DY 26: Posters - Statistical Physics, Stochastic Thermodynamics

Time: Tuesday 18:15–21:00 Location: P3

DY 26.1 Tue 18:15 P3

Investigating crystal-liquid interface by using fundamental measurement theory — •Shang-Chun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany

The crystal-liquid interface is important in material science. To investigate crystal-liquid interface, fundamental measurement theory (FMT) within density functional theory (DFT) provides the almost accurate properties for the hard-sphere like system. In FMT, the equilibrium crystal-liquid interface has been done within DFT, but has not been tackled within dynamic density functional theory (DDFT). The dynamics play a crucial role in non-equilibrium systems, such as nucleation; however, so far only the bulk liquid phase has been done within DDFT. Thus, I attempt to model the crystal phase and crystal-liquid interface by using FMT within DDFT, and compare results with FMT within DFT.

DY 26.2 Tue 18:15 P3

Importance of many-body dispersion and temperature effects on gas-phase gold cluster (meta)stability — •Bryan R. Goldsmith, Philipp Gruene, Jonathan T. Lyon, David M. Rayner, André Fielicke, Matthias Scheffler, and Luca Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Gold clusters in the gas phase exhibit many structural isomers that are shown to intercovert frequently, even at room temperature. We performed ab initio replica-exchange molecular dynamics (REMD) calculations on gold clusters (of sizes 5-14 atoms) to identify metastable states and their relative populations at finite temperature, as well as to examine the importance of temperature and van der Waals (vdW) on their isomer energetic ordering. Free energies of the gold cluster isomers are optimally estimated using the Multistate Bennett Acceptance Ratio. The distribution of bond coordination numbers and radius of gyration are used to address the challenge of discriminating isomers along their dynamical trajectories. Dispersion effects are important for stabilizing three-dimensional structures relative to planar structures and brings isomer energetic predictions to closer quantitative agreement compared with RPA@PBE calculations. We find that higher temperatures typically stabilize metastable three-dimensional structures relative to planar/quasiplanar structures. Computed IR spectra of low free energy Au9, Au10, and Au12 isomers are in agreement with experimental spectra obtained by far-IR multiple photon dissociation in a molecular beam at 100 K.

DY 26.3 Tue 18:15 P3

Determination of elastic constants in the isothermal-isobaric ensemble — •Dominik Lips and Philipp Maass — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück, Germany

The calculation of local elastic constants in heterogeneous materials from computer simulations is an important task for applications in materials science on the nanoscale and for a better understanding of biological processes involving elastic deformations. By combining Irving and Kirkwood's definition of a continuum stress field in terms of averages over phase space functions [1], and the work of Ray and Rahman on the calculation of bulk elastic constants by equilibrium stress fluctuations [2], Lutsko succeeded to derive a stress fluctuation formula to cope with the problem of local elastic constants in heterogeneous materials [3]. This approach has been worked out in the canonical ensemble and cannot be applied in constant pressure simulations, as they are nowadays often conducted in soft matter and biological systems. We present new stress fluctuation formulas valid in the isothermal-isobaric ensemble, for both local and bulk elastic constants [4]. Useful applications of these fluctuation formulas to complex heterogeneous soft matter systems subject to external pressure will be discussed.

[1] J. H. Irving and J. G. Kirkwood, J. Chem. Phys. **18**, 817 (1950).
[2] J. R. Ray and A. Rahman, J. Chem. Phys. **80**, 4424 (1984).
[3] J. F. Lutsko, J. Appl. Phys. **64**, 1152 (1988).
[4] D. Lips and P. Maass, preprint.

DY 26.4 Tue 18:15 P3

Impact of heterogeneities in power generation and transmission line admittances on power grid stability — •Matthias Wolff, Pedro Lind, and Philipp Maass — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück, Germany

In theoretical studies, power grids are often investigated assuming topological simplifications, namely neglecting the heterogeneous features of transmission lines and generators. These grid heterogeneities, however, play an important role and need to be taken into account to predict critical states for failure. We analyze their impact on the grid stability based on the dynamical equations for the voltage phase angles and frequencies in the synchronous machine model [1], which we apply to an IEEE test grid. It is shown that disregarding heterogeneities can lead to biased estimates of the grid stability [2]. This conclusion is drawn by comparing the stability of the heterogeneous IEEE test grid with a partially and fully homogenized version of this network.

[1] T. Nishikawa and A. E. Motter, New J. Phys. 17, 015012 (2015).
[2] M. Wolff, P. Lind and P. Maass, preprint.

DY 26.5 Tue 18:15 P3

Machine learning quantum phases of matter beyond the fermion sign problem — •Peter Broecker[1], Simon Trebst[1], Juan Carrasquilla[2], and Roger Melko[2,3] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada — [3]Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada

Many-fermion systems exhibit some of the most intriguing physical phenomena in condensed matter physics such as the formation of non-Fermi liquids, superconductivity, or Mott insulators with fractionalized excitations. Exact analytical methods for the study of such fascinating phenomena are scarce and numerical tools are called for. However, one of the most powerful methods at our disposal - quantum Monte Carlo sampling - is often hampered by the fermion sign problem, which manifests itself most strikingly in the exponential growth of statistical errors and thus an exponential slowdown of the sampling. Here, we present the use of artificial neural networks as a powerful approach that is able to learn and distinguish quantum phases of matter despite the sign problem.

DY 26.6 Tue 18:15 P3

Nonequilibrium thermodynamics in the strong coupling and non-Markovian regime based on a redefined system-environment partition — •Philipp Strasberg — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany — Complex Systems and Statistical Mechanics, Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

I propose a method to study the thermodynamic behaviour of small systems beyond the weak coupling and Markovian approximation, which is different in spirit from conventional approaches. The idea is to redefine the system and environment such that the effective, redefined system is again coupled weakly to Markovian residual baths and thus, allows to derive a consistent thermodynamic framework for this new system-environment partition. Besides general conclusions, I will also present particular model systems demonstrating the feasibility of this approach.

DY 26.7 Tue 18:15 P3

Apparent Entropy Production in Networks with Hidden Degrees of Freedom — •Matthias Uhl, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The fluctuation theorem for entropy production is a remarkable symmetry relation for the distribution of produced entropy that holds universally in non-equilibrium steady states of Markovian systems. However, in systems with degrees of freedom that are hidden from the observer, it is not possible to infer the amount of produced entropy exactly. Previous work [1] suggested that a relation similar to the fluctuation theorem may hold at least approximately for such systems if one considers the apparent entropy production. By extending the notion of apparent entropy production to discrete bipartite systems we investigate which criteria have to be met for such a modified fluctuation theorem to hold in the large deviation limit and how the deviations

from the regular fluctuation theorem can be used to infer information on the hidden degree of freedom.
[1] J. Mehl, B. Lander, C. Bechinger, and U. Seifert, Phys. Rev. Lett. **108**, 220601 (2012)

DY 26.8 Tue 18:15 P3

Dissipationless precision by counting the time spent in a state — •Somrita Ray and Andre C Barato — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany.

We analyze the relation between precision and dissipation for a random variable that is the time a stochastic trajectory spends in a state. We find that for this random variable, precision can be obtained with an arbitrarily low energetic cost. This result is in contrast with the thermodynamic uncertainty relation for the currents, which establishes a minimal energetic cost for precision in a current like random variable. On the technical side, we obtain a general analytic expression for the dispersion of the time that a stochastic trajectory spends in a cluster of states for a unicyclic network.

DY 26.9 Tue 18:15 P3

Work and Power in the Strong Coupling Regime — Martí Perarnau-Llobet[1,3], •Henrik Wilming[2], Arnau Riera[3], Rodrigo Gallego[2], and Jens Eisert[2] — [1]Max-Planck-Institut fur Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [3]Institut de Ciencies Fotoniques (ICFO), The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain

We combine recent results in thermodynamics and the theory of equilibration in closed quantum systems to discuss work extraction of a quantum thermal machine strongly coupled to a heat bath. Giving the corrections to the weak-coupling limit, in particular we show that a finite coupling strength necessarily leads to irreversibility due to built-up of correlations. We then discuss the power of such strongly coupled thermal machines, showing that optimal power is reached for intermediate coupling strengths where the work per cycle is not optimal. Finally we exemplify all our results in the Caldeira-Leggett model. To analyze power in this model we also present new results regarding equilibration times in the Caldeira-Leggett model which might be of independent interest.

DY 26.10 Tue 18:15 P3

On the Role of Latent Variables in Stochastic Thermodynamics — •Jannik Ehrich and Andreas Engel — Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Hidden variables play an important role for the entropy balance in stochastic thermodynamics. By constructing a general bipartite Markov chain we elaborate on several limiting cases including the setup of a sensor, a measurement-feedback-loop and a hidden Markov model. We derive and explain fluctuation theorems relevant to each of these setups. This view promises a unified approach for the understanding of the role of latent variables in stochastic thermodynamics.

DY 26.11 Tue 18:15 P3

Percolation transition of Fortuin-Kasteleyn clusters for the three-dimensional $\pm J$ random-bond-Ising model — •Hauke Fajen and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

We investigated the behavior of the Wolff algorithm for the $\pm J$ Random-Bond-Ising model on a three-dimensional lattice. We studied the percolation transition of the Fortuin-Kasteleyn clusters. Our motivation is that the Wolff algorithm works best when the percolation transition temperature T_p and the phase transition temperatureT_c coincide. Fortuin-Kasteleyn clusters are constructed be randomly drawing subsets of bonds from all satisfied bonds of a given spin configuration. Each satisfied bond is considered with a possibility of $1-e^{-2J/T}$. Therefore we studied the percolation temperature T_p as a function of the fraction p of antiferromagnetic ($-J$) bonds. To measure the percolation probability we used the Swendsen-Wang algorithm to construct the Fortuin-Kasteleyn clusters. It's already known that the Wolff algorithm doesn't work efficiently for $p = 0.5$. Our results show that $T_p > T_c$ for most values of p, only near $p = 0$ T_p is equal T_c. We also studied an effective cluster size near p_c (ferromagnet-spin-glass transition) in the spin-glass phase. Nevertheless, close to T_c the effective cluster sizes remain small, showing that the Wolff algorithm is not efficient for all values $p > p_c$.

DY 26.12 Tue 18:15 P3

Phase diagram and critical phase transitions of driven granular matter in quasi 2d — •Thomas Schindler and Sebastian Kapfer — Theorie 1, FAU Erlangen

Driven granular matter exhibits a rich variety of nonequilibrium phases [1,2]. Recently, a critical transition to a state with quadratic order has been reported, with several critical exponents measurable [3]. We study this set-up by computer simulations, which consists of spherical particles between two horizontal plates. The particles are agitated by vibrating the plates in vertical direction. The energy injection is balanced by energy loss through inelastic collisions of the granular particles. Thus, the system reaches a steady state which exhibits phase behavior similar to equilibrium systems. The gap between the plates is about two particle diameters allowing the particles to form - besides fluid-like states - hexagonal and quadratic bilayers. We determine the relevant parameters for formation of ordered states, present a numerical phase diagram for this system, and study phase coexistence and criticality.
[1] Melby et al, J.Phys. Condens. Matter **17**, S2689 (2005)
[2] Reyes and Urbach, Phys. Rev. E **78**, 051301 (2008)
[3] Castillo et al, Phys. Rev. Lett. **109**, 095701 (2012)

DY 26.13 Tue 18:15 P3

A Linear Programming Approach to Graph-Coloring — •Daniel Grujic and Alexander K. Hartmann — Institut of Physics, University of Oldenburg

