



Modelling specific ion effects in solutions using integral equation theories

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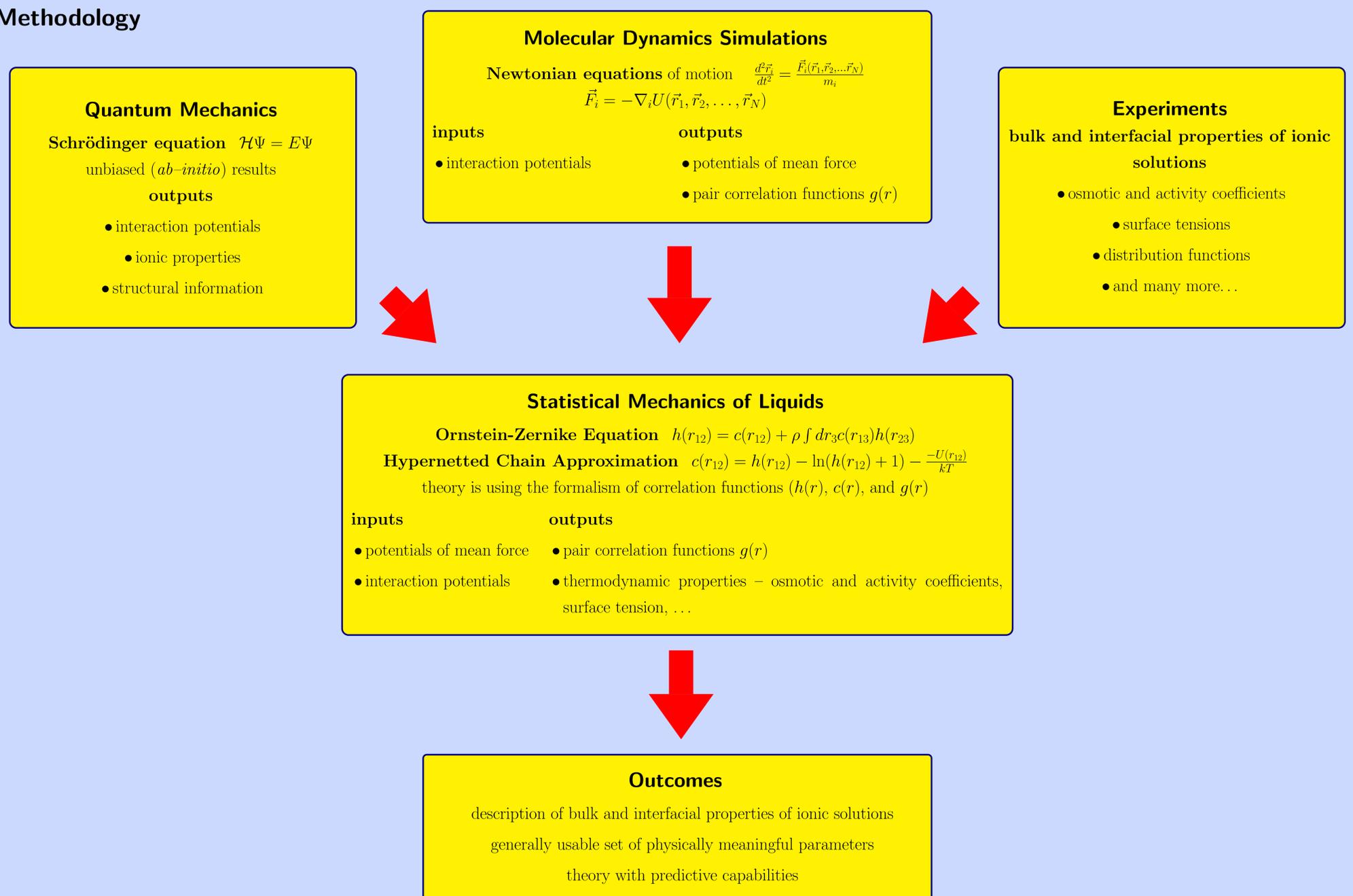
Introduction Ions play an important role in many natural, biological, and technological processes. As a consequence, various experimental techniques are used to assess properties of ionic solutions. A theoretical description of these solutions can provide complementary information, and can be also used for predictions of their properties without the need to perform experiments.

We use the integral equation theory (namely the Ornstein-Zernike equation with the Hypernetted Chain closure relation) for obtaining such models of ionic solutions.

Our study requires very close collaboration with specialists from other fields of (not only) physical

chemistry. The development of reliable interaction potentials would not be possible without the methods of computational chemistry, namely molecular dynamics simulations and quantum mechanical calculations. The Poisson–Boltzmann equation can be used for modeling of the interfaces of ionic solutions and, therefore, provides interesting insights into the physics of the interfacial behavior of ions. It is also an important source of material for comparison with the integral equation theory. Finally, experiments (when available) provide essential data that can be used for benchmarking and validating theoretical findings.

Methodology



Goals of the work We are aiming at obtaining precise and predictive description of properties of ionic solutions. The most important steps of this project will be:

- development of new **physically sound** solvent averaged interaction potentials
- definition of suitable fitting parameters, if needed
- description of both **bulk and surface properties of ionic solutions**
- description of **dissociation phenomena** - pK of weak electrolytes in mixtures and buffers
- application of the results in biology, biochemistry, engineering, ...

Collaborations

- **Roland Netz, Dominik Horinek** (TU München)
– molecular dynamics and quantum mechanical calculations
- **Matthias Boström** (Linköping University)
– description of solution interfaces using the Poisson–Boltzmann equation