# DY 7: Statistical physics II (general)

Time: Tuesday 9:30–13:00 Location: HÜL 386

**Invited Talk** DY 7.1 Tue 9:30 HÜL 386

**Statistical Mechanics of sytems with long range interactions.** — •David Mukamel — The Weizmann Institute of Science, Rehovot, Israel

Systems with long range interactions, in which the two-body potential decreases at large distances, R, with a rate slower than $1/R^d$ in d dimensions are discussed. These systems are non-additive, and as a result they display unusual thermodynamic and dynamical properties which are not present in systems with short range interactions. In particular, the various statistical mechanical ensembles are not equivalent and the microcanonical specific heat may be negative. Long range interactions may also result in breaking of ergodicity, making the maximal entropy state inaccessible from some regions of phase space. In addition, in many cases long range interactions result in slow relaxation processes, with time scales which diverge in the thermodynamic limit. Various models which have been found to exhibit these features are discussed. Relevance of these studies to collective behavior of non-equilibrium driven systems is pointed out.

DY 7.2 Tue 10:00 HÜL 386

**Green-Kubo formalism for solids** — •Henk van Beijeren — Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands — Zentrum Mathematik, Bereich M5 Technische Universität München D-85747 Garching bei München (bis Juli 2009), Germany

The Green-Kubo formalism yields macroscopic transport equations on the basis of the microscopic equations of motion, by postulating the existence of a set of slowly varying microscopic phase functions, whose dynamics allow for a closed macroscopic description. These functions always include the long-wavelength Fourier components of energy, momentum and mass densities. In systems with broken symmetries the order parameters describing these have to be added. In solids these primarily are displacement fields, describing the displacements of the atoms from their equilibrium positions. The resulting macroscopic equations are the elastic equations describing propagation and damping of sound and Fourier's law of heat conduction. The Green-Kubo formalism expresses the transport coefficients and damping constants occurring in these equations in terms of time integrals of current-current time correlation functions.

I will present the general structure of these equations together with the Green-Kubo expressions for transport and damping coefficients. If time allows I will consider mode-coupling predictions for the long time behavior of the correlation functions relevant for heat diffusion. I will discuss divergences of transport coefficients and their finite-size renormalization.

DY 7.3 Tue 10:15 HÜL 386

**Theory of anisotropic electric conductivity of random resistor network on a Bethe lattice** — •Fyodor Semeriyanov, Marina Saphiannikova, and Gert Heinrich — Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069, Dresden, Germany

We propose a theory of anisotropic electric conductivity of composites filled by particles of anisometric shape. This theory is a generalization of the model of random resistor network proposed by Stinchcombe [1]. Using the Bethe lattice approach, we obtained an analytical solution and verified it by means of computer simulations. Namely, we performed a Monte Carlo simulation for the random resistor network on regular 2D and 3D lattice with resistors of orientation-dependent value and computed electrical conductivity in the parallel and the normal direction of applied voltage. The simulation time increased dramatically as the resistor concentration p approached the percolation threshold pc. The advantage of the analytical approach is that it allows to access this critical region by means of e-expansion, e=p-pc. We obtained the first term to be independent of direction, whereas the second was found to be anisotropic. These results are important in connection with experimental data for carbon-filled systems. Finally, we present a dynamic model for shear-induced effects based on a kinetic equation controlling resistor concentration.

This work was supported by the BMBF grant CarboNet No. 03X0504E.

[1] R.B. Stinchcombe, J. Phys. C 7, 179, 1974.

DY 7.4 Tue 10:30 HÜL 386

**Pair-factorized Steady States on Arbitrary Graphs** — Bartlomiej Waclaw[1], Julien Sopik[2], Wolfhard Janke[3], and •Hildegard Meyer-Ortmanns[4] — [1]Institute of Theoretical Physics, Leipzig University, 04009-Leipzig, Germany — [2]SES, Jacobs University, 28725-Bremen, Germany — [3]Institute of Theoretical Physics, Leipzig University, 04009-Leipzig, Germany — [4]SES, Jacobs University, 28725-Bremen, Germany

