MAR09-2008-002510

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Simulation studies of DNA translocation through a nanopore ([†])

ANIKET BHATTACHARYA, University of Central Florida

The experimental studies of voltage driven translocation of a single stranded DNA through a α-hemolysin pore, have stimulated a lot of activities as the phenomenon is rich in fundamental science involved and its prospective technical applications for detecting DNA/RNA sequences. While it is the attributes of heteropolymer translocation that are the key ingredients for prospective new sequencing methods, these experiments have generated stimulating theoretical and numerical studies directed toward a seemingly much simpler problem of homopolymer translocation through a nanopore. The earlier theoretical work of Muthukumar, Sung and Park, and by Kardar and his collaboartors[2] have been supplemented by more recent theoretical work by Dubbledam *et. al* and Panja *et. al*[3]. During this talk I will show results from Langevin dynamics simulation carried out on a coarse-garined bead-spring model of DNA-polymer both for the unbiased and driven translocation[4]. During the first part of the talk, after a brief review of the current theories of DNA translocation, specifically mentioning the underlying assumptions, I will compare simulation results with those predicted by different theories. Particularly, I will show numerical results for the translocation exponent α defined as $\langle\tau\rangle \sim N^{\alpha}$ and the exponent for the s-coordinate β defined as $\langle s^2(\tau)\rangle \sim \tau^{\beta}$, and discuss how the numerical values differ as one chooses slightly different pore width and geometry. In the second part of my talk I show how a model *attractive nanopore* can distinguish the sequence of a heteropolymer[4] and discuss possibility of making a device based on this idea.

[†]work done in collaboration with Kaifu Luo, Tapio Ala-Nissila, See-chen Yin, Andrey Milchev and Kurt Binder

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