DY 6: Poster Session I

Time: Monday 16:00–18:00 Location: Poster B2

DY 6.1 Mon 16:00 Poster B2

Statistics of distinguishable particles and resolution of the Gibbs paradox of the first kind — •Hjalmar Peters — Universität Karlsruhe

In physics, there are two distinct paradoxes, which are both known under the name of "Gibbs paradox". In the following, the spurious increase in entropy when combining two gases of the same kind will be referred to as the Gibbs paradox of the first kind (GP1). The GP1 only arises if the gases consist of distinguishable particles. The analysis of the GP1 shows that, for systems of distinguishable particles, it is generally uncertain of which particles they consist. For the statistical description of a system of distinguishable particles, an underlying set of particles, containing all particles that in principle qualify for being part of the system, is assumed to be known. Of which elements of this underlying particle set the system is composed, differs from microstate to microstate. The uncertainty about the particle composition contributes to the entropy of the system. Systems for which admissible compositions with equal particle number are equiprobable will be called *harmonic*. Harmonic systems with the same underlying particle set are always correlated; hence, for harmonic systems, the entropy is no longer additive and loses its thermodynamic meaning. A quantity derived from entropy is introduced, the *reduced entropy*, which, for harmonic systems, replaces the entropy as thermodynamic potential. It can be shown that distinguishable and indistinguishable identical classical particles are physically equivalent. The resolution of the GP1 is demonstrated applying the previously found results.

DY 6.2 Mon 16:00 Poster B2

Cutting the Energy Range in Multicanonical Monte Carlo Simulations — •Steffen Karalus[1,2], Wolfhard Janke[1], and Michael Bachmann[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Soft Matter Systems Research Group, Institut für Festkörperforschung (IFF-2), Forschungszentrum Jülich, Germany

For a bead-and-spring polymer model, we investigate the dependence of several observables on the energy boundaries in a multicanonical Monte Carlo simulation. As expected, the results of the reweighting of statistical quantities to a certain temperature deviate seriously if a substantial part of the corresponding energy distribution lies outside the predefined energy range. However, structural quantities like the end-to-end distance are less affected than the energy itself.

DY 6.3 Mon 16:00 Poster B2

From an atomistic to a path integral representation of molecules in adaptive simulation — •Adolfo Poma and Luigi Delle Site — Max Planck Institute for Polymer Research, Ackermannweg 10, D - 55128 Mainz , Germany

We present a method to carry out an adaptive representation from a classical to a quantum description of molecules. This method captures the delocalization of particles from its quantum contribution, which mainly affects the static properties in liquids. This approach is tested on a model system of tetrahedral molecules. A coarse grained (CG) procedure was used to reduce the number of degrees of freedom from a path integral representation (QM) to one effective CG site. Our method maintains the thermodynamic equilibrium among the two description allowing the change of representation on the fly. Our studies will address the possibility of studying the process of bond breaking in soft matter systems.

DY 6.4 Mon 16:00 Poster B2

Quantum corrections in the strong friction limit: Perturbation theory and applications — •Stefan A. Maier and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The strong friction regime at low temperatures is analyzed systematically starting from the formally exact path integral expression for the reduced dynamics. This quantum Smoluchowski regime allows for a type of semiclassical treatment in the inverse friction strength so that higher order quantum corrections to the original quantum Smoluchowski equation [PRL **87**, 086802 (2001), PRL **101**, 11903 (2008)] can be derived. Drift and diffusion coefficients are determined by the equilibrium distribution in position and are directly related to the corresponding action of extremal paths and fluctuations around them. The inclusion of higher order corrections reproduces the quantum enhancement above crossover for the decay rate out of a metastable well exactly. Our results are also applied to study transport in quantum ratchets.

DY 6.5 Mon 16:00 Poster B2

Coupling different levels of resolution in molecular dynamics. — •Simon Poblete, Matej Praprotnik, Kurt Kremer, and Luigi Delle Site — Max-Planck-Institut fuer Polymerforschung, Mainz, Germany.

Simulation schemes that allow to change molecular representation in a subvolume of the simulation box while preserving the equilibrium with the surrounding introduce conceptual problems of thermodynamic consistency. In this work we present a general scheme based on thermodynamic arguments which ensures thermodynamic equilibrium among the molecules of different representation. The robustness of the algorithm is tested for two examples, namely an adaptive resolution simulation, atomistic/coarse-grained, for a liquid of tetrahedral molecules and an adaptive resolution simulation of a binary mixture of tetrahedral molecules and spherical solutes.

DY 6.6 Mon 16:00 Poster B2

Shape and Pinching-Off of Dew Droplets — •Johannes Blaschke, Tobias Lapp, Björn Hof, and Jürgen Vollmer — MPI for Dynamics & Self-Organization, 37073 Göttingen, Germany

For sessile droplets of a circular cap shape Family and Meakin have shown that the size distribution of dew droplets on flat surfaces is described by a scaling law [1]. In the case of water droplets hanging from a substrate the scaling ansatz has to be augmented to account for shape distortion by gravity and droplets dripping off.

The distorted 3-dimensional profile, $h(r)$, for such stationary hanging droplets is determined by minimizing the total energy functional (for rotationally-symmetric droplets) [2]:

$$E[h(r)] = \pi \int_0^R r \left(2\sigma \sqrt{1 + h'(r)^2} - \rho g\, h(r)^2 \right) \mathrm{d}r$$

We explore the effect of gravity on the relationship of volume, $V(R) = 2\pi \int_0^R rh(r)\,\mathrm{d}r$, to radius of the wetted area on the substrate, R, and how this is dependent on the contact angle.

An analysis of the energetic stability of these droplet profiles yields the maximum size of the droplets before they are ripped off the substrate by gravity. In order to verify the model, real droplets of a known volume are hung off a substrate and their profiles are compared to the theoretical predictions. Finally, the implications on Family and Meakin's scaling theory are discussed.

[1] F. Family, P. Meakin, Phys. Rev. A **40**, 3836 (1989)
[2] H. C. Wente, Pacific J. Math. **88**, 421 (1980)

DY 6.7 Mon 16:00 Poster B2

Monte Carlo simulations without detailed balance — •Heitor Fernandes, Martin Weigel, and Tanja Schilling — Institut für Physik, Johannes-Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Monte Carlo simulations are used to study simple systems where the underlying Markov chain satisfies the necessary condition of global balance but does not obey the more restrictive condition of detailed balance. These non-reversible Markov chains generate correct stationary distributions and have been used for a long time with the aim of decreasing autocorrelation times between consecutive measurements in sequential updates for spins systems and, e.g., for the checkerboard decomposition used in parallel architectures.

The aim of this work is to explore schemes where non-reversible dynamics is present. Our approach is based on splitting the dynamics into a set of replicas, where each of them represents a biased movement in reaction-coordinate space. This introduction of an additional bias in a given replica is compensated for by choosing an appropriate dynamics on the other replicas such as to ensure the validity of global balance.

