Dissertation Announcement

Announcing the Final Examination of Aiqun Huang for the Degree of Doctor of Philosophy in Physics

Date: Wednesday, March 30, 2016
Time: 2:00 pm – 5:00 pm
Room: PSB 445 (UCF Main Campus)
Dissertation title:
Conformations and Dynamics of Semi-Flexible Polymers

Abstract:

In this thesis, we investigate the conformations, transverse fluctuations and dynamics of two-dimensional (2D) semi-flexible polymers both in the bulk and under channel confinement. We present unified scaling relations in regard to various quantities of interest for a broad range of combinations of chain length and chain stiffness using Langevin dynamics simulation. We also present a three-dimensional (3D) heterogeneous semi-flexible chain model for a double stranded DNA (dsDNA). Our model not only confirms the established findings for homogeneous dsDNA, but also predicts new physical phenomenon for heterogeneous dsDNA. The problems studied in this dissertation are relevant to analysis of the conformations and dynamics of biopolymers (such as DNA) in living organisms, and also offer insights for developing devices which operate on the single-molecule level.

In particular, we present a unified description for the dynamics of building-blocks (monomers) of a semi-flexible chain. We consider the full range of flexibility from the case where the chain is fully flexible (no stiffness at all) to the case where the chain behaves like a rod (infinite stiffness). Our theory predicts qualitatively different sub-diffusive regimes for the monomer dynamics originating from the chain stiffness by studying the mean square displacement (MSD) of the monomers before the chain dynamics become purely diffusive.

For the conformations in the bulk, we present results confirmed and agreed by two completely different models of semi-flexible polymers, with one of which is the bead-spring model (studied by Langevin dynamics) in the continuum space, the other (studied by Monte Carlo) is a self-avoiding walk chain on the square lattice, where only discrete bond angles are possible. We point out the universal features of chain conformations and fluctuations which are independent of the models.

For the conformations under channel confinement, we discover qualitatively different conformations and dynamics of the chain as a function of the channel width and chain stiffness, and show how globule like shapes ("de Gennes blobs") for more flexible chains continuously go over to shapes in the form of deflections from the wall ("Odijk limit") for more stiff chains. We provide theoretical arguments how these regimes occur and interpolate among each other as one varies different parameters of the model. We also demonstrate the effect of physical dimensions (either 2D or 3D) on these regimes and argue that since in 2D the excluded volume (EV) effect is more severe compared to 3D, certain regimes do not exist in 2D.

Finally, we study a model of a dsDNA , where both base-pairing and base-stacking interactions are accounted for albeit at a low computational cost compared to the other existing models. Our model correctly recovers the stiffness for dsDNA and ssDNA at different temperatures. Under most conditions of interest, a dsDNA can locally denature and form bubbles due to thermal fluctuations. At a critical temperature, a dsDNA undergoes a phase transition, in which the two strands of dsDNA completely melt to two single strands (two ssDNA). By considering EV interactions and calculating the bubble size distribution, recent studies have shown that this denaturation process is a first order transition. We show that for a homogeneous dsDNA made of only AT or GC pairs, our simulation results agree with the previous conclusion of first order transition, however, for sequences of periodic AT and GC regions, when the periodic size is relatively large compared to the sequence length, we show that the bubble size distribution exhibits peaks expressing the sequence pattern, and more importantly, the denaturation is no longer a first order transition.

All these studies reported in the dissertation are relevant to the physics of living systems.

Outline of Studies:
Major: Physics

Educational Career:
M. S. University of Central Florida, USA, 2013
M. S. Nanjing University, China, 2011
B. Eng. Zhengzhou University, China, 2008

Committee in Charge:
Dr. Aniket Bhattacharya (Chair)
Dr. Suren Tatulian
Dr. Viatcheslav Kokoouline
Dr. Andres Campiglia (External Committee Member)

Approved for distribution by Dr. Aniket Bhattacharya, Committee Chair, on March 24, 2016.

The public is welcome to attend.