Implicit model for water and electrolytes with a field theory approach.

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It is difficult to overstate the importance of electrostatic interactions in water in nanometric structures, biological organelles or nanofluidic devices to name a few. At this scale water can not be modeled by an homogeneous dielectric medium but its molecular structure has to be taken into account. Explicit models of water which consists in simulating all the molecules of the liquid phase are broadly used to study the electrostatic environment in nanometric devices. However, they are so time-consuming that it is difficult to scale to systems bigger than few nanometers.

An exciting alternative is to develop a continuous model describing the properties of water and electrolytes at the nanometric scale. Density and polarization fiels functionals have shown to be a promising tool as they can capture some key properties of water such as its structure factor or the dipole-dipole correlations induced by the hydrogen bonds network[1,2]. These tools need to be refined and it is the objective of this traineeship: building a better field theory for water and electrolytes.

The construction of a phenomenological semi-microscopic model for a solvent starts with a good knowledge of its molecular structure and the traineeship will be organized in two steps:

1) **Field Theory**: Propose an expression for the functional of density and polarization that capture the structural and dielectric properties of water and electrolytes and forsee the profile of electrostatic field in nanometric confinement geometries.

2) **Molecular dynamics simulations**: Study the properties of water molecules in the surrounding of ions and dielectric spheres (hydrophilic and hydrophobic). We aim at characterizing both the polarization, the correlations in presence of an inclusion and the geometric arrangement of the molecules.

A PhD could be envisaged after the traineeship. The midterm perspective of this work is to propose an implicit model for electrolytes treating solvant molecules and ions on the same footing. On a longer term perspective, such models could be used to study ion transports in biological processes.

This traineeship will necessitate and develop skills both in theoretical calculations and in programming. It will be supervised by Hélène Berthoumieux at LPTMC, Sorbonne Université and Maximilien Levesque at ENS Paris.

1) H. Berthoumieux, *Gaussian field model for polar fluids as a function of density and polarization: Toward a model for water*, JCP, **2018**, (148).
2) G. Jeanmairet *et al.*, *Molecular Density Functional Theory of Water*, JCP, **2013**, (4).