We start by applying this method to a mean field Ising model, splitting the system into two replicas: one trying to increase magnetization and the other trying to decrease it. For this simple test system, our results show that the altered dynamics is able to reduce the dynam-

ical critical exponent, in agreement with results from Turitsyn et al. (arXiv:0809.0916). Generalizations of this scheme to 2D-Potts models using canonical and multicanonical ensembles are discussed.

DY 6.8 Mon 16:00 Poster B2

Domain walls and optimal droplets in the SOS model — •Karsten Schwarz and Heiko Rieger — Theoretische Physik, Universität des Saarlandes

Domain walls, optimal droplets and disorder chaos at zero temperature are studied numerically for the solid-on-solid model on a random substrate. The ensemble of random curves represented by the domain walls obeys Schramm's left passage formula with $\kappa = 4$ (or $\kappa \approx 3$ for two ends not fixed) whereas their fractal dimension is $d_s = 1.25$, and therefore their behaviour can't be described by a Schramm-Loewner evolution. We also investigated optimal droplets with a lateral size between L and $2L$ and detected the same fractal dimension as we found for the domain walls above. But the energy for these low excited states saturates at a value of $\mathcal{O}(1)$ for $L \to \infty$. So arbitrarily large excitations exist which cost only a small amount of energy.

DY 6.9 Mon 16:00 Poster B2

Spin dynamics: quantum master equation in phase space for a spin in a uniform external field — •Bernard P.J. Mulligan[1], William T. Coffey[2], Yuri P. Kalmykov[3], and Serguey V. Titov[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Trinity College Dublin, Ireland — [3]Universite de Perpignan, France — [4]Russian Academy of Sciences, Russia

The dynamics of a quantum spin in an external field is presented in the representation (phase) space of polar and azimuthal angles via a master equation for the quasiprobability distribution of spin orientations, allowing the averages of quantum mechanical spin operators to be calculated just as the classical case from the Weyl Symbol of the operator. The phase space master equation has essentially the same form as the classical Fokker-Planck equation, allowing existing solution methods (matrix continued fractions, integral relaxation times, etc.) to be used.

DY 6.10 Mon 16:00 Poster B2

Entropy of lattice triangulations — •Johannes Reinhard and Klaus Mecke — Institut für theoretische Physik Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Unimodular triangulations of a rectangular planar grid of size $m \times n$ are an important tool in computational geometry and statistical physics. They have an extensive entropy in the macroscopic limit, i.e. the number of possible triangulations scales as $e^{s_0 mn}$. We define an energy functional with a known ground-state degeneracy and calculate the number of triangulations using a multicanonical sampling Monte Carlo algorithm. We test the results against the exact number of triangulations, which is known for systems smaller than 6×7. Bulk and surface terms are determined for the entropy.

Our scheme can be generalized and applied for solving approximately a multitude of combinatorial problems. As a by-product we obtain the distributions of edge-lengths and vertex-degrees in random lattice triangulations.

DY 6.11 Mon 16:00 Poster B2

Investigation of a highly frustrated point packing problem — •Andre Müller, Sebiha Sahin, Michael Kwasnicki, Frederic Stein, Tobias Preis, Elmar Schömer, and Johannes J. Schneider — Center for Computational Research Methods in Natural Sciences, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We consider a highly frustrated point packing problem. The task of this problem is to place a proposed number of points on the nodes of a square lattice in the way that the radius of the circumcircle around the points is minimized and that each Euclidean distance value between each pair of points only occurs once. We show that this latter constraint leads to a large frustration effect by comparison with the corresponding unfrustrated system. We solve this problem by using simulated annealing, study the dynamics of the cooling process, and demonstrate that this problem exhibits interesting features, including scaling laws, e.g., for the radius of the circumcircle.

DY 6.12 Mon 16:00 Poster B2

Investigation of the kissing number problem — •Sebiha Sahin, Andre Müller, Elmar Schömer, and Johannes J. Schneider — Center for Computational Research Methods in Natural Sciences, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We consider a problem which originates in its current form from a famous dispute between Sir Isaac Newton and the Scottish mathematician David Gregory in the year 1694. The question was how many equal spheres can touch a sphere of the same radius in their midst, without any overlaps. Newton correctly thought that the limit was 12; Gregory thought that a 13th could fit. The proof that Newton was correct was provided by Schütte and van der Waerden in 1953. Only for a few higher dimensions, the value of this kissing number is exactly known. Mostly, only lower and upper bounds to the kissing number can be estimated. We propose a heuristic optimization approach to this problem in higher dimensions and study the dynamics of the optimization process.

DY 6.13 Mon 16:00 Poster B2

Morphometric Relationship for Thermodynamic Properties of Confined Hard Sphere Fluids — Stefan Kuczera, •Klaus Mecke, and Gerd Schröder-Turk — Institut für Theoretische Physik 1, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Thermodynamical properties of confined fluids depend on the shape of the confining cavity. König *et al.* have shown by density functional theory that for hard-sphere fluid and for simple pore shapes this dependence is expressed as a simple linear combination of four terms, namely the volume of the cavity, its interfacial area and integrated mean curvature and its Euler characteristic [1]. We extend this work by studying the equilibrium fluid density in cavities of complex shape by grand-canonical Monte Carlo simulation. The confining cavities are given by the periodic labyrinthine domains bounded by so-called triply-periodic minimal or constant mean curvature surfaces. The complexity of these cavity shapes is (a) the negative Gaussian curvature of the pore-solid interface and (b) their labyrinthine character with finite domain thicknesses. We numerically determine the boundary terms of thermodynamic quantities and compare them with analytic results.

[1] P.-M. König, R. Roth, and K. Mecke, Morphological thermodynamics of fluids: shape dependence of free energies, Phys. Rev. Lett. 93, 160601 (2004)

DY 6.14 Mon 16:00 Poster B2

Multithreading Monte Carlo simulations of polymer models — •Jonathan Gross[1], Wolfhard Janke[1], and Michael Bachmann[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Soft Matter Systems Research Group, Institut für Festkörperforschung (IFF-2), Forschungszentrum Jülich, 52425 Jülich, Germany

We discuss the advantages of parallelization by multithreading on multicore CPUs and GPUs for parallel tempering Monte Carlo computer simulations of an exemplified bead-spring model for homopolymers. Since the sampling of a large ensemble of conformations is a prerequisite for the precise estimation of statistical quantities such as typical indicators for conformational transitions like the peak structure of the specific heat, the advantage of a strong increase in performance in Monte Carlo simulations cannot be overestimated. Employing multithreading on standard multicore CPUs is a first step and utilizing the massive power of the large number of cores on graphics processing units (GPUs), available in modern but standard graphics cards, is a second one. We have compared both approaches and find a noticeable increase of efficiency when porting parts of the code to the GPU.