A variety of stochastic processes out-of-equilibrium may be summarized under the name of stochastic mass transport models. We shall consider variations of mass transport models with interactions leading to pair-factorized steady states on arbitrary graphs. Usually the hopping rates are the primary quantities that are specified to model a given transport process, and the stationary states are determined thereafter. Here we consider the reverse question. Given a pair-factorized steady state over an arbitrary (connected) graph, we ask which hopping rates could have led to this state. We give an answer in terms of hopping rate classes that include frequently studied special cases. By construction all the hopping rates within one class lead to the same stationary state, but differ in their conserved current. For special cases we then present results on the phase structure in terms of liquid versus condensed phases. Finally, we shall indicate extensions towards full factorization over k-cells on arbitrary graphs, of which pairs (i.e. 2-cells) are just a special case.

DY 7.5 Tue 10:45 HÜL 386

**On the critical properties of DLA clusters** — Lev Shchur[1], Anton Menshutin[1], and •Vladimir Vinokour[2] — [1]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We introduce variable size of the probe particles to estimate harmonic measure and extract fractal dimension of DLA clusters taking two limits, of vanishingly small probe particle size and of infinitely large size of a DLA cluster. We generate 1000 DLA clusters consisting of 50 million particles each using off-lattice killing-free algorithm developed in the early work. We found that effective fractal dimension D(N,b) measured using probe particles of size b and ensemble of the clusters of size N may be collapsed onto one curve as function of the variable b/Rdep, where Rdep is the radius of deposition. Thus, using smaller radius of the probe particles we get larger effective size of cluster. We extend our program and method for the case of clusters with the local anisotropy and investigate clusters with local symmetry of order 3 through 8. Results of simulation may be interpreted in the following way: i) there is strong repulsion between cluster branches for the local symmetry larger than 5, and all generated structures belongs to the one universality class of the off-lattice DLA with fractal dimension D=1.7104(5); 2) for symmetry lower than 5 structures seems to belong to the universality class of anisotropic fractals with D=3/2; 3) the case with 5 main branches is the marginal one - even lowest level of the noise reduction moves structures to the class of anisotropic fractals.

DY 7.6 Tue 11:00 HÜL 386

**Heterogeneous nucleation in the Ising model** — •David Winter, Peter Virnau, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz

Nucleation is typically enhanced by the presence of a wall because the free energy of a droplet in contact with a wall is reduced in comparison to the free energy of a droplet in the bulk. The difference between the homogeneous and the heterogeneous case can be described by Turnbull's formula which determines the free energy of a droplet as a function of the contact angle given by Young's equation. In this work, we test this simple model with Monte Carlo simulations of the 3d Ising model.

**15 min. break.**

DY 7.7 Tue 11:30 HÜL 386

**MD simulation of the formation of pharmaceutical particles by rapid expansion of a supercritical solution** — •Frank Römer and Thomas Kraska — Institute for Physical Chemistry, University Cologne, Luxemburger Str.116, 50939 Köln, Germany

Rapid Expansion from Supercritical Solution (RESS) is a method for the production of small particles down to the nanometer size for various substances including pharmaceuticals. The substance is dissolved in a supercritical solvent, typically carbon dioxide, and then expanded in a nozzle. This leads to lowering of the solubility and hence to a very high supersaturation. As a consequence the solute precipitates from the solution. We investigate this process by molecular dynamics simulation. An equilibrated supercritical solution is expanded by successive expansion of the simulation box. The parameters of the expansion are chosen to closely follow the path of an adiabatic expansion while preventing the phase separation of the solvent. The particles obtained in this way are investigated with respect to their structure and properties.

DY 7.8 Tue 11:45 HÜL 386

**Ultrametricity structure in the subspace of quasi optimum configurations of packing problems** — •Johannes Josef Schneider, Andre Müller, and Elmar Schömer — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We consider the problem of finding the densest closed packing of hard discs with proposed different radii in a circular environment, such that the radius of the circumcircle is minimal. With our heuristic optimization approach based on simulated annealing, we are able to get optimum and quasi optimum configurations for this packing problem [1]. The subspace of these configurations exhibits the property of ultrametricity,

[1] André Müller, Johannes J. Schneider, Elmar Schömer, Packing a multidisperse system of hard discs in a circular environment, accepted by Phys. Rev. E, 2008.

