DY 22: Statistical Physics (general)

Time: Wednesday 15:00–18:30 Location: H48

DY 22.1 Wed 15:00 H48

Density fluctuations and self-diffusion along saturation in dense liquids: acoustic data and lattice model — Alexander Goncharov, Vyacheslav Melent'ev, and •Eugene Postnikov — Kursk State Univesity, Kursk, Russia

We consider the density fluctuations in fluids along a saturation line (both liquid and vapour phases) especially in the region closed to the malting point. Corresponding data are extracted from acoustic (speed of sound) and thermophysical (heat capacity ratio) measurements. The analysis of the dependence for reduced fluctuations (ratio of fluctuations of real media and ideal gas under the same PVT conditions) allow to determine the region of exponentially decaying dependencies, which is universal for a large amount of substances (liquid noble gases, chained hydrocarbons and their halogen substituted).

The considered theoretical lattice model (grand canonical statistic ensamble) argues that this region corresponds to absence of structure transitions but the presence of geometrical rearrangements of particles. The derived correspondence between these fluctuational characteristics and self-diffusion properties confirms the outlook about universality of universal scaling law for atomic distribution [Dzugutov, Nature, 381 (1996), 137] non only for simple (spherically symmetric) particles but for constituents of chained hydrocarbons as well.

DY 22.2 Wed 15:15 H48

Method for prediction of thermophysical, acoustic and structure properties of liquids with the framework of cluster model — Gennady Melnikov[2], •Vyacheslav Verveyko[1], Marina Verveyko[1], and Yury Melikhov[1] — [1]Kursk State University, Kursk, Russia — [2]South-West University, Kursk, Russia

The proposed by authors distribution function of clusters with respect to number of particles allows to obtain the isothermal equation of state, which provides the method for prediction of thermophysical, acoustic and structure properties of simple liquids without a knowledge of an explicit form for the radial distribution function and adjustable intermolecular interaction potential. As well, structure and relaxation processes could be analyzed too.

The calculations are evaluated for liquefied noble gases and several hydrocarbons. Their comparison with the known experimental data shows a high exactness of the proposed method and its advances for the prediction of the mentioned properties in a wide range of state parameters.

G.A. Melnikov, V.N. Verveyko et al. Int. J. Therm. 32 (2011), 901.
G.A. Melnikov, V.N. Verveyko et al. High Temperature. 50 (2012), 214.

DY 22.3 Wed 15:30 H48

Common features of simple water models — •Lotta Heckmann and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Germany

The rich phase diagram and the anomalies of water continue to inspire theoretical and numerical studies. Simplified models for water that do not aim at accurately describing molecular structure, but rather at matching general properties of water, have been successful at revealing the mechanisms and principles behind the special behaviour of this substance. In particular, the association of a lower local density with a stronger binding energy is an important ingredient in such models. Several models have been introduced that include this feature and that produce, among other transitions, phase transitions between a high-density and a low-density liquid phase. We compare three of these models, which are at first sight rather different, and investigate in particular the water anomalies and the phase transition line between the two liquid phases of these models. Our objective is to identify common characteristics and to extract the minimal ingredients required for a successful water model.

DY 22.4 Wed 15:45 H48

Grand-Canonical-like molecular dynamics — •Han Wang, Carsten Hartmann, Christof Schuette, and Luigi Delle Site — Institute for Mathematics, Freie Univ. Berlin

In this presentation, we describe a general theoretical analysis, and show numerical tests of the reliability of the adaptive resolution simulation (AdResS) technique in sampling the Grand Canonical ensemble. We demonstrate that the correct density and radial distribution functions in the hybrid region, where molecules change resolution, are two necessary conditions for considering the atomistic and coarse-grained regions in AdResS equivalent to subsystems of a full atomistic system with an accuracy up to the second order with respect to the probability distribution of the system. Moreover, we show that the work done by a thermodynamic force in the transition region, that is a force originally derived on the basis of empirical thermodynamic considerations, is formally equivalent to balance the chemical potential difference between the different resolutions. From these results follows the main conclusion that the atomistic region exchanges molecules with the coarse-grained region in a Grand Canonical fashion with an accuracy up to (at least) second order. Numerical tests, for the relevant case of liquid water at ambient conditions, are carried out to strengthen the conclusions of the theoretical analysis. This fruitful combination of theoretical principles and numerical evidence candidates the adaptive resolution technique as a natural, general and efficient protocol for Grand Canonical Molecular Dynamics for the case of large systems.

DY 22.5 Wed 16:00 H48

Levy flights search in potential — •Vladimir Palyulin, Alexei Chechkin, and Ralf Metzler — Chair for Theoretical Physics, Inst for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

Problem of target search has a long history. There are many theoretical and experimental works which discuss whether Levy flights, Brownian motion or intermittent search strategy is the most efficient way for a particle or predator to find the target. We introduce a new convenient measure of search efficiency and compute it for Brownian and Levy search with and without potential bias. This measure shows non-trivial behavior which depends on Levy flights exponent, initial distance of a particle from the target and drift velocity. Analytical and numerical results show that either Brownian or Levy flights can be efficient depending on the initial conditions. Cumulative probability to reach a target ever is also calculated. Analytical and numerical results are obtained from fractional Fokker-Planck equation and supported by Monte-Carlo simulations.

15 min. break.