DY 6.15 Mon 16:00 Poster B2

Folding and unfolding of a triple-branch DNA hairpin molecule with four conformational states — •Sandra Engel[1], Anna Alemany[2,3], Nuria Forns[2,3], Philipp Maass[1], and Felix Ritort[2,3] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Departament de Física Fonamental, Universitat de Barcelona, Spain — [3]CIBER-BBN Networking center on Bioengineering, Biomaterials and Nanomedicine, Spain

Single-molecule experiments provide new insights into biological processes hitherto not accessible by measurements performed on bulk systems. Here we report on a study of the kinetics of a triple-branch hairpin molecule with four conformational states by pulling experiments with optical tweezers and theoretical modelling. Three distinct force rips associated with different transitions between the conformational states are observed in the folding and unfolding trajectories. By

applying transition rate theory to a free energy model of the molecule, probability distributions for the first rupture forces of the different transitions are calculated. Good agreement of the theoretical predictions with the experimental findings is achieved for various pulling speeds.

DY 6.16 Mon 16:00 Poster B2

Genome Folding at the 30 nm Scale — •Philipp M. Diesinger[1] and Dieter W. Heermann[2] — [1]Institute of Theoretical Physics, Heidelberg, Germany / MIT, Cambridge, USA — [2]Institute of Theoretical Physics, Heidelberg

We present a Monte Carlo model for genome folding at the 30-nm scale with focus on linker-histone and nucleosome depletion effects. Depletion of linker histones and nucleosomes affects, massively, the flexibility and the extension of chromatin fibers. Increasing the amount of nucleosome skips can lead either to a collapse or to a swelling of chromatin fibers. We show that depletion effects may even contribute to chromatin compaction. Furthermore, we find that predictions from experimental data for the average nucleosome skip rate lie exactly in the regime of maximum chromatin compaction.

We determine the nucleosome pair distribution function of chromatin. We show that chromatin nanostructure might in principle be accessible by 2D high-resolution light microscopy: Our simulations show that even in the case of fibers with depletion effects and after a projection, the main dominant peaks can still be identified.

Furthremore, we compare our simulations with 5C data of a gene desert as well as FISH data and find that only fibers with random depletion of linker histones or nucleosomes can explain the probability of random chromatin contacts on small length scales that play an important role in gene regulation. Missing linker histones and nucleosomes might not just be randomly occuring simple unavoidable defects but instead they might even play a regulatory role in gene expression.

DY 6.17 Mon 16:00 Poster B2

Morphological Influences on Colloidal Transport in Porous Structures — •Christian Scholz[1], Yujie Li[1,2], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The morphological properties of artificial quasi two-dimensional micro porous structures are studied and related to transport properties of colloidal particles on a single particle level. The structure of the samples which are created with soft lithography are characterized using pore size distributions, percolation thresholds and Minkowski functionals, where the Euler index is used as a fast and robust measure to identify differences between designed and fabricated structures. We present first results where we demonstrate how small changes in the sample morpholoy lead to significant differences in the particle trajectories and the corresponding mean squared displacements.

DY 6.18 Mon 16:00 Poster B2

Diffusive Transport of light in a two-dimensinal disordered packing of disks:analytical approach to transport mean free path — •Zeinab Sadjadi[1] and MirFaez Miri[2] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany — [2]Institute for Advanced Studies in Basic Sciences, Zanjan, 45195-1159, Iran

We study photon diffusion in a two-dimensional random packing of monodisperse disks as a simple model of granular media and wet foams. We employ ray optics to follow a light beam or photon as it is reflected by the disks. For the intensity reflectance at the disks two models are presented. In the first model the intensity reflectance of disks is assumed to be a constant r . We present an analytic theory based on persistent random walk of photons and express the transport-mean-free path l^* in terms of the velocity of light in the disks and host medium, radius R and packing fraction of the disks, and the intensity reflectance. Then in a more realistic model we choose the Fresnel intensity reflectance and take into account the dependence of intensity reflectance on the incident angle of light, refractive indices if disks and host medium and other parameters. We examine our analytic results by performing numerical simulation.

DY 6.19 Mon 16:00 Poster B2

Quantitative analysis of fluctuations and irreversibility of optically trapped microspheres — •Olaf Ueberschär and Friedrich Kremer — Universität Leipzig; Institut für Experimentelle Physik I; Linnéstraße 5; D-04103 Leipzig

We present an experimental verification of several universal theorems of stochastic thermodynamics by means of optical tweezers. The theoretical and experimental investigation of this novel branch of modern thermodynamics promises in various ways to be of great benefit for the quantitative understanding and application of processes at the micro- and nanometre scale in the fields of physics, biochemistry and applied technology. Utilizing the formal framework established by U. Seifert and others around 2005 and following the experimental approaches of G. M. Wang et al. first published in 2002, we experimentally demonstrate the validity of several pertinent fluctuation theorems for special non-equilibrium states of optically trapped colloids. Our results in this context exceed the scope of Wang et al. 2002-2005 by a considerable margin. Fluctuation theorems which came into the focus of theoretical research about 15 years ago describe the emergence and quantitative evolution of macroscopic irreversibility from the microscopic point of view of stochastic thermodynamics. Moreover, we present a new method for the experimental determination of the radius and the temperature of a single optically trapped colloid by directly analyzing the thermal equilibriums fluctuations of the bead. This technique may be utilized for the optimisation of several other optical tweezers experiments which show a high requirement for quantitative precision.

DY 6.20 Mon 16:00 Poster B2

Directed Brownian motion of asymmetric particles in a time-dependent potential — •Martin Reichelsdorfer and Klaus Mecke — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudstr. 7, 91058 Erlangen

The motion of an asymmetrically shaped particle in a heat-bath can be directed if it is kept far away from thermal equilibrium. This can be achieved by a time-dependent spatial-symmetric potential. As a model system a hard convex body with one translational degree of freedom which experiences an harmonic restoring force with exponentially decreasing spring constant is studied in an ideal gas. Fluctuation theorems are tested and the efficiency is determined.

DY 6.21 Mon 16:00 Poster B2

Effect of negative resistance in the transport of a dimer system — •Steffen Martens[1], Dirk Hennig[2], and Lutz Schimansky-Geier[1] — [1]Department of Physics, TSP, Humboldt Universität zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany — [2]Department of Mathematics, University of Portsmouth, Lion Terrace, Portsmouth, Hampshire PO1 3HF

The one-dimensional as well as the two-dimensional overdamped Langevin dynamics of a dimer system consisting of two harmonically interacting components are studied. Both components are absorbed at the same spatially periodic substrate potential and are coupled to the same external heat bath. In contrast to previous works, we consider the impact of an inhomogeneous forcing, viz., an external localized point force applied at only one of the two components, on the dynamic of the dimer system. For the one-dimensional case, two accurate approximations for the center of mass mobility and its diffusion coefficient are obtained for weak and strong couplings. It turns out that the mobility of a dimer as a function of the competing length scales of the system, that are the period of the substrate potential and the equilibrium distance between the two constituents, shows a resonance behavior. More precisely there exist a set of optimal parameter values maximizing the mobility. Interestingly, while in the one-dimensional case the mobility as a function of the noise strength is a monotonic function of the latter in 2D we found the effect of negative resistance, i.e., the mobility possesses a minimum at a finite value of the noise strength for a given overcritical external force magnitude.

