DY 3: Complex energy landscapes (addendum to SYEL)

Time: Monday 14:00–16:00 Location: H42

DY 3.1 Mon 14:00 H42

Coupling in glass-forming systems: From MD simulation to generalized KCM models — •Christian Rehwald and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster

Macroscopic glass-forming systems can be regarded as superposition of coupled elementary units, whose dynamics can in turn be described within the framework of the potential energy landscape and the concept of metabasins. This treatment of supercooled liquids leads to "coupled energy landscapes" for which we present a different concept to describe this coupling.

We study a binary mixture Lennard-Jones liquid for different system sizes and calculate local waiting times generated by particle displacements to gain detailed information about coupling events. While the waiting time distributions of local exchange events can be used to measure the coupling strength, the identification of the underlying processes requires greater effort. For this purpose we use the iso-configurational ensemble of a suitably prepared configuration to understand in detail the response to a single local relaxation event. Furthermore, we work out the essential differences between strong and weak coupling.

These MD results can be used to define a generalized KCM model. It turns out that the model can reproduce many properties of glass-forming systems, e.g. different finite size effects of D and τ_α or the growth of dynamical length scales (χ_4).

DY 3.2 Mon 14:15 H42

Phase diagrams of nanoparticles in various thermodynamic ensembles: Lattice-based Monte-Carlo Simulations of Pt-Rh — •Christian Stahl, Johan Pohl, and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 32, D-64287 Darmstadt

The equilibrium phase diagrams of Pt-Rh nanoparticles, which represent a binary model system with order-disorder transitions, are investigated as a function of particle size. Lattice-based Monte-Carlo simulations in the canonical and semi-grand canonical ensemble are carried out using a refined bond-order simulation (BOS) mixing model. With decreasing particle size, order-disorder transitions shift towards lower temperatures and higher Pt concentration, while phase fields of ordered intermetallic phase broaden and the two-phase areas shrink, which is mainly due to Pt segregation to the surface. Furthermore, we observe that the order-disorder transition becomes of second order for small particles, which is reflected in the size-dependence of Warren-Cowley short range order parameters. Finally, we investigate the phase transition in the microcanonical ensemble using a novel simulation technique for direct sampling of the density of states and hence the entropy of the system. In the region of high energy that is not accessible in the canonical and semi-grand canonical ensemble, we observe decomposition of the components.

DY 3.3 Mon 14:30 H42

Ground states of random-field Ising magnets around the upper critical dimension — •Björn Ahrens and Alexander K. Hartmann — University of Oldenburg

We consider the random-field Ising magnet (RFIM) around the upper critical dimension which is $d_u = 6$. The RFIM consists of ferromagnetically coupled Ising spins with an additional quenched local random field. To ensure unique ground-states we choose Gaussian random fields with zero mean and a tuneable standard deviation h. When varying h, each realization of the disorder exhibits a rather complex energy landscape, in particular close to the ferromagnetic-paramegnetic phase transition. We obtain the ground state numerically [A.K. Hartmann, Practical Guide to Computer Simulations, World Scientific 2009]. For each realisation of disorder we map the random field to a graph with suitible chosen edge capacities [Picard and Ratliff, Networks 5, 357 (1975)]. For these graphs we calculate the maximum flow using a fast max-flow/min-cut algorithm, developed in algorithmic graph theory, which allows us to address large system sizes. Therein the minimum cut corresponds to a ground-state configuration of the system.

Using finite-size scaling, we obtain critical scaling exponents for correlation length, energy, magnetisation and susceptibility. The results for $d = 5$ to $d = 7$ are compared with the mean-field exponents of the RFIM, since from $d_u = 6$ on the mean-field exponents are expected to hold.

DY 3.4 Mon 14:45 H42

A dedicated algorithm for calculating ground states for the triangular random bond Ising model — •Oliver Melchert and Alexander K. Hartmann — Institut für Physik, Universität Oldenburg, Carl-von-Ossietzky Str. 9-11, 26111 Oldenburg, Germany

Triggered by the exchange of ideas between computer science and theoretical physics, several disordered systems with complex energy landscapes can now be analyzed numerically exact through computer simulations [1] by using fast combinatorial optimization algorithms.

For example, the ground-state problem for the planar $2d$ random bond Ising model (RBIM) can be mapped to an auxiliary minimum-weight perfect matching problem, solvable in polynomial time. Consequently, the GS properties as well as minimum-energy domain wall (MEDW) excitations can be analyzed for large systems [2].

Here, we introduce a dedicated algorithm for the $2d$ RBIM on planar triangular lattices that improves on the running time of existing algorithms. Further, we investigate the critical behavior of the corresponding $T = 0$ ferromagnet to spin-glass transition, signaled by a breakdown of the magnetization, using finite-size scaling analyses of the MEDW excitation energy. Finally, we contrast our numerical results with previous simulations and presumably exact results [3].

