DY 62: Glasses and Glass transition (joint session DY/CPP)

Time: Friday 10:00–11:45 Location: H19

DY 62.1 Fri 10:00 H19

Unified Formulation of Fractional Relaxation — •Tillmann Kleiner and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart

Susceptibility functions that involve stretching exponents which are derived from fractional dynamics [1] reproduce the excess wing of α-relaxation peaks that has been observed in dielectric spectra of glass forming materials [2]. The contemporary formulation of fractional dynamics requires two distinct approaches to describe the relaxation motion and the response of the system to periodic excitations. The former uses fractional Liouville-Caputo derivatives in the time domain and the latter multiplication with the susceptibility function in the frequency domain. Both approaches impose severe restrictions on the past history of the involved electric field that are unrealistic in an experimental situation. Due to the occurrence of memory effects this poses a serious problem. In this contribution a unified description of fractional dynamics is presented where fractional derivatives are defined using distributional convolution. The resulting response functions are stretched multinomial Mittag-Leffler functions. This formulation extends the mentioned approaches to all experimentally relevant situations in a consistent way and exposes a high degree of convenience.

[1] R. Hilfer, Analysis **36**, 49-64 (2016)
[2] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)

DY 62.2 Fri 10:15 H19

Ion and Molecule Transport in Nanopores - a NMR Study — •Christoph Säckel, Sarah Schneider, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

We analyze ion and molecule transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While biological ion channels are highly selective and sensitive, they lack the robustness for technological applications. In contrast, silica pores are well-established in industrial environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favourable properties of both types of pores. It is therefore necessary to understand the influence of the confinement on the temperature-dependent ion and molecule transport. We systematically vary the pore parameters and study effects on the dynamics with ^{1}H, ^{2}H and ^{7}Li nuclear magnetic resonance (NMR). We combine homogeneous and gradient field NMR to selectively investigate water and ion dynamics on broad time and length scales in the supercooled regime. Both the local and long-range dynamics of ions and water show a slowdown with decreasing pore size. In addition, our data indicates more heterogeneous dynamics for the liquid in confinement than in bulk. Both the slowdown and heterogeneity can be explained by a slower layer of solution at the pore walls and bulk-like dynamics in the pore centre. Self-diffusion shows an Arrhenius-like behaviour of the solution in confinements, while bulk samples are best described by a VFT fit.

DY 62.3 Fri 10:30 H19

Glass transition of water-like models in bulk and confinement — •Robin Horstmann and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Tetrahedral network formers have a special position among glass-forming liquids. Their well defined local prefered structures cause significant structural changes with temperature but often render the transfer of models of supercooled liquids, e.g. density scaling, difficult. We use molecular dynamics simulations to examine two families of water-like molecules, based on the SPC/E and TIP4P/2005 water models, that vary only in their partial charges to systematically alter the strength of the hydrogen-bonds and, hence, the relevance of tetrahedral order.[1] The varied inter-molecular interactions spread dynamics over a wide temperature range with the glass transition temperature T_g and the high temperature activation energy E_∞ both changing by a factor of five. Additionally, we study water-like systems in neutral confinements and find unchanged tetrahedral structure but slowed molecular dynamics. To describe the glassy slowdown, we assume that the activation free energy can be split into a constant value E_∞ and an exponentially growing contribution $E_c(T)$.[2] Common ratios of E_∞/T_g and $E_c(T)/T_g$ are found indicating that the high temperature results can be used to rescale the glassy slowdown in bulk and confinement.

[1] R. Horstmann and M. Vogel, J. Chem. Phys. **147**, 034505 (2017)
[2] B. Schmidtke et al., Phys. Rev. E **86**, 041507 (2012)

DY 62.4 Fri 10:45 H19

Effects of fractional freezing on the structure and dynamics of deeply cooled confined water — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

The properties of confined water are of enormous importance in nature and technology. In particular, the effects of partial freezing on structure and dynamics is largely relevant for, e.g. geology, cryopreservation and our understanding of the glass transition of water [1]. To obtain a better understanding of the properties of the liquid fraction molecular dynamic simulations were performed with the TIP4P/Ice water model. This model was chosen for its good agreement with several water and ice properties. A series of frozen confinements with different pore diameters were made to analyze the structure and dynamics of the water layer remaining liquid upon deeply cooling, between pore wall and ice crystals. The partial freezing results in altered water dynamics, most importantly, the non-Arrhenius behavior of weakly supercooled bulk water is replaced by an Arrhenius behavior. Confined and bulk water have in common that the structure is disturbed at low temperatures. Either trough the existence of two interfaces in the case of the frozen confinement or through partly forming ice nuclei in the bulk.