DY 6.22 Mon 16:00 Poster B2

Application of the Maximum Entropie Method for Heterogeneous Diffusion Systems — •Mario Heidernätsch, Michael Bauer, and Günter Radons — Chemnitz University of Technology, D-09126 Chemnitz, Germany

Nowadays a range of experimental methods is used for the investigation of single molecule diffusion. Especially Single Molecule Tracking (SMT) and Fluorescence Correlation Spectroscopy (FCS) are suitable methods to probe small systems with high temporal or spatial resolution. However, as the examined systems became smaller, environmental inhomogeneities for instance on interfaces or of the surrounding liquid are causing observed heterogeneous diffusion processes. In FCS the Maximum Entropie Method (MEM) is a well tested technique

to obtain a distribution of diffusivities from measured autocorrelation curves [1]. With the help of our distribution of scaled squared displacements [2] we are now able to apply the Maximum Entropie Method also in Single Molecule Tracking.

[1] P. Sengupta, K. Garai, J. Balaji, N. Periasamy, S. Maiti, Biophys. J. **84** (2003), pp 1977-1984
[2] M. Bauer, M. Heidernätsch, D. Täuber, C. von Borczyskowski, G. Radons, Diffusion Fundamentals III **11** (2009), pp. 70.1-70.2

DY 6.23 Mon 16:00 Poster B2

Characterization of heterogeneous single molecule diffusion in ultra-thin liquid films from the probability density of scaled squared displacements — •Michael Bauer and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz, Germany

Our objective is to characterize the behavior of heterogeneous diffusion processes observed from single molecule trajectories. Such processes arise in many physical and biological applications, for instance in ultra-thin liquid films. A change of diffusion properties between different liquid layers and a projection of the particle's trajectory onto the two-dimensional plane lead to dynamic heterogeneities in the observed motion of the molecules [1]. Due to averaging, conventional methods like mean square displacement calculations conceal the effects originating from these inhomogeneities. Consequently, interesting parameters like distinct diffusion coefficients cannot be determined from averaged data. Hence, investigations based on the probability density of scaled squared displacements offer a promising approach to identify and characterize properties of the observed inhomogeneous diffusion process. We consider moments of the probability density and calculate time-dependent diffusion coefficients along with their fluctuations. Furthermore, our analysis is extended to static heterogeneities originating from modified compartments near the substrate. A map of probability densities enables the distinction between static and dynamic heterogeneities.
[1] M. Bauer et al., Diffusion Fundamentals 11(70):1–2, 2009.

DY 6.24 Mon 16:00 Poster B2

Brownian motion of heated particles — •Daniel Rings[1], Dipanjan Chakraborty[1], Markus Selmke[2], Romy Radünz[2], Frank Cichos[2], and Klaus Kroy[1] — [1]ITP, Uni Leipzig, Germany — [2]EXP1, Uni Leipzig, Germany

We derive the generalized Markovian description for the non-equilibrium Brownian motion of a heated particle in a simple solvent with a temperature-dependent viscosity. Our approximate analytical results for the generalized fluctuation-dissipation and Stokes-Einstein relations compare favorably with measurements of laser-heated gold nano-particles and provide a practical rational basis for emerging photothermal tracer techniques. We also compare our analytic results with a numerical solution of the hydrodynamic equations and find good agreement after a parameter-free but non-trivial rescaling. To gain insight into the microscopic basis for the effective equations and boundary conditions, we study the heat and solvent flow around the particle in molecular resolution by means of GPU-enhanced parallel MD simulations.

DY 6.25 Mon 16:00 Poster B2

Numerical calculation of the filter efficiency of fibrous aerosol filters — Egbert Zienicke and •Hartmut Grille — Institut für Physik, TU Ilmenau, 98684 Ilmenau, Gemany

An important environmental task is the suppression of soot emission from Diesel engines in traffic. New EU and US norms do not only set limits for the total mass of soot per km, but also prescribe the maximally allowed number of particles. The challenge for the construction of Diesel particle filters is the maximization of the filter effectivity and the minimization of the pressure drop.

The computation of the effectivity of a fibrous filter is based on the single fiber efficiency, which is obtained by numerical integration of the particle trajectories in the Kuwabara cell around a single fiber. The soot particle paths are influenced by (i) Stokes friction in the flow of the exhaust gas, (ii) Brownian motion and (iii) the particle inertia. The single fiber efficiency depends on the flow velocity, particle size, fiber diameter, the filter porosity, and the exhaust gas temperature. For the goal of designing more efficient filters a large part of this parameter space has to be treated with sufficient statistics. As each trajectory can be computed independently, this task is an ideal candidate for parallelization. This has been realized with Nvidia graphic cards in the CUDA frame work. We compare our numerically received single fiber efficiencies with experimental data and analytical approximations.

DY 6.26 Mon 16:00 Poster B2

Diffusive transport of ballistic particles in hard-spheres systems — •Markus Spanner[1], Felix Höfling[3], Gerd Schröder-Turk[1], Klaus Mecke[1], and Thomas Franosch[2,1] — [1]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics and CeNS, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, D-80333 München, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom

We study critical diffusive transport in porous media at the percolation threshold by simulating the trajectories of ballistic tracer particles. The porous medium is given by quenched configurations of hard non-overlapping spheres and the size of the tracer particle is adjusted to be the largest possible sphere that can traverse the system in all directions, i.e. the system is at its percolation threshold. Results for the diffusion coefficient at different hard-sphere densities are compared with results for point-like tracers in systems of a Boolean model of uncorrelated overlapping spheres from [1]. Our system of correlated obstacles should represent a more realistic model for porous media than the previous system of uncorrelated spheres. We are interested if sub-diffusive motion in the hard-sphere system still has the same value for the exponent z in $\delta r^2(t) \propto t^{-2/z}$ as in the system of overlapping spheres with a point like tracer, because the probability for narrow channels in the system might or might not influence this exponent.
[1] F. Höfling, T. Franosch, E. Frey, Phys.Rev.Lett. 96, 165901(2006)

DY 6.27 Mon 16:00 Poster B2

Measuring Hindered Transport and Self-Diffusion by Means of Optical and NMR Methods — •Tom Kirchner[1], Christian Chmelik[1], Helge Bux[2], Jürgen Caro[2], Lars Heinke[1], Florian Hibbe[1], Tobias Titze[1], and Jörg Kärger[1] — [1]University of Leipzig, Faculty of Physics and Earth Science, Linnéstr. 5, D-04103 Leipzig, Germany — [2]Leibniz University Hannover, Callinstr. 3a, D-30167 Hannover, Germany

Infrared micro-imaging and pulsed field gradient NMR allow to obtain the transport and
selfdiffusivities of a probe molecule in the same host material and over comparable
length scales. In a systematic study, we compare directly both quantities in one and the same system,
namely methanol in a representatve of the famous novel group of nanoporous materials (MOF
ZIF-8). Following this approach, an unexpected behaviour has been obtained: the self-diffusion of
methanol notably exceeds the transport diffusion in a wide range of loadings. This finding is rationalized by considering the strong intermolecular interaction and
the dominating role of inter-cage hopping in mass transfer in the systems under study.