Invited Talk DY 22.6 Wed 16:30 H48

Entropy based approaches to transport — •Thomas Christen — ABB Corporate Research, CH-5405 Baden, Schweiz

The quasi-stationary distribution function for a gas of independent particles, which are not in local thermal equilibrium (LTE) but strongly interact with an LTE medium, can often be described by a linear Boltzmann transport equation (BTE). In order to make use of a truncated expansion of the distribution function in terms of moments that satisfy generalized hydrodynamic equations, an appropriate closure method is required. An often used closure method is based on constrained entropy maximization. We show that a closure based on constrained entropy production minimization is superior to entropy maximization, and mitigates some well-known errors of the latter. As an example, we discuss non-LTE radiation in an LTE-plasma and show how average heat transport coefficients can be determined for realistic absorption spectra. As a second example, we illustrate the approach for electric conduction in low-dimensional structures.

DY 22.7 Wed 17:00 H48

Massively parallel Monte Carlo for many-particle simulations on GPUs: Application to the liquid-hexatic transition of hard disks — Joshua A. Anderson, Eric Jankowski, Sharon C. Glotzer, and •Michael Engel — Chemical Engineering, University of Michigan, USA

Parallel algorithms for Monte Carlo simulations of thermodynamic ensembles of particles have received little attention because of the inherent serial nature of the statistical sampling. In this talk, we present a massively parallel method that obeys detailed balance and its implementation for a system of hard disks on the GPU [1]. We reproduce results of serial high-precision Monte Carlo runs to verify the method [2]. This is a good test case because the hard disk equation of state over the range where the liquid transforms into the solid is

particularly sensitive to small deviations away from the balance conditions. Our results confirm the first-order nature of the hard disk liquid-hexatic phase transition. Phase coexistence is visualized for individual configurations via the local orientations, and positional correlation functions are computed. The performance of our method to sample configuration space and approach equilibrium is compared with the local Monte Carlo method, the event-chain Monte Carlo algorithm, and event-driven molecular dynamics.

[1] J.A. Anderson et al., arXiv:1211.1646
[2] J.A. Anderson et al., arXiv:1211.1645

DY 22.8 Wed 17:15 H48

From the number of detritus lines to hysteresis memory – On the statistics of dominant extreme values — •Sven Schubert and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz, Germany

We are interested in the statistics of the number of dominant extreme values and its evolution in time. What are dominant maxima? They are to a time series what the pattern of seaweed and detritus residues on the beach is to the amplitudes of the arriving water waves.
In the first part of the talk, results are presented on the statistics of the number of dominant maxima of a sequence of i.i.d. continuous random variables. One finds that the number of dominant maxima is a nonstationary variable. It shows ageing and its expectation value is diverging logarithmically as the time approaches infinity.
The sequence of dominant maxima memorizes certain local maxima from a time series. This decreasing sequence of maxima is a simplified version of the memory of a Preisach model of hysteresis where an alternating series of dominant minima and maxima is stored. The second part of the talk elucidates this connection and discusses the implications of the results presented to the memory length of the Preisach model of hysteresis.

DY 22.9 Wed 17:30 H48

Chaoticity and thermalization in the mean-field disordered Bose-Hubbard model — •Olivier Tieleman[1], Charalampos Skokos[1,2], and Achilleas Lazarides[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

We study chaoticity and thermalization in the mean-field disordered Bose-Hubbard model. A symplectic integration method allows us to obtain both full trajectories through phase space and maximum Lyapunov exponents, characterizing the chaoticity of the trajectory. We then compare long-time averages of some observables to thermal expectation values and study how the system approaches a thermal state, testing the hypothesis that the ergodicity of trajectories through phase space is closely linked to their chaoticity.

DY 22.10 Wed 17:45 H48

Statistical Physics of Lattice Triangulations in Arbitrary Dimensions — •Benedikt Krüger, Johannes F. Knauf, and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

Triangulations are a common tool in physics, e.g. for discretization of complex structures in classical and quantum geometry. They can be used for approximating smooth curved objects with piecewise flat simplices as elementary building blocks. We study the statistical properties of lattice triangulations in arbitrary dimensions numerically. Defining elementary flips between different triangulations, Markov-Chain Monte-Carlo simulation methods can be applied. Using the Wang-Landau algorithm we can directly calculate the density of states (DOS) and the total number of lattice triangulations for different system sizes. By applying different energy functionals we examine canonical partition sums and phase transitions.

DY 22.11 Wed 18:00 H48

Quasiparticle parameterization of meanfields, Galilean invariance and universal conserving response function — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The form of meanfield and density functional parameterization in terms of current, energy and density are examined by the restriction of Galilean invariance. It is found that besides a density functional only one parameter remains which is usually condensed in the effective mass. The universal response with respect to density, momentum and energy is found in the sense that the response becomes independent on actual parameterization of the local equilibrium provided the conservation laws are enforced. The sum rules by frequency moments and the compressibility sum rule impose further restrictions which determines the last parameter.

DY 22.12 Wed 18:15 H48

Asymmetry in the search for the best and the worst configurations of complex problems — •Johannes Josef Schneider — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, 55099 Mainz, Germany

Usually, the search for exact ground states of complex problems is considered to be as difficult as the search for states with highest cost function values, at least in the absence of symmetry breaking constraints. In this talk, I will show that there are indeed complex problems, for which the worst solution can be determined computationally much easier than the best configuration, although both tasks have to be considered as complex. Computational results are presented for the traveling salesman problem and the portfolio optimization problem.