[1] Cerveny, S. et al., Chem. Rev., **2016**, *116* (13)

DY 62.5 Fri 11:00 H19

Decoding of the Toric Code: A High Temperature Series Analysis — •Benedikt Placke[1], Nikolas Breuckmann[2], and Ananda Roy[1,3] — [1]JARA Institute for Quantum Information, RWTH Aachen University — [2]Department of Physics and Astronomy, University College London — [3]Insitut de Physique Théorique, CEA Saclay

The decoding of several topological quantum codes (TQC) can be mapped onto statistical physics models (SPM). This mapping relates the successful decoding of the error syndrome of the TQC to a certain phase of the respective SPM. The error-correction performance of several TQC-s have been analyzed using Monte Carlo (MC) simulations of the corresponding SPM. We, on the other hand, use high-temperature series expansion (HTSE) to analyze the decoding performance of the toric code. In contrast to zero temperature simulations, which estimate the threshold of the minimum-weight perfect-matching decoder, our method naturally provides an estimate of that of the maximum-likelihood decoder. First, we analyze the full phase diagram of the 2D random-bond Ising model by computing HTSE to a higher order than previously performed. From our analysis, we estimate the accuracy threshold of the toric code in absence of measurement imperfections. We compare our result to those obtained by MC simulations and network model analysis. Then, we perform HTSE of the zero-field free-energy and the Wilson loop order parameter in the 3D Ising gauge theory in the presence of quenched disorder. The latter model describes the decoding of the toric code subject to measurement errors.

DY 62.6 Fri 11:15 H19

Local and translational dynamics of water in various confinements investigated via ^{1}H and ^{2}H NMR — •Simon Schoner, Max Weigler, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Confined water is interesting for several reasons. On the one hand the topic is highly relevant in biology or geology where water is often found in soft or hard confinements, water around proteins or in rods being prime examples. On the other hand confined water allows one to investigate liquid water at low temperatures, where normally crystallization would occur, and, in this way, to obtain insights into the heavily debated glass transition of water. We investigate the dynamics of water confined in various rigid matrices using ^{1}H and ^{2}H NMR experiments. One goal is to obtain information on the influence of different kinds of confinements and pore sizes on the self diffusion and the structural relaxation of water. Especially, we address the question whether trans-

lational diffusion and local reorientation are affected by confinement in a comparable way. First measurements with D_2O and H_2O indicate similar correlation times and diffusion coefficients for both MCM-48 and MCM-41 confinements with comparable pore sizes between 2 and 3 nm.

DY 62.7 Fri 11:30 H19

Universal hidden order in amorphous cellular geometries — •Gerd E Schröder-Turk — Murdoch University, Perth, School of Engineering and IT, WA 6150, Murdoch, Australia

Partitioning space into cells is central to many fields of science and technology, as well as to resource distribution problems in economics and telecommunication. The nature of cellular partitions is often defined by optimization with respect to certain properties, such as interface area in the Kelvin problem, packing density in the Kepler problem, or cell centrality in the Quantizer problem. In all known cases, the optimal solutions are crystalline configurations with long range order. To date, no optimization problem has been identified where the optimal solution is a disordered configuration. Amorphous, or disordered, structures are generally considered to be intermittent meta-stable states that prevent the system from attaining the optimal ordered structures. Here we use Lloyd's iteration to demonstrate the existence and stability of a special disordered state in the three-dimensional Quantizer problem, despite the existence of lower-energy crystalline configurations. Akin to a thermodynamic phase, this state is universal. Specifically, irrespective of the level and type of disorder in the initial configurations, we find a convergence to the same amorphous state, representing configurations characterized by the same structure factor and energy distributions. This highly degenerate state is characterised by an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity.