

DY 27: Poster - Statistical Physics, Critical Phenomena, Brownian motion

Time: Tuesday 18:15–21:00

Location: Poster C

DY 27.1 Tue 18:15 Poster C

Phase separation in mixtures of soft particles in 2D: A dynamical DFT study — ●ALEXANDER KRAFT and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We investigate binary mixtures of soft particles (e.g. of Gaussian core type) in a two-dimensional system within the framework of density functional theory and dynamical density functional theory. Depending on system parameters, we observe homogeneous mixing or a phase separation of both species. In order to classify the system behaviour, we calculate the phase diagram, i.e. the spinodal and binodal lines, based on thermodynamic stability conditions. Furthermore, we compare the regions of thermodynamic stability with estimates based on linear stability analysis of the homogeneously mixed system. In contrast to previous studies [1,2], in this work, we focus on a two-dimensional system, in order to gain access to the behaviour in flat geometries or on surfaces. We also discuss possible control strategies for the manipulation of the phase separation process.

[1] A. A. Louis, P. G. Bolhuis, and J. P. Hansen, *Phys. Rev. E* **62**, 7961 (2000)

[2] A. J. Archer and R. Evans, *Phys. Rev. E* **64** (2001)

DY 27.2 Tue 18:15 Poster C

P-T-V equations of state for III-V compound semiconductors — ●ALRIK STEGMAIER, ULRICH VETTER, and HANS HOFSSÄSS — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Equations of state (EoS) for solids are necessary for relating the state variables to each other and an important application is the description of the technologically important III-V compound semiconductors at different temperatures and pressures.

While many general EoS for solids exist, the introduction of a temperature dependence is not unique [1] and the materials considered here have negative thermal expansion coefficients at low temperatures [2], hampering a simple but accurate description. Further more, EoS are often not easily invertible [3] and several constraints have been suggested for isothermal EoS for solids that are not fulfilled by all formulations [4].

Here several EoS for III-V compound semiconductors are compared against experimental data and the results of ab-initio calculations. As a result a general P-T-V equation of state is proposed that is relatively accurate, simple, invertible and approximately fulfills the constraints reported in the literature for such an equation.

[1] R. E. Cohen et al., *Am. Mineral.*, 85(4), 338-344, 2000

[2] G. Dolling and R. A. Cowley, *Proc. Phys. Soc.*, 88, 463, 1965

[3] M. Etter and R. E. Dinnebier, *J. Appl. Cryst.*, 47, 384-390, 2014

[4] P. K. Singh and A. Dwivedi, *Indian J. Pure & Appl. Phys.*, 50, 734-738, 2012

DY 27.3 Tue 18:15 Poster C

Bi-stable state on the prestructured surface: Free energy calculation — ●OLEG BULLER, LISA GÖTTE, and ANDREAS HEUER — Institut für Physikalische Chemie, WWU, Münster

Attachment of molecules on a prepatterned surface by vapor deposition displays a wide variety of resulting structures. We are interested in the single stripe and double stripe prepattern. For the case of a single stripe geometry an instability is observed forming a bulge. A second stripe close-by can destabilize the bulge leading to the agglomeration of the molecules in-between the stripes. We model this system by a kinetic Monte Carlo model and calculate the relative free energies by using Markov State sampling techniques. We analyze the influence on the stripe distance and the amount of particles forming a bulge.

DY 27.4 Tue 18:15 Poster C

The Voronoi liquid — ●CÉLINE RUSCHER, JÖRG BASCHNAGEL, and JEAN FARAGO — Institut Charles Sadron, Strasbourg, France

Voronoi tessellations are defined as a mathematical partition of the space where a cell containing the point of interest is defined through the points of space which are the closest from this point than from any other. In soft matter physics Voronoi tessellations are widely used to probe the local environment of particles.

We describe here a new model of fluid called the Voronoi fluid where the force field is directly expressed through the intrinsic properties of the Voronoi tessellations. Due to its definition this monodisperse fluid presents many-body interactions and there is no excluded volume. Moreover the force field derives from a potential energy which exhibits scaling properties.

Thermodynamics and microscopic observables of the Voronoi fluid are both investigated through numerical simulations. Similarities with simple liquids have been observed however some differences occur. For instance an unexpected relation between the pair correlation function and the chemical potential has been found and the dynamic structure factor exhibits an unusual behavior in the hydrodynamic regime.

Finally we observed that when the Voronoi fluid crystallizes into a BCC an atypical behavior appears. Below the melting point particles move leaving the whole structure unchanged. As the motion seems to be a collective phenomenon these rearrangements appear to be a good indicator that the model can be extended to probe glass-forming systems.