We study phase transitions in the combinatorial optimimization problem [1] in particular Graph-Coloring for Erdős-Rényi random graphs with N nodes and M edges. Graph coloring is an assignment of q colors to vertices in a way that no two adjacent vertices share the same color. To find such a solution we use the simplex algorithm known from linear programming (LP). Similiar studies were performed previously for other NP-hard problems like the Vertex-Cover problem [2] and the Travelling-Salesman problem [3]. We use a LP relaxation, which can lead to incomplete solutions where a node has multiple colors. We find that the LP is able to find complete solutions for small connectivities $c = \frac{2M}{N}$ which means the problem is "easy" there. At the critical connectivity c_{crit} a phase transition occurs. Beyond the critical point we find incomplete solutions with high probability. We try different methods to eliminate such incomplete solutions such as different types of *cutting planes*. We also try a pseudo-optimization, where we assign specific colors to specific nodes in advance and let the LP try to retain the colors. Both approaches lead to different critical thresholds c_{crit}.
[1] A. K. Hartmann, M. Weight, *Phase Transitions in Combinatorial Optimization Problems*, Wiley-VCH, Weinheim (2005)
[2] T. Dewenter, A. K. Hartmann, Phys. Rev. E **86**, 041128 (2012)
[3] Hendrik Schawe, Alexander K. Hartmann, EPL **113**, 30004 (2016)

DY 26.14 Tue 18:15 P3

Multifractal finite-size scaling at the Anderson transition in the unitary symmetry class — Jakob Lindinger, Andreas Buchleitner, and •Alberto Rodríguez — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We carry out a full characterisation of the Anderson transition in the unitary symmetry class. We apply multifractal finite-size scaling [A. Rodriguez, L. J. Vasquez, K. Slevin, R. A. Römer, Phys. Rev. B 84, 134209 (2011)] to the 3-D Anderson model subjected to a random magnetic field, and estimate the critical parameters as well as the multifractal exponents with high precision using wavefunction data of systems up to $L^3 = 150^3$. We also examine the scaling of the probability density function and the spatial correlations of the wavefunctions intensities as the system undergoes the transition.

DY 26.15 Tue 18:15 P3

Characterisation of the superfluid to Mott insulator transition from multifractal fluctuations in Hilbert space — •Jakob Lindinger, Andreas Buchleitner, and Alberto Rodríguez — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Recent theoretical work has revealed multifractality in Hilbert space as a generic feature of certain many-body systems even in the absence of disorder. The study of multifractal fluctuations in Fock space is particularly significant in the context of many-body localisation and

Anderson localisation in random graphs, where the potential existence of an extensive non-ergodic multifractal phase is currently under an intense debate which has led to a controversy. Inspired by these results, we explore the possibility of identifying fingerprints of the superfluid to Mott insulator transition in the fluctuations of the many-body wavefunction in Hilbert space. We present preliminary numerical and analytical results obtained for the Bose-Hubbard model.

DY 26.16 Tue 18:15 P3

Analysis of bifurcations in stochastic biological networks with few nodes — •Marc Mendler, Johannes Falk, and Barbara Drossel — Technische Universität Darmstadt, Institut für Festkörperphysik

We investigate how intrinsic noise, which is due to small molecule numbers, influences the occurrence, position and critical parameter values of saddle-node and hopf bifurcations in reaction networks with few nodes.

In recent years new experimental techniques have enabled researchers to observe and analyse biological systems at the single cell level. At those scales intrinsic noise can play a significant role and alter the system's behaviour. In order to describe such systems correctly, one has to utilize stochastic methods.

Based on the Fokker Planck equation we investigate how the number and position of local maxima of the stationary distribution changes and relates to the position of fixed points and bifurcations in the deterministic description. We apply these methods to stochastic saddle-node and hopf bifurcations. Using simple example systems, we also compare our analytical results with numerical simulations.