DY 15: Statistical Physics - general

Time: Tuesday 9:30–12:30 Location: BH-N 334

DY 15.1 Tue 9:30 BH-N 334

Extracting Canonical Information from Grand Potential Density Functional Theory — •Daniel de las Heras and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Studying averaged quantities that compress the full many-body information into digestible, analyzable and experimentally measurable quantities lies at the core of essentially all condensed matter physics. Moreover, suitable averaging often simplifies theoretical treatments. An example is the use of the grand canonical ensemble, which permits fluctuations in the total number of particles, in the formulation statistical mechanical liquid state theories. The structuring and self-assembly of real systems, however, can depend crucially on the precise number of particles in the system. In particular small systems, such as e.g. finite colloidal clusters, are better analyzed canonically, where the number of particles is fixed.

We present a general and formally exact method to obtain the canonical one-body density distribution and the canonical partition sums from direct decomposition of classical density functional results in the grand canonical ensemble [1]. The method is relevant for treating finite systems.

[1] D. de las Heras, and M. Schmidt. Accepted in Phys. Rev. Lett. (2014).

DY 15.2 Tue 9:45 BH-N 334

Canonical approach to equilibrium properties of interacting quantum gases — Quirin Hummel, Juan Diego Urbina, and •Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

It is generally accepted that the equilibrium properties of quantum gases give the same results for the canonical and grand canonical ensemble. For finite systems well below the thermodynamic limit, however, this equivalence breaks down. The total number of particles cannot be fixed within the grand canonical formalism where this quantity is subject to thermal and quantum fluctuations. This poses a serious problem, as most of the powerful techniques to deal with quantum and interaction effects in quantum gases are based on the grand canonical formalism.

In this contribution we present a purely canonical approach, with the specific intention to obtain virial-type expansions for finite systems of interacting identical particles, including the equation of state and (local and non-local) pair correlations. In our formalism the canonical partition function is given by a finite expansion in the inverse temperature, thus providing a closed explicit form for the quantum equation of state. We also discuss the thermodynamic limit and the effect of interactions and particle symmetry on the many-body spectra.

DY 15.3 Tue 10:00 BH-N 334

Calculating the density of states for materials with nested sampling — •Robert Baldock[1], Livia Bartók-Pártay[2], Albert Bartók-Pártay[3], Mike Payne[1], and Gábor Csányi[3] — [1]Department of Physics, University of Cambridge — [2]Department of Chemistry, University of Cambridge — [3]Department of Engineering, University of Cambridge

We present the developed nested sampling algorithm for calculating the density of states of materials. Having obtained the density of states, one can calculate the partition function and perform statistical mechanics in full. We demonstrate calculation of the complete pressure-temperature phase diagram for aluminium (using an EAM potential), and a binary Lennard-Jones "alloy" that exhibits an order-disorder transition.

Thermal distributions for virtually any structural quantity can be calculated from the output of Nested Sampling. Such distributions are obtained in seconds at any temperature.

DY 15.4 Tue 10:15 BH-N 334

Weak thermal contact is not universal for work extraction — •Henrik Wilming, Rodrigo Gallego, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The free energy difference to the equilibrium state limits the amount of work that can be extracted on average from a system out of thermal equilibrium. This bound can be saturated by protocols putting the system and a bath into weak thermal contact (WTC), i.e., bringing the system into a Gibbs state at the bath's temperature. Surprisingly, the same bound holds true when the contact to the heat bath is modelled by more general proccesses, which have the only restriction that when the system already is in equilibrium, it cannot be brought out of it. In that sense, WTC is universal for work extraction.

In this work, we introduce the study of work-extraction protocols under restrictions encountered in realistic devices at the nano-scale. We consider limitations on the maximum energies in the system and on the local structure of many-body Hamiltonians. Remarkably, we find that WTC then loses its universality: There is a gap between the work the can be extracted with WTC and with more general operations. Our work highlights the relevance of operational frameworks such as those of thermal operations and Gibbs preserving maps, as they can improve the performance of thermal machines, and provides a unifying framework of incorporating natural restrictions in quantum thermodynamics.

