Mathematical, Algorithmic and Numerical Solutions to enhance Electrostatic Calculations for Biomolecules in Electrolytic Solutions

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This PhD thesis is structured in two Parts, reflecting the two main project we have worked on: the study of electrostatic in biomolecules within electrolytic solutions, and the analysis of state relations in oscillator chains. At first glance, these topics might seem unrelated. However, they are deeply connected by a common goal: understanding the behavior of complex systems through the lens of mechanics and thermodynamics, and their mathematical formulations. Both projects start from the same idea to develop models that capture physical phenomena, especially in cases where standard numerical and analytical approaches can produce misleading results if the underlying physical and mathematical principles of thermodynamics are not properly respected.

In the first Part, we focus on modeling electrostatic interactions of biomolecules in electrolytic solvents using continuum electrostatic models. We derive the Poisson-Boltzmann equation (PBE) and its linearized and general forms. The PBE is a relevant partial differential equation commonly used in biophysical applications to estimate the electrostatic energy of biomolecular systems immersed in electrolytic solutions. We further analyze the linear PBE, offering new analytical insights and proposing a numerical model to solve it efficiently. This model is implemented in the software `NextGenPB`. We validate our approach through comparisons with analytical benchmarks presented in this thesis, as well as with well-established software. Finally, we demonstrate the solver's applicability to real-size systems, showing its potential for practical use in realistic scenarios.

In the second Part, we investigate a previously discovered linear relation, that connects the average distance between pairs of consecutive particles with their kinetic energy, applies to quite a large set of one-dimensional particle systems known to produce anomalous transport. This relation is microscopic in nature, since the quantities involved are neither averaged over many particles, neither over very large times. Nevertheless, its robustness under variations of the external parameters, and the limited set of quantities it involves qualify it as a state equation, analogously to thermodynamic relations. We provide conditions for which the relation can be violated within a limited range of parameters values, and we find that it can be extended to two dimensional networks of coupled oscillators. The validity of this relation further shows that the states of aggregation of matter in low dimensional systems are often different from standard

macroscopic ones.