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Rodlike Electrolytes using Lattice Boltzmann

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Abstract – We solve the Poisson-Boltzmann equation for a cylinder electrolyte in the Debye-Hückel approximation using lattice-Boltzmann technique.

The problem of an electrical potential distribution for a charged surface immersed in an electrolyte solution is quite well explained by Poisson-Boltzmann (PB) theory. The distribution of ions close to a charged planar surface is described by Gouy-Chapman mean field theory [1]. This problem and their deviations underneath several electrochemical and biological processes such electron and ion transfer across interfaces [2].

On the other hand, electrostatic interactions play a central role in the structure and function of polymers, macromolecules, drug design and cells in Biology [3]. There are important industrial applications, such as stabilization of charged colloidal suspensions and flocculation processes [4]. Also, we can find very important cylindrical biopolymers as DNA, RNA, actin filaments, viruses, etc., playing a central role in the biological processes and by themselves, they are examples of highly charged cylindrical electrolytes that display a very rich dynamics as condensation and bundle formation [5-6].

Much theoretical work has been done along years. PB equation can be considered as a mean field theory that gives into account of the electrostatic interactions between the charges in an ionic solution. In its linear approximation, called Debye-Hückel theory, we can solve analytically a spherically charge distribution. The problem arises when we ask for rodlike charge configurations. In 1951 Fuoss [7], proposes an analytical solution for a cylindrical isolated molecule assuming a superposition of fields in the case where the Poisson-Boltzmann equation is nonlinear. The Painlevé type solutions are involved for a cylindrical polyelectrolyte, proposing an explanation of highly charged cylindrical molecules and its response of the mobile ion distributions [8]. A refinement and extension of the Painleve approach is given in [9]. Also, amazing phenomena can be found in strongly charged electrolytes as the so called counterion condensation, basically a linear polyelectrolyte reduces their line charge density because of the polielectrolyte line charge overreach a given critical value [10].

Because of the enormous complexity of the problem makes very difficult to give analytical solutions, therefore the computational method is a fairly enough approach. We found a novel and very insightful method to give solution to the Poisson Boltzmann equation using lattice Boltzmann [11].

This work presents the electrostatic potential for one and various rodlike electrolytes giving full insight of the physics.

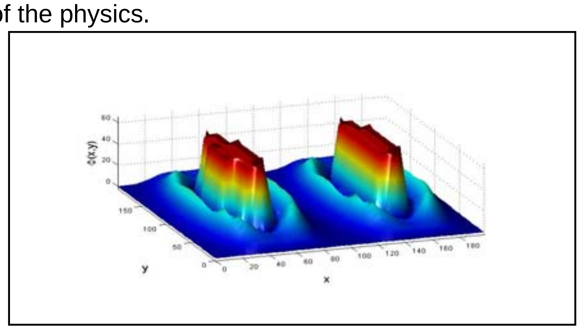

Figure 1: Electric potential for two rodlike electrolytes.

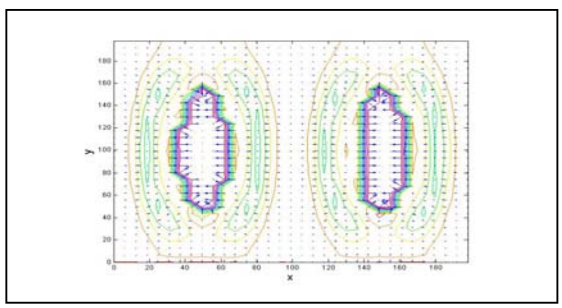

Figure 2: Electric field for two rodlike electrolytes.

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