Bachelor/Masterarbeiten Themen

Prof. Dr. Ana-Sunčana Smith – Lehrstuhl für Theoretische Physik I

1. Orientational dynamics of water

The dynamical structure of liquid water is often characterized as a fluctuating network of hydrogen bonded molecules, in which specific molecular motions, such as restricted translations and rotations, contribute to many practically important phenomena (e.g. acoustics). Because of the experimental difficulties of exploring the structure and dynamics of liquid-state water, molecular dynamics simulations have proved to be a valuable tool over the years. We intend to investigate the orientational dynamics of pure water represented by simple models (SPC/E, TIP4P2005, etc.) at ambient conditions. The orientational dynamics will be quantified through the orientational and angular velocity correlation functions of water molecules and related to its local structure. A logical extension of the project would be trying to gain an insight into the water orientational dynamics in different environments, such as the presence of hydrophobic objects (particles, walls) or external electric fields.

2. The role of long-range interactions in the calculation of the friction coefficient of a Brownian particle

A large and heavy colloidal particle, the so-called Brownian particle, experiences a friction force arising from systematic collisions with solvent molecules which is directly proportional to its velocity, and the proportionality constant is the friction coefficient. Unfortunately, it is very hard to calculate the friction coefficient directly from computer simulations using the Green-Kubo formalism. Primarily, due to finite computational resources available, the maximum size of the system available for investigation is reached before the desired thermodynamic limit is obtained. Since a large part of the computation is spent on calculating the long-ranged van der Waals (vdW) interactions it is of interest to understand their influence in the calculation of the friction coefficient. Moreover, we want to find minimal conditions in the description of the vdW interactions in order to speed up the calculations while keeping the accuracy in the description of the particle's dynamics. The system of study will be a Brownian particle interacting with a bath of solvent molecules only through the Lennard-Jones interactions.

Contact: **Dipl. Zoran Miličević**
Zoran.Milicevic@physik.uni-erlangen.de
Phone: +4991318520114

Web:
http://www.eam.uni-erlangen.de
http://theorie1.physik.uni-erlangen.de/people/asmith/

Prof. A. S. Smith
Group for Theoretical Biophysics
Institute for Theoretical Physics I