DY 7.9 Tue 12:00 HÜL 386

**GPU accelerated optimization of packing problems** — •Andre Müller, Johannes Josef Schneider, and Elmar Schömer — Department of Physics, Mathematics, and Computer Science, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We consider the problem of finding the densest closed packing of hard discs with proposed different radii in a circular environment, such that the radius of the circumcircle is minimal, and the analogous problem of hard spheres in three dimensions. Recently, the CUDA package has become a useful tool for performing simulations very fast on graphical processing units (GPUs) produced by NVidia. We will show how we implemented our optimization techniques for this problem on the GPU and we will provide results for small and medium system sizes.

DY 7.10 Tue 12:15 HÜL 386

**Finite-size effects and prediction of extreme events in the BTW model** — •Anja Garber[1], Holger Kantz[1], and Sarah Hallerberg[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Instituto de Física de Cantabria, Santander, Spain

The BTW Abelian sandpile model is a prominent example of systems exhibiting self-organised criticality. Finite-size effects are studied with special emphasis on the statistics of extreme events. Not only the avalanche size probability distribution, but also the mutual independence of large avalanches is affected. Instead of a Poissonian recurrence time distribution, a temporal repulsion of extreme events is found in the finite system that depends on the avalanche size rather than on its respective probability.

Deriving a decision variable from the time series of avalanches, this effect can be used to predict the occurrence of a particularly large event in the next time step. The larger the magnitude of these target avalanches, the better is their predictability.

DY 7.11 Tue 12:30 HÜL 386

**Reproduction of the collective behavior of the Hamiltonian Mean Field Model by means of a single forced oscillator** — •Angelo Facchini[1,2] and Stefano Ruffo[3] — [1]Center for the Study of Complex Systems, University of Siena, Italy — [2]Department of Information Engineering, University of Siena, Italy — [3]Dipartimento di Energetica "S. Stecco", University of Florence, INFN and CSDC, Italy

We force a single oscillator with the $x$ and $y$ components of the magnetization computed by integrating an $N$ particles Hamiltonian Mean Field model (*Phys. Rev. E, 52, 2361*). The equations of motion read $\ddot{x} = M_x(t)\sin(x) - M_y(t)\cos(x)$, where $M_x(t)$ and $M_y(t)$ are computed step by step and the energy is set to $U = 0.3$. We show that the motion of the particle is statistically equivalent to the motion of the $N$ particles cluster, and that the memory effect (*Comm. Nonlin. Sc. and Num. Methods, 13, 868*) observed in the life-time of the cluster is also found in the phase of the driven particle. Furthermore, we test the consistency of the single oscillator phase with that of the cluster by driving with $M_{x,y}(t)$ a system of $N$ uncoupled oscillators whose initial conditions correspond to those of the equilibrium state of the HMF model.

DY 7.12 Tue 12:45 HÜL 386

**A New Method of Tracking Feature Points in Videos** — •Mario Heidernätsch and Günter Radons — Chemnitz University of Technology, D-09126 Chemnitz, Germany

A general problem in the analysis of moving objects is to trace their path in a series of snapshots or a video. The objects are abstractly described by a set of properties/features, e.g. position, shape, color etc. To determine whether a detected feature point is the same in a series of consecutive images and to follow its path, it is necessary to find the optimal assignment by means of its features. An additional difficulty which could show up during tracking lies in the property that points stay undetected on single frames and make it inevitable to look at more than one frame at a single tracking step.

To solve this problem we propose a new tracking algorithm, which extends the idea of a connection cost matrix [1] with use of the Viterbi algorithm. On the basis of random moving fluorescent molecules we demonstrate how the algorithm works. In addition to the minimalistic a priori information of a single particle track due to the random movement, these molecules underlie the effect of photobleaching and therefore are temporary complete invisible. Thus these videos are the best "Testground" for this algorithm.

[1] I.F. Sbalzarini, P. Koumoutsakos, Journal of Structural Biology, 151, pp. 182-195, 2005