DY 15.5 Tue 10:30 BH-N 334

Ising model on two-dimensional unimodular Lattice Triangulations — •Tony Wasserka, Benedikt Krüger, and Klaus Mecke — Institut für Theoretische Physik, Staudtstr. 7, 91058 Erlangen

Unimodular triangulations of two-dimensional integer lattices can be used as real-space networks implementing certain amounts of order or disorder. We couple the well-known Ising model (which is a common prototype model for phase transitions and can be solved analytical for regular lattices) with such lattice triangulations so that nearest neighbours are defined by the edges of the triangulation. Using this setup the critical temperature and critical exponents can be measured numerically using Monte-Carlo-simulations. Introducing an order parameter for triangulations and interpreting it as an energy we determine microcanonical and canonical averages and therewith the order-dependency of these critical observables.

DY 15.6 Tue 10:45 BH-N 334

Corrections to finite–size scaling in the φ^4 model on square lattices — •Jevgenijs Kaupuzs — University of Latvia, LV-1459 Riga, Latvia

Corrections to scaling in the two–dimensional scalar φ^4 model are studied based on non–perturbative analytical arguments and Monte Carlo (MC) simulation data for different lattice sizes L ($4 \le L \le 1536$) and different values of the φ^4 coupling constant λ, i. e., $\lambda = 0.1, 1, 10$. According to our analysis, amplitudes of the nontrivial correction terms with the correction–to–scaling exponents $\omega_\ell < 1$ become small when approaching the Ising limit ($\lambda \to \infty$), but such corrections generally exist in the 2D φ^4 model. Analytical arguments show the existence of corrections with the exponent 3/4. The numerical analysis suggests that there exists also a correction with the exponent 1/2, which is detectable at $\lambda = 0.1$. The numerical tests clearly show that the structure of corrections to scaling in the 2D φ^4 model differs from the usually expected one in the 2D Ising model.

15 min. break

DY 15.7 Tue 11:15 BH-N 334

Multiply charged monopoles in cubic dimer model — •Sreejith Ganesh Jaya[1] and Stephen Powell[2] — [1]MPI PKS, Dresden, Germany — [2]University of Nottingham, UK

The classical cubic dimer model is a 3 dimensional statistical mechanical system whose degrees of freedom are dimers that occupy the edges between nearest neighbour vertices of a cubic lattice. Dimer occupancies are subject to the local constraint that every lattice point is associated with exactly one dimer. In the presence of an aligning interaction, it is known that the system exhibits an unconventional continuous thermal phase transition from a symmetry broken columnar phase to a Coulomb-phase. The transition is in the NCCP1 universality class, which also describes the Neel-VBS transition in the JQ model and the S=1/2 Heisenberg model with suppression of hedgehog defects. Using Monte-Carlo simulations of a pair of defects in a background of fluctuating dimers, we calculate the scaling exponents

for fugacities of monopole defects of charge Q=2 and 3 in this critical point. Our estimates suggest that Q=3 monopoles are relevant and could therefore drive the JQ model away from the NCCP1 critical point on a hexagonal lattice.

DY 15.8 Tue 11:30 BH-N 334

Critical adsorption and Casimir forces in systems with a globally constrained order parameter — •Markus Gross[1,2], Oleg Vasilyev[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Institut für Theoretische Physik IV, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Typically, critical phenomena are investigated in the grand canonical ensemble, in which the order parameter is free to fluctuate without constraints. However, confining systems with a locally conserved order parameter – such as fluids in a closed environment – imposes a global constraint on the order parameter and thereby changes its fluctuation spectrum. This situation is naturally encountered in particle- or hydrodynamics-based simulations, such as Molecular Dynamics or Lattice Boltzmann methods. Here, we explore the consequences of the global order-parameter conservation on critical adsorption at walls and critical Casimir forces in a fluid film. Analytical calculations have been performed within mean-field theory as well as statistical field theory of a Ginzburg-Landau model. These results are confronted with Monte-Carlo simulations of the Ising model. Depending on the boundary conditions, the constraint is found to induce significant changes in the shape of the order-parameter profile of the adsorbed fluid. For instance, within mean field theory the divergence of the order parameter at the wall is cut-off. For certain boundary conditions, the Casimir force experienced by the critical film can have a drastically different temperature dependence as a consequence of the constraint.

