Statement of Research Plan

My general research interest lies in the field of statistical mechanics and soft condensed matter physics. These branches of physics have given me the opportunity to work in broad interdisciplinary areas such as polymer science and biological physics. Below is a summary of my past and ongoing work, and plans for the future.

Virus structure

Over the last two years, the main focus of my research has been on understanding the structure and mechanical properties of viruses.

A viral capsid consists of a single molecule of RNA or DNA surrounded by a rigid protective shell of protein --the capsid. With few exceptions, the rigid shell of spherical virus consists of a two-dimensional, icosahedral-symmetry, network of a definite number of identical copies of the capsid protein. I (with my collaborators) investigated the origin of icosahedral symmetry in spherical viruses. First, we introduced a phenomenological Hamiltonian that contained an adhesion term associated with attractive interactions between subunits and an elastic contribution arising from inhomogeneous curvature. Looking for conditions under which self-assembly leads to structures with icosahedral symmetry we found that this symmetry is not purely a generic consequence of free energy minimization but requires—in addition—optimization of the internal structure of the capsid proteins. We followed up on that work by using a minimal model for equilibrium capsid structure, which introduced an explicit interaction between protein multimers ("capsomers"). Using Monte Carlo simulation we showed that the model reproduces the main structures of viruses *in vivo* as well as important non-icosahedral structures observed *in vitro*.

In addition to explaining the origin of special symmetries of viral capsids, I am also interested in the new concepts and physical properties that protein shells bring to the material science arena. For example, their remarkable mechanical strength makes viral capsids the ideal candidates for nano-containers. With David Reguera, I just completed a research on the mechanical consequences of the icosahedral symmetry on viral capsids, and in particular on the elastic properties and failure modes of protein shells that result from their faceted nature.

In vivo experiments indicate that the presence of an enclosed "cargo" (the viral RNA or DNA) might significantly modify the final equilibrium structure of a viral particle. To elucidate the simplest physical role played by an encapsidated chain in determining the preferred size and shape of a viral particle, I plan to use mean field methods to calculate the free energy of viral particles as a function of genome length and molecular weight and of the strength of the genome/capsid attractive interaction. In instances where an analytical approach is not feasible, I intend to perform a series of Monte Carlo simulations to explore the relevance of the above-mentioned factors on the final size and shape of capsid. The theory of virion structure will be a principle component of my future research. I have recently submitted a proposal on this subject to NIH, which I will provide if requested.

Configurations of biological polymers

As part of my doctoral thesis, I studied the statistical mechanics of biopolymers. This work was mainly motivated by efforts to understand the packaging of DNA inside a cell. Most remarkably, a meter of DNA fits remarkably into a cell nucleus having a typical radius of only a few microns, and thus packed, it still manages to perform all of its biological functions. In a nucleosome—the fundamental configurational unit of chromosomal DNA packing, a portion of a DNA strand wraps almost twice around a protein spool formed from an octamer of histones. My collaborator (Joseph Rudnick) and I treated the wrapped segment of DNA in a nucleosome as an elastic rod that was free to twist and writhe subject to mechanical constraints. We showed that the presence of histone octamers provides a physical mechanism by which compact configurations of DNA are rendered stable against purely mechanical fluctuations.

Another avenue of my continuing research has involved the charged polymers, generically referred to as polyelectrolytes (PEs). In the case of neutral polymers, the worm-like chain model provides an accurate description of flexibility through the persistence length, which quantifies the correlations of unit tangent vectors parallel to the chain. However, a complete characterization of the mechanical properties of charged chains is difficult due to the existence of a number of length scales. With my collaborators, I calculated the radial distribution function of the end-to-end distance of a charged, inextensible, semiflexible chain as a function of charge density, screening length and intrinsic stiffness. We investigated the extent to which the radial distribution function of a PE is reproduced by that of a wormlike chain with an effective persistence length. Currently, in the Department of Chemistry and Biochemistry at UCLA, the group of Professor Shimon Weiss is in the process of measuring the end-to-end distances in short pieces of DNA; their results will be compared with our theory.

As a means of exploring the widespread notion that polyelectrolytes can be described in terms of uncharged worm-like chains, my collaborators and I also investigated the shape of a short PE chain subjected to equal and opposite force-couples or torques at its two ends. We found that, unlike a neutral semi-flexible polymer, which forms a constant curvature configuration under such conditions, the short segment of PE tends to flatten in the interior and accumulate curvature at its end points; this response maximally reduces electrostatic self-repulsion. In a related project, I studied the buckling instability of a charged rod. Such phenomena have far-reaching implications in nano-technology, for instance, with regard to the properties of nanoactuators, tweezers, and AFM probes. A calculation of the force required to buckle a short charged rod leads to the conclusion that, in the limit of unscreened coulomb interactions, the buckling force is independent of chain length, in marked contrast to the case of neutral chains. In the future, I plan to investigate the effect of screening on the buckling force, and I will also be looking at buckling induced by counterion fluctuations.

