DY 1: Statistical Physics (general) I

Time: Monday 10:15–13:00 Location: H47

DY 1.1 Mon 10:15 H47

Magnetic Anisotropy due to the Casimir Effect — •Georgo Metalidis[1] and Patrick Bruno[2] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

We show that the Casimir interaction between a ferromagnetic and a non-magnetic mirror gives rise to a magnetic anisotropy in the ferromagnetic layer. The anisotropy is out-of-plane for an optically isotropic non-magnetic plate. If the non-magnetic plate has a uniaxial optical anisotropy (with optical axis in the plate plane), we find an in-plane magnetic anisotropy. In both cases, the magnetization orientation with the lowest energy is given by the competition between polar, longitudinal and transverse contributions to the magneto-optical Kerr effect, and will depend on the interplate distance. Results for a magnetic plate made out of iron, and non-magnetic plates of gold (optically isotropic), quartz, calcite and barium titanate (all uniaxially birefringent) are presented.

DY 1.2 Mon 10:30 H47

Calculating statistical field theories beyond the mean-field level by employing self-interaction renormalized actions — •Stephan Baeurle[1], Garii Efimov[2], and Evgenij Nogovitsin[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätstr. 31, 93053 Regensburg, Germany — [2]Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia — [3]Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russia

Mean-field theories are widely used as comparative theoretical tools throughout all areas of natural and engineering sciences. They are capable in many instances to deliver useful insights in properties and behavior of multi-body systems at relatively moderate computational costs. However, there are a multitude of cases where the mean-field approach provides either inaccurate or even qualitatively wrong results. In this presentation we introduce a new beyond mean field calculation approach based on an alternative exact formulation of the partition function integral, which relies on the method of Gaussian equivalent representation GER originally developed in quantum field theory. With this new approach, we remove divergent contributions from the action, related to particle self-interaction, by employing the concept of normal product in conjunction with Cauchy's integral theorem. We show that the related thermodynamic and structural quantities possess better approximation characteristics and statistical convergence properties in Monte-Carlo sampling, than the ones derived from the original field-theoretic formulation of the partition function integral.

DY 1.3 Mon 10:45 H47

Fast Converging Path Integrals for Time-Dependent Potentials — •Antun Balaž[1], Ivana Vidanović[1], Aleksandar Bogojević[1], and Axel Pelster[2,3] — [1]Scientific Computing Laboratory, Institute of Physics Belgrade, Belgrade, Serbia — [2]Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany — [3]Universität Potsdam, Campus Golm, Potsdam-Golm, Germany

We calculate the short-time expansion of the propagator for a general many-body quantum system in a time-dependent potential to orders that have not been accessible before, thus extending a previously developed approach for time-independent potentials [1]. To this end the propagator is expressed in terms of a discretized effective potential, for which we derive and analytically solve a set of recursion relations [2]. Such a discretized effective potential can be used to substantially speed up numerical Monte Carlo simulations for path integrals, or to set-up various analytic approximation techniques to study dynamic properties of quantum systems in time-dependent potentials. The analytically derived results are numerically verified by treating several simple one-dimensional models.

[1] A. Balaž, A. Bogojević, I. Vidanović, A. Pelster, Phys. Rev. E **79**, 036701 (2009)
[2] A. Balaž, I. Vidanović, A. Bogojević, A. Pelster, arXiv:0912.2743

DY 1.4 Mon 11:00 H47

Quantum master equations in phase space applied to the Brownian motion in a periodic potential: comparison of various kinetic models for Wigner's function — Liam Cleary[1], •William T. Coffey[1], William J. Dowling[1], Yuri P. Kalmykov[2], and Serguey V. Titov[3] — [1]Trinity College Dublin, Ireland — [2]Université de Perpignan, France — [3]Russian Academy of Sciences, Russia

A comparison of the master equations for the time evolution of the Wigner distribution function $W(x,p,t)$ in phase space (x,p) for various quantum kinetic models of dissipation is presented by considering the quantum Brownian motion of a particle in a cosine periodic potential $V(x) = -V_0\cos(x/x_0)$. The dynamic structure factor, averaged spectrum of the structure factor and escape rate are evaluated for each model via matrix continued fractions in the manner customarily used for the classical Fokker-Planck equation. The escape rates so yielded are compared with that given analytically by the quantum-mechanical reaction rate solution of the Kramers turnover problem.

DY 1.5 Mon 11:15 H47

Quantum–induced symmetry breaking explains infrared spectra of CH_5^+ isotopologues — •Alexander Witt, Sergei D. Ivanov, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

Protonated methane, CH_5^+, has been investigated intensively using a host of different experimental and theoretical techniques since decades, see Ref. [1] for a review. The challenge to theory arises from its shallow potential energy surface which leads to dynamical equivalence of the hydrogen atoms often referred to as "scrambling". It has been shown that this is driven by quantum fluctuation effects of the nuclei [2].
Ab initio MD in combination with techniques based on Feynman's formulation of quantum statistical mechanics in terms of path integrals allows us to fully reproduce the experimental IR spectra of all isotopologues of CH_5^+. Moreover, an analysis technique developed in–house enables full assignment of spectral features to molecular motions.
[1] P. Kumar P. and D. Marx, Phys. Chem. Chem. Phys. **8**, 573 (2006)
[2] D. Marx and M. Parrinello, Nature **375**, 216 (1995)