DY 15.9 Tue 11:45 BH-N 334

Equilibrium of a mesoscopic system in a damping induced inhomogeneous space — •Arijit Bhattacharyay — Indian Institute of Science Education and Research, Pune, India

Complex molecules like proteins, colloids etc can often have conformation dependent damping due to varied proximity of its constituents from each other at different conformational states. The dynamics of such systems in the conformation space, when in equilibrium with a homogeneous heat bath, is generally considered to be a stochastic dynamics with multiplicative noise. The origin of the multiplicative noise is related to the inhomogeneity of the conformation space caused by damping on top of which there can exist inhomogeneity of space caused by a conservative force field as usual. I would argue that, the equilibrium distribution of such systems has to be of a modified Maxwell-Boltzmann form resulting from a stochastic dynamics with additive noise. In this approach, putting the stochastic problem to an additive noise form would be the prerequisite for equilibrium. The results at the limit of constant damping would be recovered.

DY 15.10 Tue 12:00 BH-N 334

Electrical charging effects on sliding lubrication properties of a model confined ionic liquid — •Rosario Capozza[1], Andrea Benassi[2], Andrea Vanossi[3,1], and Erio Tosatti[1,4] — [1]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [2]Empa, Materials Science and Technology, Uberlandstrasse 129, 8600 Dubendorf, Switzerland — [3]CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy — [4]International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34014 Trieste, Italy

Ionic liquids lubricants, used under conditions of nanometric confinement between parallel plates or tip-surface gaps, explore the dependence of friction upon charging, suggestive of some electrical control of friction. Using a simple ionic liquid model, we first study by molecular dynamics the friction between parallel plates under conditions of successive layering reached by squeezout under an increasing inter-plate force. We then simulate the frictional changes brought about by different charging states of the plates, related to charging-induced switches corresponding to squeezout (or suck-in) transitions between different layering states as predicted by local minima in the charge-dependent enthalpy curves. Although the actual frictional behavior obtained does depend upon the assumed features and parameters of the model liquid and its interaction with the plates, the broader scenario obtained for charging effects, its relationship to the equilibrium layering and its enthalpy characterization appear of general value.

DY 15.11 Tue 12:15 BH-N 334

Towards a General Theory of Extremes for Observables of Chaotic Dynamical Systems — •Valerio Lucarini — Institute of Meteorology, University of Hamburg, Hamburg, Germany — Department of Mathematics and Statistics, University of Reading, Reading, UK

In this paper we provide a connection between the geometrical properties of a chaotic dynamical system and the distribution of extreme values. We show that the extremes of so-called physical observables are distributed according to the classical generalised Pareto distribution and derive explicit expressions for the scaling and the shape parameter. In particular, we derive that the shape parameter does not depend on the chosen observables, but only on the partial dimensions of the invariant measure on the stable, unstable, and neutral manifolds. The shape parameter is negative and is close to zero when high-dimensional systems are considered. This result agrees with what was derived recently using the generalized extreme value approach. Combining the results obtained using such physical observables and the properties of the extremes of distance observables, it is possible to derive estimates of the partial dimensions of the attractor along the stable and the unstable directions of the flow. Moreover, by writing the shape parameter in terms of moments of the extremes of the considered observable and by using linear response theory, we relate the sensitivity to perturbations of the shape parameter to the sensitivity of the moments, of the partial dimensions, and of the Kaplan-Yorke dimension of the attractor.