DY 27.5 Tue 18:15 Poster C

Behavior of electronic states on random Voronoi-Delaunay lattices in the orthogonal and the unitary universality class — ●MARTIN PUSCHMANN¹, PHILIPP CAIN¹, MICHAEL SCHREIBER¹, and THOMAS VOJTA² — ¹Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — ²Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, USA

The random Voronoi-Delaunay lattice (VDL) is defined as a set of bonds between randomly positioned sites. The bonds connect neighboring Voronoi cells and are obtained by the Delaunay triangulation. The resulting topologically disordered lattice features strong anticorrelations between the coordination numbers of neighboring sites. The disorder fluctuations therefore decay qualitatively faster with increasing length scale than those of generic random systems. A recent study showed that this modifies the Harris and Imry-Ma criteria and leads to qualitatively changes of the scaling behavior at magnetic phase transitions [1]. We consider the transport of non-interacting electrons on two- and three dimensional random VDLs without and with magnetic fields. The electronic wave functions are analyzed by multifractal analysis. Without magnetic fields, we obtain results in accordance to the orthogonal universality class [2]. Applying magnetic fields introduces a phase shift to the local wave function. This shift is proportional to the area of the local Delaunay triangle. We show how the topological aspect affects the behavior of the wave functions in magnetic VDLs and whether this is compatible with unitary universality class.

[1] PRL 113, 120602 (2014) [2] EPJ B 88, 314 (2015)

DY 27.6 Tue 18:15 Poster C

Spin glasses with variable frustration — ●RAVINDER KUMAR^{1,2}, MARTIN WEIGEL¹, and WOLFHARD JANKE² — ¹Applied Mathematics Research Centre, Coventry University, Coventry, UK. — ²Institut für Theoretische Physik, Leipzig University, Leipzig, Germany.

Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behavior in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure [1].

[1] Efe Ilker and A. Nihat Berker, *Phys. Rev. E* 89, 042139 (2014).

DY 27.7 Tue 18:15 Poster C

Using entanglement to discern phases in the disordered one-dimensional Bose-Hubbard model — ANDREW M. GOLDSBOROUGH^{1,2} and ●RUDOLF A. RÖMER² — ¹JARA Institute for Quantum Information, RWTH Aachen University - D-52056 Aachen, Germany — ²University of Warwick, Coventry CV4 7AL, UK

We perform a matrix-product-state based density matrix renormalisation group analysis of the phases for the disordered one-dimensional

Bose-Hubbard model. For particle densities $N/L = 1, 1/2$ and 2 we show that it is possible to obtain a full phase diagram using only the entanglement properties, which come for free when performing an update. We confirm the presence of Mott insulating, superfluid and Bose glass phases when $N/L = 1$ and $1/2$ (without the Mott insulator) as found in previous studies. For the $N/L = 2$ system we find a double-lobed superfluid phase with possible re-entrance.

DY 27.8 Tue 18:15 Poster C

Characterization of multifractality at the Anderson transition from wavefunction dynamics — CHI-HUNG WENG, ANDREAS BUCHLEITNER, and ●ALBERTO RODRIGUEZ — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

While stationary numerical techniques to obtain the multifractal spectrum from eigenstates close to the Anderson transition have been extensively studied, the implications of multifractality on the dynamics close to the critical point, and in particular the validation of the different proposed dynamical scaling laws involving multifractal exponents have not received comparable attention. The dynamical approach may however be crucial for the characterization of multifractality from experimental data of the expansion of wave packets in disordered potentials. For this task, we consider several scaling laws: the scaling of the return probability with time, the decaying profile of the time-dependent wavefunction with distance, and the scaling of the long-time return probability with system size. We present a thorough analysis of the regimes of validity of these scaling laws and their suitability to obtain a reliable estimate of the multifractal exponent D_2 from the dynamics of a localized initial excitation in a critical power-law random banded matrix model.

DY 27.9 Tue 18:15 Poster C

Optimal performance under limited control of periodically driven, stochastic heat engines — ●MICHAEL BAUER¹, KAY BRANDNER^{1,2}, and UDO SEIFERT¹ — ¹II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — ²Department of Applied Physics, Aalto University, 00076 Aalto, Finland

We investigate the performance of periodically driven, stochastic heat engines under optimal driving in the linear response regime. The Onsager coefficients for such machines obeying Fokker-Planck dynamics have recently been developed and illustrated with an overdamped Brownian particle, where the driving protocol allows full control on the particle [1].

Here, we are interested in the performance of such heat engines if only a limited number of degrees of freedom can be externally controlled. In a case study, we examine a heat engine consisting of an underdamped Brownian particle in a magnetic field, where the kinetic degrees of freedom cannot be controlled. We find expressions for the efficiency in analogy to the performance of thermoelectric devices and define an adequate figure of merit. In the absence of a magnetic field, more general results are obtained if the control functions are assumed to be given by the eigenfunctions of the adjoint Fokker-Planck operator. We recover the expressions of the case study and obtain a condition for the attainability of Carnot efficiency.

