

## DY 62: Critical Phenomena and Phase Transitions

Time: Friday 9:30–11:45

Location: ZEU 118

DY 62.1 Fri 9:30 ZEU 118

**Quasiparticles as Detector of Topological Quantum Phase Transitions** — ●SOURAV MANNA<sup>1</sup>, SRIVATSA NAGARA SRINIVASA PRASANNA<sup>1</sup>, JULIA WILDEBOER<sup>2</sup>, and ANNE E. B. NIELSEN<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — <sup>2</sup>Department of Physics, Arizona State University, Tempe, AZ 85287, USA

Phases and phase transitions provide an important framework to understand the physics of strongly correlated quantum many-body systems. Topologically ordered phases of matter are particularly challenging in this context, because they are characterized by long-range entanglement and go beyond the Landau-Ginzburg theory. A few tools have been developed to study topological phase transitions, but the needed computations are generally demanding, they typically require the system to have particular boundary conditions, and they often provide only partial information. There is hence a high demand for developing further probes. Here, we propose to use the study of quasiparticle properties to detect phase transitions. Topologically ordered states support anyonic quasiparticles with special braiding properties and fractional charge. Being able to generate a given type of anyons in a system is a direct method to detect the topology, and the approach is independent from the choice of boundary conditions. We provide three examples, and for all of them we find that it is sufficient to study the anyon charge to detect the phase transition point. This makes the method numerically cheap.

DY 62.2 Fri 9:45 ZEU 118

**Critical Exponents of the Ising Model in Three Dimensions with Long-range Correlated Site Disorder** — ●STANISLAV KAZMIN<sup>1,2</sup> and WOLFHARD JANKE<sup>2</sup> — <sup>1</sup>Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — <sup>2</sup>University Leipzig, Institute for Theoretical Physics, Leipzig, Germany

We study the Ising model in three dimensions with site dilution with the help of Monte Carlo techniques. The dilution is long-range correlated and the correlation function decays proportional to a power law  $\propto r^{-a}$ . We derive the critical exponent of the correlation length  $\nu$  in dependence of  $a$  by combining different defect concentrations  $0.1 \leq p_d \leq 0.4$  and by applying finite-size scaling techniques to the derivative of the logarithm of the magnetization  $\partial_\beta \ln |m|$ . We study a wide range of correlation exponents  $1.5 \leq a \leq 3.5$  as well as the uncorrelated case  $a = \infty$ . Finally, we compare our results to known estimates from other works and to the conjecture of Weinrib and Halperin:  $\nu = 2/a$ .

DY 62.3 Fri 10:00 ZEU 118

**Exchange between two phases of confined water using deuteron two-dimensional exchange NMR** — ●VERENA FELLA and MICHAEL VOGEL — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Understanding the properties of water in confinement is an important task due to its many applications in life science and technology. Nano-confinement reduces the crystallization temperature of water to lower values and enables supercooling to temperatures even below the nucleation temperature. Our previous studies [Yao et al., Langmuir (2019)], [Weigler et al., J. Phys. Chem. B (2019)] identified two dynamically distinguishable fractions of water coexisting within the pores at sufficiently low temperatures. These fractions correspond to a liquid interfacial water layer and a less mobile water phase in the pore center. We conjecture that highly distorted and unstable crystal nuclei exist under extreme confinement that exhibit reorientational dynamics with time scales intermediate to the confined liquid and to bulk ice. This leads to a complex and heterogeneous system inside the pores. One of the still open questions is the potential exchange between both water species and the time scales on which it occurs. Therefore we measure <sup>2</sup>H two-dimensional NMR spectra of water in mesoporous silica materials. This method is well suited for heterogeneous systems because it directly probes exchange processes between fast and slow subensembles [Vogel, Rössler, J. Phys. Chem. A (1998)]. By varying the temperature and mixing time of the experiment we determine the time scale of these processes.

DY 62.4 Fri 10:15 ZEU 118

**Acceptance rate is a thermodynamic function in local Monte Carlo algorithms** — EVGENI BUROVSKI<sup>1</sup>, ●WOLFHARD JANKE<sup>2</sup>, MARIA GUSKOVA<sup>1</sup>, and LEV SHCHUR<sup>1,3</sup> — <sup>1</sup>National Research University Higher School of Economics, 101000 Moscow, Russia — <sup>2</sup>Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — <sup>3</sup>Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia

We study properties of Markov chain Monte Carlo simulations of classical spin models with local updates. We derive analytic expressions for the mean value of the acceptance rate of single-spin-flip algorithms (Metropolis, heat bath) for the one-dimensional Ising chain with periodic boundary conditions. For the Metropolis algorithm we find that the average acceptance rate is a linear function of energy, independent of the chain length. We further provide numerical results for the energy dependence of the average acceptance rate for the three- and four-state Potts model, and the XY model in one and two spatial dimensions. In all cases, the acceptance rate is an almost linear function of the energy in the critical region. The variance of the acceptance rate is studied as a function of the specific heat. While the specific heat develops a singularity in the vicinity of a phase transition, the variance of the acceptance rate stays finite.