DY 6.28 Mon 16:00 Poster B2

Gas sensitivity in nanoporous crystalline metal oxide: a site-bond percolation approach — •Julia Dräger[1], Stefanie Russ[2], Claus-Dieter Kohl[3], and Armin Bunde[1] — [1]Institut für Theoretische Physik III, 35392 Giessen — [2]Freie Universität Berlin, 14195 Berlin — [3]Institut für Angewandte Physik, 35392 Gießen

By means of a site-bond percolation model we study numerically and analytically the gas-induced metal-insulator transition of thin films of nanoporous crystalline metal oxides. We model the layers by a network of intergranular contacts where the conductances of the grains (sites) and of the bonds depend on the amount of adsorbed gas molecules that extract electrons from the inner part of the grains, leaving a depletion zone. While below a critical gas concentration N_c the nanoporous structure is insulating due to the absence of a conducting percolating cluster, above N_c the conductance increases rapidly. Depending on the parameters of the system (layer thickness, average grain size, coordination number) we find two different scenarios: for systems of small grains and high porosity (i.e low coordination number) the transition from a conducting towards an insulating phase arises from the disappearance of conducting grains due to the lack of charge carriers. For systems of large grains and lower porosity, on the other hand, the transition is governed by the bond percolation effect, which reflects the influence of the depletion zone on the grain necks and thus on

the bonds. Furthermore, we explore which details of the shape of the characteristic curve are due to percolation effects and which properties arise from the variation of the bonds.

DY 6.29 Mon 16:00 Poster B2

Anomalous transport in porous media III: Anomalous immiscible displacement — •Florian Doster[1] and Rudolf Hilfer[1,2] — [1]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Physics, University of Mainz, 55099 Mainz, Germany

Two phase immiscible fluid displacement in porous media shows several anomalies when compared with experiments. The standard model has been extended by distinguishing percolating and nonpercolating phases [1]. In one dimension the theory reduces to a set of ten coupled nonlinear partial differential equations. In this contribution we present numerical simulations based on a judicious coice of abnormal diffusion terms. The numerical diffusion terms are needed to stabilize the nonlinear system of partial differential equations [2,3].

[1] R. Hilfer, Physica A **371**, 209 (2006)
[2] R. Hilfer and F. Doster, Transport in Porous Media, published online, doi: 10.1007/s11242-009-9395-0 (2009)
[3] F. Doster, P. Zegeling and R. Hilfer, Physical Review E (in print)

DY 6.30 Mon 16:00 Poster B2

Anomalous transport in porous media IV: Immiscible displacement in the diffusive limit — •Oliver Hönig[1], Florian Doster[1], and Rudolf Hilfer[1,2] — [1]Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland — [2]Institut für Physik, Universität Mainz, 55099 Mainz, Deutschland

We study anomalous capillary diffusion in porous media. Capillary diffusion arises during macroscopic multiphase flow when capillary forces become dominant. We extend recent results on a generalised fractional flow formulation [1] into the diffusive limit.

[1] F. Doster and R. Hilfer, preprint

DY 6.31 Mon 16:00 Poster B2

Anomalous diffusion in inhomogeneous viscosity landscapes — •Markus Burgis, Volker Schaller, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, D-95440 Bayreuth

We find anomalous diffusive motion for Brownian particles in inhomogeneous viscosity landscapes and we investigate the dependence of the anomalous power laws on the shape of the viscosity land scape. For a Brownian particle placed in the vicinity of a local minimum of the viscosity subdiffusion is predicted.

In contrast superdiffusion is found for the particle in the vicinity of a local maximum of the viscosity as well as in the region of a linearly varying viscosity. In the case of a heated particle in a binary mixture with different viscosities for pure components the thermodiffusion (Soret effect) induces a concentration gradient around the particle and therefore simultaneously the viscosity gradient. This leads to anomalous diffusion of the particle affected by memory effects.

We compare the results of simulations based on the Langevin equation for the particle motion and diffusion equation for the concentration field with the appropriate model incorporated memory effects.

DY 6.32 Mon 16:00 Poster B2

Noise Effects in Ferromagnetic Systems — •Thomas Bose and Steffen Trimper — Martin-Luther-University, Halle, Germany

We study a model for ferromagnetic materials describing the propagation of spin waves under the influence of deterministic and stochastic forces. The analysis is performed referring to the classical limit by introducing a stochastic Landau-Lifshitz-Gilbert equation (LLG). The stochastic force has a finite correlation time τ leading to a non-Markovian process. The LLG is transformed into an equivalent equation for the corresponding probability distribution. Approximate equations for the mean values and the correlation functions, respectively, are derived. In general, the Gilbert damping leads to a decay of the spin wave amplitude. Whereas, this situation can change when both the deterministic and the stochastic forces act simultaneously on the system. In this case we found a phase diagram in terms of the Gilbert damping parameter α, the correlation strength of the random noises D and the correlation time τ.

DY 6.33 Mon 16:00 Poster B2

Power–Law Level–Statistics due to Dynamical Tunneling — Arnd Bäcker, Roland Ketzmerick, Steffen Löck, and •Normann Mertig — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Germany

We study level–spacing statistics for systems with a mixed phase space, in which regions of regular and chaotic dynamics coexist. Assuming statistical independence of the corresponding subspectra, spacings are described by the Berry–Robnik distribution. However, due to dynamical tunneling, regular and chaotic states are coupled. This leads to small avoided crossings which vary in size over many orders of magnitude, depending on the regular state involved. We demonstrate that this implies a power law of the level–spacing distribution for small spacings. It is analytically and numerically shown that the power-law exponent semiclassically scales linearly with the effective Planck constant.

DY 6.34 Mon 16:00 Poster B2

Transport in Correlated Random Media — •Otto Dietz[1], Ulrich Kuhl[1], Hans-Jürgen Stöckmann[1], Felix M. Izrailev[2], and Nykolay M. Makarov[2] — [1]Fachbereich Physik, Universität Marburg, Germany — [2]Instituto de Física, Universidad de Puebla, Mexico

We investigate the microwave transport properties of quasi-one-dimensional channels with correlated disorder. The correspondence between quantum and classical wave equations allows to use classical waves to understand electron transport properties in new low dimensional materials like nanowires and graphene stripes. Theoretical studies predict that the transport should strongly depend on the correlation of the disorder for bulk [1] and surface [2] disorder. These correlations can be created by inserting brass bars or copper cylinders into the waveguide and allow for a precise prescription of the transport properties of a given frequency region. Previous studies could confirm these results [3] in a one-dimensional channel with bulk disorder. We were able to expand these observations to various types of disorder. We found a strong non-evanescent transport unpredicted by theory in disordered systems in a frequency range where only evanescent transport is expected. This shows the limit of the propagating mode model and allows for estimating the range of its applicability in new nano experiments.

[1] J. C. Hernández Herrejón et al., Physica E 40, 3137 (2008).
[2] M. Rendón et al., Phys. Rev. B 75, 205404 (2007).
[3] U. Kuhl et al., Phys. Rev. Lett. 100, 126402 (2008).

