to the power of the laser beam. These predictions have been tested experimentally. Some numerical estimates have been made and the order-of-magnitude estimates agree well with the experimental figures. We have suggested a possible mechanism for emergence of birefringent properties in the RBC in the folded state.

5.2 Future Directions

An interesting problem to address in future is the distinction between different knot classes while constructing the partition function. The energetics and topology of knotted molecules can be studied both analytically as well as by simulation methods and compared against single molecule experiments on knotted polymers by Quake *et al.* [8]. Another problem of interest is to understand the elastic properties of polymer networks using the knowledge of the elasticity of individual filaments. In recent years, there has been a lot of interest in physics at the micro and nano scales. The scales of interest cover the range from molecules to living cells. At these scales, thermal fluctuations become extremely important and entropic effects cannot be neglected. This is quite different from the macroscopic world where energy dominates over entropy and thermal fluctuations are negligible. Soft condensed matter systems are entropy dominated. This field has become topical today because of applications in biology and recent advances in micromanipulation and optics. This field of research involves a rich cross-fertilization of ideas between biologists, theoretical physicists and mathematicians. Many interesting phenomena, that require sophisticated mathematical techniques for modelling, have been observed; for example Cozarelli *et al.* [9] have shown that the enzyme gyrase brings two segments of a DNA molecule together, cuts both of the backbones of one of the segments, inserts the other intact segment and rejoins the cut backbones thus changing the linking number of the DNA in units of two. To quote Bauer *et al* "Understanding the mechanism of supercoiling and the consequences of this structural features of DNA, however, presents problems of considerable mathematical complexity. Fortunately there are two branches of mathematics that offer substantial help in this effort: topology, which studies the properties of structures that remain unchanged when the structures are deformed, and differential geometry, which applies the methods of differential calculus to the study of curves and surfaces.” [10]. Put together with statistical mechanics, differential geometry and topology have been and will continue to be powerful tools in the study of soft materials.

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