Translocation

I also studied the problem of translocation of a polymer through a membrane pore. This system has very recently been the subject of intense research by both experimentalists and theorists. One version of this problem involves proteins that are thought to "ratchet" the polymer through the pore. The result of our research turned out to be both novel and exciting in that we found that the role of binding particles is quite different from what had been suggested by previous studies on the subject. We discovered that non-equilibrium effects contribute significantly to the dynamics of the passage of the chain through the pore, and moreover, we found that the hypothesis of a biased/ratcheted motion of the chain into the cell does not completely explain the underlying phenomena. More explicitly, we established that binding particles actually pull the chain into the cell; the force they exert can be attributed to a free energy gradient, modified by dynamical effects associated with the time required for binding particles to diffuse and associate with the chain.

In the future, I plan to investigate the chain release scenario by which a viral genome leaves its capsid. It has been speculated that in some plant and animal viruses, translation by the ribosome of the host cell provides the deriving force for viral genome translocation.

Entropic competition and knots

I have also started working with Professor Mehran Kardar at MIT, undertaking research on the entropic exponents of self-avoiding polymers. Using canonical Monte Carlo simulations, we introduced a new numerical method to obtain the universal exponents of partition functions of polymers with different constraints and/or topologies. The method was successfully tested for closed polymers decorated with sliding rings. Recently, we have applied the method to calculate the entropic exponents γ_1 and γ_2, characterizing the number of configurations for the attachment to an impenetrable probe of the polymer by one end, or at its midpoint. We discovered that these entropic exponents vary continuously with the angle formed by the tip of the probe.
In the future, I plan to utilize the entropic competition method to assess the effective degrees of freedom associated with knots. Knots and entanglement frequently appear in closed polymers and play a major role in numerous biological systems. I have performed off-lattice simulations that were, unfortunately, limited by finite size effects. I will take advantage of a new, much more promising, approach which places a knot on a lattice. Iterations of the system will proceed via moves that preserve knot topology.

Casimir forces

Recent experiments on the wetting of ^{4}He have shown that the film becomes thinner in the superfluid phase. Until recently this difference in film thickness has remained unexplained. So-called Goldstone modes, associated with the broken symmetry of the superfluid state, have been known to be responsible for part, but not all, of the thinning. We have shown that the flow field generated by *surface* fluctuations leads to a Casimir type force favoring thinner superfluid films. The combination of surface fluctuations and Goldstone modes is sufficient to account for the entirety of the thinning of the film in the superfluid phase. In the future, I plan to explore the role of critical fluctuations in generating unexpectedly large film thinning in the immediate vicinity of the superfluid transition.

Statement of Teaching Philosophy

Since I am the first one with a graduate degree in my family, I appreciate the importance of good teachers in the life and aspiration of young adults. I believe that all good teachers have the skills to make complex concepts clear, simple, and connected to the real world. Beside problem solving skills, I believe that students should develop critical thinking so as to be able to tackle scientific problems and be prepared to practice their profession ethically. My teaching assistant experience at the undergraduate level leads me to believe that I possess the qualities and potential to become an effective teacher and a supportive mentor of students at all levels of advancement. As a teaching assistant, I have worked diligently to present physical concepts to my students in accessible ways, and in 1998 I had the honor of receiving an Outstanding Teaching Award in the Physics Department at UCLA. I feel ready and eager to begin teaching at all levels as a new faculty member.

I am persuaded that independent research is a vital part of the learning experience at both undergraduate and graduate levels. Therefore, I plan not only to direct students' research efforts towards productive conclusions, but also to promote independent thinking on the part of the students. I would like to encourage free exchange of ideas within the research group and strongly support the students taking charge of developing their own research initiatives. In my opinion, the final goal of physics education is shaping an individual into becoming a creative and honest researcher able to provide society with technical answers to its current problems and to anticipate the future ones.

My diverse research projects in statistical physics and soft condensed matter allow me to interact with present group at Indiana University, and to advise students with various strengths and from different backgrounds. I also expect these projects to enrich and contribute to the kinds of new courses and seminars I intend to implement in a Physics department.

Finally, it is also my strong conviction that it is essential for today's young physicists not only to have technical ability but also to know how to step forward with an initiative, to communicate their ideas effectively and to implement these ideas. I possess a strong interest in promoting curricular and extracurricular activities that foster all these qualities in physics students.