DY 6.35 Mon 16:00 Poster B2

Singular statistics revised — •Timur Tudorovskiy, Ulrich Kuhl, and Hans-Jürgen Stöckmann — Fachbereich Physik, Renthof 5, D-35032 Philipps-Universität Marburg

We analyze the "singular statistics" of pseudointegrable Šeba billiards and show that taking into account growing number of resonances one observes the transition from "semi-Poissonian"-like statistics to Poissonian. This observation is in agreement with an argument that a classical particle does not feel a point perturbation. However, our findings contradict results reported earlier (P. Šeba, Phys. Rev. Lett. **64**, 1855 (1990)).

DY 6.36 Mon 16:00 Poster B2

Superconducting measurement of two microwave billiards with constant width shape — Stefan Bittner[1], Barbara Dietz[1], Maksim Miski-Oglu[1], Pedro Oria Iriarte[1], •Birgit Quast[1], Achim Richter[1,2], and Florian Schäfer[1,3] — [1]Institute for Nuclear Physics Darmstadt — [2]ECT* Trento — [3]LENS, University of Florence

Convex quantum billiards of constant width are characterized by a phase space which is separated into two parts corresponding to clockwise and anti-clockwise motion. We present experimental results for two microwave billiards of constant width shape, where each part of phase space consists of a chaotic region and a tiny region of regular motion located around the separation line in the Poincaré surface of section. Classically, the transition from clockwise to anti-clockwise motion is forbidden, whereas in the quantum system this is possible via dynamical tunneling. The aim of the microwave experiments is the investigation of spectral properties and the tunneling effects, which leads to a splitting of the degeneracies due to the clockwise/anti-clockwise symmetry. The resonance spectra obtained by superconducting measurements primarily contain dubletts. The few existing singuletts are due to the diameter orbit and their location in the resonance spectra are predictable. Therefore our attention is concentrated on the dubletts and results on their spectral properties and their splittings

will be presented. The work presented in this poster was supported by the DFG within the SFB634

DY 6.37 Mon 16:00 Poster B2

Quantum signatures of partial barriers in phase space — Arnd Bäcker, Roland Ketzmerick, and •Matthias Michler — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

In generic Hamiltonian systems classical transport in the chaotic sea is limited by partial barriers, which allow a flux Φ given by the turnstile area. Quantum mechanically they are even more restrictive for Planck's constant $h \gg \Phi$, while for $h \ll \Phi$ classical transport is recovered. This transition is qualitatively well understood, however, many quantitative questions are still open.

We construct a kicked system with a particularly simple phase-space structure, having two chaotic regions separated by one dominant partial barrier. We find a universal scaling with the single parameter Φ/h and the transition at $\Phi/h = \pi^2/4$. The results are not described by the random matrix model for partial barriers [Bohigas et. al. 1993]. Alternative quantum models for this transition are presented.

DY 6.38 Mon 16:00 Poster B2

Microwave measurements on graphene-like structures — •Sonja Barkhofen[1], Ulrich Kuhl[1], Hans–Jürgen Stöckmann[1], and Fabrice Mortessagne[2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Laboratoire de Physique de la matière condensée, CNRS UMR 662, Université de Nice -Sophia Antipolis- 06108 Nice cedex 2, France

Electrons in graphene lattices close to the K point can be described by the Dirac equation because of their linear dispersion with k, thus allowing to study quantum electrodynamic phenomena in the solids [1]. We rebuilt graphene's hexagonal structure with high permittivity index discs in a microwave set-up. A tight binding regime for the coupling was found by varying the distance of two or three coupled scatterers. At the Dirac point a vanishing triangular density of states is found via reflection measurements, whereas measurements at corners showed edge states at the Dirac point.

[1] G.W. Semenoff, Phys. Rev. Lett. 51 (1984) 2449

DY 6.39 Mon 16:00 Poster B2

Reappearance of Flooded Regular States in Open Quantum Systems with a Mixed Phase Space — Arnd Bäcker[1], •Lars Bittrich[1], Roland Ketzmerick[1], Ulrich Kuhl[2], and Hans-Jürgen Stöckmann[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

For closed systems with a mixed phase space, it was shown that quantum mechanically flooding of regular islands may occur. This happens when the Heisenberg time is larger than the tunneling time from the regular region to the chaotic sea. In this case the regular eigenstates disappear. For open systems we investigate the phenomenon of flooding and disappearance of regular states, where the escape time occurs as an additional time scale. We discuss the reappearance of regular states in the case of strongly open systems. This is demonstrated numerically for quantum maps and experimentally for a mushroom shaped microwave resonator.

DY 6.40 Mon 16:00 Poster B2

Quality Factor Dynamics in Coupled Circular Microcavities — •Jeong-Bo Shim[1], Jan Wiersig[1], Mohamed Benyoucef[2], and Oliver Schmidt[2] — [1]Institut für Theoretische Physik, Universität Magdeburg, Postfach 4120, D-39016 Magdeburg, Germany — [2]Institute of Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

In this work, we study the spectral properties of two identical circular microdisks which are coupled through evanescent field. The system is experimentally realized with semiconductor quantum dots, and the spectrum and qualtiy factors of this system are traced, continuously varying the refractive index of one of the microcavities by heating. In this process, the spectrum shows clear level repulsion whenever the resonances are induced in both of the cavities. However, the quality factors are behaving in different ways depending on the symmetry. We analyze this observation theoretically and numerically and find a good agreement with the experimental data. Also, a simple theoretical model to grasp the physical essence of this system is presented.

DY 6.41 Mon 16:00 Poster B2

Temporal decay of open quantum billiards — Stefan Bittner[1], Bruno Camargo[1], Barbara Dietz[1], Maksim Miski-Oglu[1], •Pedro Oria-Iriarte[1], Birgit Quast[1], Achim Richter[1,2], and Florian Schäfer[1,3] — [1]Institut für Kernphysik, Technische Universität Darmstadt, D-64289, Darmstadt, Germany — [2]LENS, University of Florence, I-50019 Sesto-Fiorentino, Italy — [3]ECT, Villa Tambosi, Villazzano, I-38100 Trento, Italy

The decay probability in open quantum billiards with regular and chaotic dynamics is explored by means of experiments on superconducting microwave cavities with openings on the boundary. The scattering-matrix formalismus is used to quantify the leaked microwave flux at the opening. The decay behavior is closely related to the resonance widths. In the semiclassical regime, the decay resembles the corresponding classical probability of escape. The field distributions of some modes play also a crucial role.
This work is supported by DFG through SFB 634.

DY 6.42 Mon 16:00 Poster B2

Equivalence of transport coefficients in bath-induced and dynamical scenarios — •Robin Steinigeweg — Institute for Theoretical Physics, Technical University of Braunschweig, Mendelsohnstr. 3, D-38106 Braunschweig, Germany

We investigate the transport of a single excitation through a chain of weakly coupled subunits. At both ends the chain is exposed to baths which are incorporated by means of a master equation in Lindblad form. This master equation is solved by the use of stochastic unraveling in order to obtain excitation profile and current in the steady state. Completely diffusive transport is found for a range of model parameters, whereas signatures of ballistic behavior are observed outside this range. In the diffusive regime the conductivity is rather independent from the strength of the bath coupling and quantitatively agrees with the diffusion coefficient which has been derived from an investigation of the same model without baths. Also the ballistic behavior in the non-diffusive regime is in accord with results from this alternative approach.