DY 1.6 Mon 11:30 H47

Shape Dependent Partition Sums of Bounded Systems — •Anatoly Danilevich and Klaus Mecke — Institut für Theoretische Physik Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

We consider classical many-particle systems bounded by an arbitrarily shaped convex container $\mathcal{D} \subset \mathbb{R}^d$. In the asymptotic limit $\mathcal{D} \to \mathbb{R}^d$ thermodynamic potentials are expected to be extensive, meaning to be a linear combination of $d+1$ Minkowski functionals $M_i(\mathcal{D})$ (e.g. the volume, the surface area, etc.) and correction terms which decrease exponentially with the size of $\mathcal{D}$ [1]. This conjecture has been tested analytically for Ising models and for a cluster expansion of a continuous fluid model in the grandcanonical ensemble.

[1] P. König, R. Roth and K. Mecke, Phys. Rev. Lett. **93**, 160601 (2004).

DY 1.7 Mon 11:45 H47

Tensorial Minkowski Functionals as Shape Measures for Experimental Data — •Sebastian Kapfer, Klaus Mecke, and Gerd E. Schröder-Turk — Friedrich-Alexander-Universität, Erlangen, Germany

In order to establish structure–function relationships for cellular and inhomogeneous materials, quantitative and robust 'shape measures' are required that succinctly characterise the geometry of the material. In particular, if the quantities of interest are direction-dependent, tensor-valued shape measures are essential. We demonstrate that Minkowski Tensors characterise the anisotropy of disordered media in a robust way. We show that Minkowski tensors can be directly applied to experimental datasets. This is illustrated specifically for microscopy and tomography images.

Minkowski Tensors, also offering a firm mathematical foundation, consequently are promising candidates for shape measures.

For details see also: Schroeder-Turk et al., Journal of Microscopy 2009.

DY 1.8 Mon 12:00 H47

Foundation of Statistical Mechanics under experimentally realistic conditions — •Peter Reimann — Fakultät für Physik, Universität Bielefeld

We demonstrate the equilibration of isolated macroscopic quantum systems, prepared in non-equilibrium mixed states with significant population of many energy levels, and observed by instruments with a reasonably bound working range compared to the resolution limit. Both properties are fulfilled under many, if not all, experimentally realistic conditions. At equilibrium, the predictions and limitations of Statistical Mechanics are recovered. Finally, the imitation of statistical ensembles by pure (zero entropy) states is discussed [1].

[1] P. Reimann, Phys. Rev. Lett. 101, 190403 (2008); 99, 160404 (2007)

DY 1.9 Mon 12:15 H47

Performance potential for simulating spin models on GPU — •Martin Weigel — Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz

Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses. In this contribution I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards-Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis and cluster updates, as well as computional tricks such as multi-spin coding are taken into account.

DY 1.10 Mon 12:30 H47

Performance optimization of a thermoelectric generator with linear material profiles in a 1D setup — •Knud Zabrocki[1], Eckhard Müller[1], Wolfgang Seifert[2], and Steffen Trimper[2] — [1]Institute of Materials Research, German Aerospace Center (DLR), D-51170 Köln, Germany — [2]Martin Luther University Halle-Wittenberg, D-06099 Halle (Saale), Germany

Graded and segmented thermoelectric elements have been studied for a long time with the aim of improving the performance of thermogenerators that are exposed to a large temperature difference. The global optimization of a performance parameter is commonly based on a one-dimensional continua-theoretical model. Following the proposal by Müller et al., the temperature profile $T(x)$ can be calculated within a model-free setup directly from the 1D thermal energy balance, e. g. based on an independent and free variability of the material parameters the Seebeck coefficient, the electrical and thermal conductivities, $S(x), \sigma(x)$ and $\kappa(x)$ is assumed primarily. Thus the optimum current density can be determined from the maximum of the global performance parameter. Here, an analytical solution of the 1D thermal energy balance has been found for constant gradients based on Bessel functions. For particular cases of linear material profiles the authors present results for the optimization of performance parameters like the electrical power output P_{el} and the efficiency η of a thermogenerator (TEG). These results are compared with another analytical model, the constant property model (CPM) and a suitable reference for the performance is discussed.

DY 1.11 Mon 12:45 H47

Multi-GPU Accelerated Monte Carlo Simulations of the 2D Ising Model — •Benjamin Block, Peter Virnau, and Tobias Preis — Institut für Physik, Universität Mainz, Deutschland

A modern graphics processing unit (GPU) is able to perform massively parallel scientific computations at low cost. We present an implementation of the checkerboard algorithm for the two dimensional Ising model which utilizes multiple GPUs—as provided by next generation supercomputers. By combining CUDA (compute unified device architecture) with MPI (message parsing interface) on the CPU level we overcome the memory limitations of the single GPU which enables us to simulate significantly larger systems. On our test setup we were able to accelerate calculations up to 350-fold on 4 GPUs—in comparison to a single CPU core implementation. As proof of concept we reproduce the critical temperature of the 2D Ising model using finite size scaling techniques.