[1] A.K. Hartmann, *Practical Guide to Computer Simulations*, World Scientific (2009)
[2] OM, and A.K. Hartmann, Phys. Rev. B **79** (2009) 184402
[3] J. Bendisch, Physica A 245 (1997) 560

DY 3.5 Mon 15:00 H42

Free-energy barriers of the 3D Edwards-Anderson-Ising spin glass model — •Andreas Nussbaumer, Elmar Bittner, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany

We investigate the three-dimensional Edwards-Anderson-Ising spin glass model using a combination of the multioverlap algorithm and parallel tempering methods. By using this combined algorithm we are able to perform simulations at much lower temperatures for the Edwards-Anderson-Ising model than previous studies. This is necessary to investigate the spin glass phase well below the spin-glass transition $T_g = 1.109(10)$ [M. Hasenbusch et al., Phys. Rev. B 78, 214205 (2008)]. In this talk we focus on the hierarchy of free-energy barriers which we determined from the measured overlap distributions for lattices up to $L = 12^3$ and temperatures down to $T = 0.5$.

DY 3.6 Mon 15:15 H42

Lower critical dimension of vector spin glasses — •Frank Beyer and Martin Weigel — Institut für Physik, KOMET 331, Johannes-Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

The free energy landscape of $O(n)$ vector spin glasses is simplified considerably in the limit of an infinite number of spin components ($n \to \infty$), i.e., for the spherical spin glass. This simplification comes about through the fact that in the limit of a large number of spin components the ground state of a finite system occupies only a finite-dimensional subspace in spin space. As a consequence, for each system size there exists a finite, critical number n^* of spin components above which the ground-state energy does not change upon further adding spin dimensions, such that the system effectively describes a spherical spin glass. Here, this observation is exploited for investigating the stability of the ordered phase of the spherical spin glass as a function of the spatial dimension of the lattice. Using the concept of the defect energy, we numerically determine the stiffness exponents for lattices of various spatial dimensions $d = 2, 3, \ldots$ and use these results to estimate the lower critical dimension of the model. The results are compared to estimates resulting from field-theoretic calulcations.

DY 3.7 Mon 15:30 H42

Investigation of overlaps between quasioptimum configurations of a multidisperse packing problem — •Johannes J. Schneider, Michael Kwasnicki, Andre Müller, and Elmar Schömer — Center for Computational Research Methods in Natural

Sciences, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We consider a multidisperse system of N hard disks with integer radii $r_i = i$, $i = 1, \ldots, N$, which have to be packed in a circular environment in the way that the radius of the circumcircle is minimized. With our packing algorithm, which was rated by the Time Magazine to be one of the 50 best inventions of the year 2009, we were able to match or beat all world records established during an international contest, in which 155 groups from 32 countries competed [1]. Besides these new world record configurations, we obtained a huge number of quasi optimum solutions. We could show that the subspace of these quasi optimum solutions exhibits an ultrametric structure [2]. Here we have a more precise look at the matrix of overlap values between the various quasioptimum configurations and show whether block structures such as in Parisi's solution of the SK model occur.

[1] A.M., J.J.S., E.S., Phys. Rev. E 79, 021102, 2009.
[2] J.J.S., A.M., E.S. Phys. Rev. E 79, 031122, 2009.

DY 3.8 Mon 15:45 H42

Efficient exploration of energy landscapes — •Martin Mann[1] and Konstantin Klemm[2] — [1]Bioinformatik, University of Freiburg, Germany — [2]Bioinformatik, University of Leipzig, Germany

Many physical and chemical processes, such as folding of biopolymers, are best described as dynamics on large combinatorial energy landscapes. A concise approximate description of dynamics is obtained by partitioning the micro-states of the landscape into macro-states. Since most landscapes of interest are not tractable analytically, the probabilities of transitions between macro-states need to be extracted numerically from the microscopic ones, typically by full enumeration of the state space.

Here we suggest a Markov chain Monte-Carlo sampling method for transition matrix estimation [1]. The idea is to explicitly explore boundaries between macro-states. To this end, we confine the dynamics into a single macro-state b and find and count possible transitions from b to all adjacent macro-states. This strategy allows to select the regions of the landscape to be explored and to tune the desired accuracy of the estimated transition probabilites. At difference with earlier approaches, the memory requirement scales linearly with the number of non-zero transition probabilities to be determined.

For landscapes of the number partitioning problem and an RNA switch molecule we show that the method allows for accurate probability estimates with significantly reduced computational cost.

[1] M. Mann, K. Klemm, e-print arXiv:0910.2559