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Theory of Interacting Polyelectrolytes Under Confinement

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Abstract

During my thesis work I have investigated the problem of polyelectrolyte characterization and in particular how to interpret the experimental data to obtain the mass and gyration radius of short polyelectrolytes. This is usually a challenging problem for experimentalists to deal with. For example, the interpretation of the static light scattering data to obtain the gyration radius becomes increasingly inaccurate as the size of the chain becomes very much smaller then the light wavelength. Also, the interpretation of membrane osmomometry data is complicated by the leakage of the solute of low molecular weight polymers and so forth. There are, however, a number of approaches to deal with these problems.

In the first chapter of my thesis I obtained a crossover formula of the second virial coefficient of polyelectrolytes that correctly reproduces the perturbative and asymptotic polymer regimes in addition to the salt concentration dependence at high-to-medium salt concentrations. This formula will then be combined with similar crossover formula for the radius of gyration to interpret the later from the second virial coefficient measurement.

On the technical side of the story, the crossover formula was obtained by combining the renormalization group equation(to the first nontrivial order in epsilon) with the direct d=3 computation of the perturbative expansion(to the second order in the two coupling constants) obtained from double inverse Laplace transform.

The second chapter of my dissertation is about the translocation phenomena. Translocation is a phenomena of threading a polymer through narrow pores and/or channels. This is very promising technique to measure the molecular weight of every individual polymer in the solution. Indeed, the polymer chain threading through the pore blocks the flow of electric current that also flows through the pore. By the duration of the current blockade the length of polymer chain can be obtained.

Unfortunately, there are a number of problems this approach encounters. One of them is that the only so far practically obtainable nanometer-size pore is the alpha hemolysine one which has a complicated internal layout- a spherical(more or less) vestibule. This nasty feature makes current blockade vs time data harder to interpret. There is a way to bypass this problem. Recently a number of research groups began to modify the pore via the directed mutagenesis to reduce the time the chain spends in the vestibule.

In my work I theoretically investigated translocation of the polyelectrolyte chain through a spherical cavity with tunable charge. The results provide some guidelines on how to reduce the influence of the vestibule on the translocation time if we are to medify the chain in addition to the decorating the pore with charges. This work includes a number of interesting techniques. It is based on the self-consistent field theory which gives us nonlinear Schroedinger and Poisson-Boltzmann

equations. These equations are then solved numerically via a finite difference schemes.

Lets point out possible extensions of this work. The SCFT technique is a primary computational tool for polyelectrolyte brushes and melts. Those things can be useful for the rapidly developing technology of pore gating, brush filtration and brush lubrication, just to name a few.

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