[1] K. Brandner, K. Saito, and U. Seifert, Phys. Rev. X 5, 031019 (2015)

DY 27.10 Tue 18:15 Poster C

Aging Universality Classes in Surface Growth Models — ●JEFFREY KELLING¹, GEZA ODOR², and SIBYLLE GEMMING^{1,3} — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — ²MTA-EK-MFA Institute of Technical Physics and Materials Science, Budapest, Hungary — ³Institute of Physics, TU-Chemnitz, Germany

Extensive dynamical simulations of a 2 dimensional driven dimer lattice gas are presented, which can be mapped to (2+1) dimensional surface growth in the Kardar-Parisi-Zhang (KPZ) or Edwards-Wilkinson universality classes. From this autocorrelation and autoresponse functions have been determined for the KPZ universality class and the underlying lattice gas. Studying the effects of different dimer lattice gas dynamics revealed strong differences in the aging behavior of the

stochastic cellular automaton (SCA) and the random sequential update models. We show numerical evidence for nontrivial corrections as well as different universal scaling behaviors.

DY 27.11 Tue 18:15 Poster C

Transport of colloidal particles under the impact of time-delayed feedback control — ●SARAH A. M. LOOS and SABINE H. L. KLAPP — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We explore possibilities to analytically investigate the influence of time-delayed feedback control on transport and diffusion of overdamped Brownian particles in one dimension [1]. In particular, we consider particles in static external potentials supplemented by linear feedback forces, where the delayed particle position serves as control target. We use both, the equation of motion which is given by a non-Markovian Langevin equation, and the equation of the temporal evolution of the corresponding probability density field, i.e., the delayed Fokker-Planck equation [2,3]. We have thus access to the fluctuating trajectories as well as to the deterministic evolution of the density field. We focus on theoretical predictions of transport and diffusion properties such as the mean particle position and the mean squared displacement. In order to validate our analytical findings, we compare them with numerical results obtained by Brownian dynamics simulations. We further discuss possible applications to the case of interacting particles.

[1] R. Gernert, et al., arXiv:1511.00413 (2015).

[2] S. Guillouez et al., Phys. Rev. E 59, 3970 (1999).

[3] T. D. Frank, Phys. Rev. E 71, 031106 (2005).

DY 27.12 Tue 18:15 Poster C

Effective Perrin Theory for a Liquid of Infinitely Thin Brownian Needles — ●SEBASTIAN LEITMANN¹, FELIX HÖFLING², and THOMAS FRANOSCH¹ — ¹Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — ²Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany, and Institut für Theoretische Physik IV, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Liquids of infinitely thin Brownian needles of length L are considered up to reduced densities of $n^* = nL^3 > 10^3$ deep in the semidilute regime $n^* > 1$. By a stochastic simulation of a liquid of subsequent moving particles, we corroborate the scaling behavior n^{*-2} of the diffusion coefficients of a needle liquid. We find excellent agreement between the intermediate scattering function in the semidilute regime and a full analytic solution for a freely moving rod with the transport coefficients obtained from stochastic simulation as input parameters. We argue, that the single-needle dynamics in the liquid is asymptotically insensitive to the dynamic rearrangement of the surroundings. Therefore, we map the problem to the movement of a single needle in a frozen disordered array of needles, which enables us to characterize the dynamics in a considerably wider time window.

DY 27.13 Tue 18:15 Poster C

Random matrices and condensation into multiple states — ●SINA SADEGHI and ANDREAS ENGEL — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Germany

Condensation is a collective phenomenon that ubiquitously occurs in nature. A well-known example in physics is the Bose-Einstein condensation of a bosonic gas in equilibrium into its ground state at low temperature. Recently, it has been shown that a driven-dissipative bosonic gas may condensate into multiple states rather than into a single one [Phys. Rev. Lett. 111, 240405 (2014)] and a connection between such non-equilibrium condensation and evolutionary game theory has been established [Nat. Comm. 6, 6977 (2015)]. In the present work we employ statistical mechanics methods from disordered systems to investigate static properties of condensation in a general framework. We aim at showing how typical properties of random interaction matrices play a vital role in manifesting the statistics of condensate states. To this end we study the interplay between the condensation problem and zero-sum games with random pay-off matrices. We show for the game theoretical problem that as far as static quantities are concerned spherical and simplex constraints for the degrees of freedom are equivalent. This is advantageous also in the case of condensation since the number of order parameters is reduced which simplifies the analysis.