DY 62.5 Fri 10:30 ZEU 118

**Lindemann melting criterion in two dimensions** — ●SERGEY KHRAPAK — Institut fuer Materialphysik im Weltraum, Deutsches Zentrum fuer Luft- und Raumfahrt (DLR), 82234 Wessling, Germany

It is well known that the conventional Lindemann's melting criterion is not applicable to two-dimensional (2D) solids, because long-wavelength density fluctuations cause the mean square displacement to diverge logarithmically with system size. Here it is demonstrated that the Lindemann's criterion can be re-formulated for 2D solids using statistical mechanics arguments. With this formulation the expressions for the melting temperature are essentially equivalent in three and two dimensions. Moreover, in two dimensions the Lindemann's melting criterion practically coincides with the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young melting condition of dislocation unbinding. Examples of application are provided.

15 min. break.

DY 62.6 Fri 11:00 ZEU 118

**Fermionic Criticality Out-of-Equilibrium** — ●BERNHARD FRANK — Max-Planck-Institut für Physik komplexer Systeme — Dresden

Critical Fermions, like strange metals, exhibit correlation functions with universal, anomalous power laws, which lead to deviations from Fermi liquid results both for thermodynamic and transport quantities. Coupling a massless bosonic degree of freedom to the Fermi surface provides one mechanism to create these unconventional states of matter that so far have only been studied in thermal equilibrium. However, recent experiments combine semi-conductor devices with optical cavities and therefore mandatorily require a theoretical formulation that takes into account the intrinsically driven-dissipative nature of the photon in order to understand the electronic many-body state. Based on Keldysh quantum field theory we study a simple two-dimensional model for a strange metal out-of-equilibrium. Compared to the situation in the ground state one observes increased decay rates in the low-energy sector of the fermionic spectrum as well as a violation of the thermal fluctuation dissipation relation caused by the enhanced bosonic fluctuations generated by the drive.

DY 62.7 Fri 11:15 ZEU 118

**Bond-flip Monte Carlo based on exact results for the square lattice  $\pm J$  Ising model** — JAN BÜDEFELD and ●FRED HUCHT — Fakultät für Physik, Universität Duisburg-Essen

We present preliminary results on a Monte Carlo method with single bond-flip dynamics for the square lattice Ising model with  $\pm J$  couplings and arbitrary boundary conditions. Using a recently derived exact expression for the free energy of a system with arbitrary nearest neighbor couplings  $J_{ij}$  on the torus, we propose an efficient update scheme for the calculation of the free energy change under a bond flip. We numerically calculate the density of states of the bond ensemble and discuss advantages and disadvantages of the method.

DY 62.8 Fri 11:30 ZEU 118

**Detecting hidden and composite orders in layered models via machine learning** — ●WOJCIECH RZADKOWSKI<sup>1</sup>, NICOLO DEFENU<sup>2</sup>, SILVIA CHIACCHIERA<sup>3</sup>, ANDREA TROMBETTONI<sup>4</sup>, and GIACOMO BIGHIN<sup>1</sup> — <sup>1</sup>Institute of Science and Technology Austria (IST Austria), Am Campus 1, 3400 Klosterneuburg, Austria — <sup>2</sup>Institut für Theoretische Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — <sup>3</sup>Science and Technology Facilities Council (STFC/UKRI), Daresbury Laboratory, Keckwick Lane, Daresbury, Warrington WA44AD, United Kingdom — <sup>4</sup>CNR-IOM DEMOCRITOS Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy

Recently, machine learning is applied to the study of phase diagrams

of spin models. After initial success with supervised approaches, unsupervised techniques are being extensively developed.

We use an unsupervised technique to study layered spin models where composite order parameters may emerge as a consequence of the interlayer coupling. We determine their phase diagram, applying an algorithm based on convolutional neural networks to the raw Monte Carlo data. Remarkably our technique [1] is able to characterize all the system phases also in the case of hidden order parameters, i.e. order parameters whose expression in terms of the microscopic configurations would require additional preprocessing of the data fed to the algorithm.

[1] W. Rzadkowski, N. Defenu, S. Chiacchiera, A. Trombettoni, G. Bighin, arXiv:1907.05417 (2019)