DY 6.43 Mon 16:00 Poster B2

Diffusion in a finite, non-isotropic Anderson model — •Hendrik Niemeyer[1] and Robin Steinigeweg[2] — [1]University of Osnabrueck, Physics Departement, Germany — [2]University of Braunschweig, Physics Departement, Germany

We investigate the existence of diffusive dynamics at various wavelengths in a single-particle 3D Anderson model by solving the full time-dependent Schroedinger equation. This model features a coarse-grained structure: The lattice is divided into layers and the hoppings between layers differ from the hoppings within the layers. Criterions for the transport behaviour of the system are introduced by analyzing the time evolution of the expectation value of the Fourier components of the spatial particle density. We come to the conclusion that a diffusive corridor w.r.t. wavelengths exists featuring the same diffusion constant for every energy interval. This confirms results from the time-convolutionless projection operator technique applied to the same model.

DY 6.44 Mon 16:00 Poster B2

Dephasing in networks with traps: from Quantum to Random Walk — •Tobias Schmid, Oliver Mülken, and Alexander Blumen — Albert-Ludwig Universität Freiburg, Physikalisches Institut

Earlier works have demonstrated the transfer of excitons on networks from initial sites to traps due to classical random motion in contrast to quantum motion. By utilising the Liouville-von-Neumann (LvN) equation approach, a simple dephasing via Lindblad operators in the quantum case is introduced. The transition between random and quantum motion depending on the coupling strength to the bath is observed for different networks. The limiting cases of coherent motion for weak coupling and as well as the Zeno limit for strong coupling are demonstrated.

DY 6.45 Mon 16:00 Poster B2

Thermodynamics of quantum systems: work and heat in finite systems — •Heiko Schröder and Günter Mahler — Universität Stuttgart, 1. Institut für Theoretische Physik, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Over the past decade there has been growing interest in the thermo-

dynamics of quantum systems and their parts. In order to tackle this challenge it is necessary to identify what thermodynamic role (heat or work source) each part plays in a given system and, thus, how the exchanged energy may be split into heat and work. We present a definition of finite quantum mechanical work sources and illustrate the concept by means of the behavior of a system consisting only of a single spin coupled to a harmonic oscillator [1]. We give a generalized definition of heat and work and measures for the quality of work transfer based on the previous results and the concept of a local effective measurement basis (LEMBAS [2]).

[1] H. Schröder and G. Mahler, arXiv:0911.5236
[2] H. Weimer et al., Europhys. Lett. 83 (2008), 30008

DY 6.46 Mon 16:00 Poster B2

Effective Quantum Jarzynski estimator for embedded subsystems — •Jens Teifel and Günter Mahler — Universität Stuttgart, Germany

We consider a composite quantum system. An effective description for local observables, e.g. energy, will be used in order to analyze the behavior of a given subsystem. This local behavior (process) might arise from external driving via an explicitly time-dependent local Hamiltonian or due to the effect of the surrounding quantum systems (or a combination of both). If the investigated subsystem is in a thermal state, we call the total state partially thermalized. Starting from such states we explore the possibility to formulate Jarzynski relations for the respective subsystems.

DY 6.47 Mon 16:00 Poster B2

Quantum Thermodynamics and periodic quantum measurements — •Thomas Jahnke and Günter Mahler — Universität Stuttgart, 1. Institut für Theoretische Physik, Pfaffenwaldring 57, 70550 Stuttgart

It is known from Quantum Thermodynamics [1] that the Schrödinger dynamics of a closed bi-partite quantum system typically enforces a stationary thermalized state on the smaller subsystem. This seems to be at variance with the common picture of classical statistics, according to which the individual system continues to move through its allowed space of microstates such that the respective thermal state is established as the infinite time average only.

Here we argue that the link between these two descriptions can be found in terms of observations from the outside: Projective measurements of the environment influence the system dynamics due to "cojumps" and destruction of system-environment correlations.

Concretely, we investigate a two-level system (TLS) coupled to an environment consisting of many spins, the magnetization of which is measured periodically. Considering the ensemble average, we derive an analytical solution for the dynamical attractor state reached after many measurements.

DY 6.48 Mon 16:00 Poster B2

Two Ising-coupled quantum spins in the presence of a bosonic bath — •Peter Philipp Orth[1], Karyn Le Hur[1], David Roosen[2], and Walter Hofstetter[2] — [1]Department of Physics, Yale University, New Haven, CT 06520, USA — [2]Institut für Theoretische Physik, Goethe Universität, 60438 Frankfurt/Main, Germany

A system of two coupled quantum spins in contact with a common harmonic oscillator bath is a paradigm for the study of the interplay between quantum control and dissipation. It also constitutes the elementary building block of a quantum computer. Using the time dependent numerical renormalization group (TD-NRG), we study the system's rich dissipative dynamics arising from the competition between spin-spin and spin-bath coupling, and compare it to a perturbative Bloch-Redfield approach. As an example, we show that spin oscillations can be synchronized using the bath induced interaction. We also address how the well-known localization quantum phase transition of the single spin-boson model is affected by the presence of a second spin. We employ the NRG to calculate the zero temperature phase diagram as a function of dissipation and Ising coupling, for both ohmic and subohmic baths. In the subohmic case, we study the scaling of spin expectation values and entanglement entropy close to the phase transition.

DY 6.49 Mon 16:00 Poster B2

Quantum Monte Carlo simulations for the dynamics of the spin-boson model with a structured environment — •Charlotte Escher and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, 89069 Ulm

Based on a numerically exact path integral Monte Carlo approach we investigate the real-time dynamics of the dissipative quantum mechanical two-state system. The dissipation in our case is due to the interaction with an environment whose spectral density is not purely Ohmic, but instead shows additional resonances at characteristic frequencies. Models with this kind of structured environment are of relevance for qubit devices in condensed matter systems and quantum optics (dissipative Jaynes-Cummings model).

DY 6.50 Mon 16:00 Poster B2

Scaling behaviour in a minimal model for block copolymer microdomain ordering — •Christian Riesch and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We simulate microphase separation and subsequent microdomain ordering processes in lamellae- and cylinder-forming block copolymers using a coarse-grained model, based on a modified Cahn-Hilliard equation. This model has often been studied by use of cell dynamics simulations. We compare the ordering of stripes in 2D simulations with the ordering of cylinders in thin films (3D simulations). Evolution of microdomain order is tracked by four different quantities. Orientational correlation length and average curvature represent global measures of order. Densities of characteristic defects, such as dislocations and disclinations, provide insight into the mechanisms promoting growth of long-range microdomain order. We discuss the influence of noise and film thickness on power laws observed in measures of order and compare different numerical techniques in terms of accuracy and efficiency.

DY 6.51 Mon 16:00 Poster B2

Multiscale modeling of nanostructured polymer materials using field-theoretic methodologies — •Stephan Baeurle[1], Takao Usami[2], and Andrei Gusev[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätstr. 31, 93053 Regensburg, Germany — [2]Polymer Design Laboratory, Mitsubishi Chemical Group Science and Technology Research Center, Yokkaichi, Mie 510-0885, Japan — [3]Department of Materials, Institute of Polymers, ETH, CH-8093 Zurich, Switzerland

Understanding the chemistry and physics of polymer systems challenges scientists from a wide spectrum of research areas, ranging from polymer science to molecular electronic structure theory. One of the characteristic features of polymer systems is that their physics involve a multitude of different length and time scales, which generally render the determination of their structure and physical properties on a detailed level computationally exhaustive. To overcome this difficulty, novel field-theoretic methodologies based on the mean field approximation have been developed in the past decade for materials engineering, and have proven to deliver reliable results in the calculation of mesoscopic models of polymer melts and highly concentrated polymer solutions. In this presentation we demonstrate that the field-theoretic approach is not only an effective formalism for treating highly concentrated polymer systems on the mesoscopic level of description, but that it is also a promising theoretical tool, to solve the multiscale problems arising in the calculation of nanostructured polymer materials.

DY 6.52 Mon 16:00 Poster B2

Field-induced ordering, non-local susceptibilities and non-affine noise in 2D colloidal crystals — •Kerstin Franzrahe[1], Surajit Sengupta[2], and Peter Nielaba[1] — [1]Department of Physics, University of Konstanz, Germany — [2]CAM, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India

Ordering phenomena in monolayers interacting with a substrate are studied by MC-simulations of binary hard-disk mixtures. Here the influence of a substrate is modelled by a 1D spatially periodic external potential. For the field-free case the thermodynamic stability of space-filling lattice structures for such mixtures is analysed[1]. As these structures are stable only in high pressure environments, the phase behaviour of a binary 50% mixture with a diameter ratio $\sigma_B/\sigma_A = 0.414$ exposed to a substrate potential is studied in detail[1-3].

Furthermore our focus is on the elasticity of 2D soft matter systems. Using a coarse graining procedure the local strain fields and hence the elastic moduli can be computed from the local displacement fields. We show that for a triangular, harmonic lattice coarse graining local strains obtained from MC-simulations generates non-trivial, non-local strain correlations. These may be understood within a generalised, Landau type elastic Hamiltonian[2,4]. Apart from the smooth, affine strain fields, this procedure also gives rise to a noise field made up of non-affine displacements. [1] K. Franzrahe, P. Nielaba, Phys. Rev. E

79, 051505, (2009); [2] K. Franzrahe et al., J. Phys.: Cond. Mat. **20**, 404218, (2008); [3] K. Franzrahe, P. Nielaba, Phys. Rev. E **76**, 061503, (2007); [4] K. Franzrahe et al., Phys. Rev. E **78**, 026106, (2008).

DY 6.53 Mon 16:00 Poster B2

The Talbot effect observed in a liquid crystal convection experiment — •Stephan Messlinger, Wolfgang Schöpf, Ingo Rehberg, and Werner Pesch — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

This poster is identical to DY 6.54.

DY 6.54 Mon 16:00 Poster B2

The Talbot effect observed in a liquid crystal convection experiment — •Stephan Messlinger, Wolfgang Schöpf, Ingo Rehberg, and Werner Pesch — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

As first discovered by Talbot [1], light with a wavelength λ passing through any diffraction grating with wavelength Λ periodically reproduces images of the grating in regular distances $z_T = \Lambda^2/\lambda$ from the original plane. In this work, we describe the Talbot effect as observed with electroconvection patterns in liquid crystals. Electroconvection occurs when an alternating electric voltage of sufficient strength is applied perpendicularly to a thin liquid crystal layer [2]. The arising flow structures involve periodic modulations of the director field and hence of the refractive index in the layer plane. Thus, the layer acts as a specific amplitude and phase grating tunable by the frequency of the applied voltage in the range of $\Lambda = 5...50\,\mu$m. As a result, z_T varies from 0.1 to 10 mm, which is conveniently accessible in standard optical setups. We present a detailed comparison to recent theoretical analyses based on a wave optics approach in the limit of small λ/Λ [3]. This method presents a considerable improvement of the traditional treatment of shadowgraphy in the framework of geometrical optics [4].

[1] H. F. Talbot, Philos. Mag. 9, 401 (1836); L. Rayleigh, Philos. Mag. 11, 196 (1881). [2] A. Buka and L. Kramer, Pattern Formation in Liquid Crystals, Springer, 1996. [3] S. P. Trainoff and D. S. Cannell, Phys. Fluids 14, 1340 (2002). [4] S. Rasenat et al., Exp. Fluids 7, 412 (1989).

DY 6.55 Mon 16:00 Poster B2

Heisenberg antiferromagnets with exchange and on-site anisotropies — •Thanh-Chung Dinh[1], Reinhard Folk[1], David Peters[2], and Walter Selke[2] — [1]Institut für Theoretische Physik, JKU Linz, Austria — [2]Institut für Theoretische Physik, JARA-SIM and RWTH Aachen, Germany

We study Heisenberg antiferromagnets in a field with exchange and quadratic as well as quartic on-site anisotropies. Using, especially ground state considerations and Monte Carlo techniques for classical magnets on cubic lattices, we determine generic phase diagrams comprising antiferromagnetic, spin-flop, biconical, and paramagnetic phases. A variety of critical and multicritical scenarios are elucidated. Our results are compared to findings on related classical and quantum anisotropic antiferromagnets in lower dimensions.

Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No. 19583-N20, and by the excellence initiative of the German federal and state governments.

References: [1] G. Bannasch and W. Selke, Eur. Phys.J. B69, 439 (2009); [2] R. Folk, Yu, Holovatch, and G. Moser, Phys. Rev.E78, 041124 (2008); [3] T.-C. Dinh and R. Folk, J. Physical Studies (2009, in print); [4] W. Selke, G. Bannasch, M. Holtschneider, I. P. McCulloch, D. Peters, and S. Wessel, Cond. Mat. Phys., Vol. 12 (4) (2009, in print).

DY 6.56 Mon 16:00 Poster B2

Study of the delocalised-localised critical transition frequency for phonons — •Sebastian Pinski and Rudolf Römer — University of Warwick, Coventry, CV4 7AL, United Kingdom

In electronic systems, unlike phononic, the mobility edge of disordered electrons is well known for the Anderson model of localization. In phononic cases it is widely believed that a similar transition exists, although evidence is slim and has been achieved mostly through the Coherent Potential Approximation. We introduce a direct diagonalisation routine to obtain all vibrational eigenmodes frequencies of a three-dimensional mass and spring model under varying degree of disorder. We find the Participation Ratios and Vibrational Density of States for system sizes L= 6, 8, 10, 12 and 15 and disorders whilst averaging over 2000 realisations for all disorder magnitudes. Preliminary results suggest that the delocalised-localised transition must exist very close to the upper end of the spectrum for all mass and spring disorders considered. A natural extension to this work is to employ the transfer matrix method to find the Lyapunov exponents of quasi one-dimensional phononic systems which should reveal an exact transition frequency.