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Editorial

Recent advances in phase transitions and critical phenomena

Festschrift on the occasion of Wolfhard Janke's 60th birthday

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Abstract. Phase transitions and critical phenomena are of ubiquitous importance from the femtometre scale in quantum chromodynamics to galaxy formation in the universe, from the folding, adsorption or denaturation of bio-polymers to the magnetisation effects in storage media, from percolation in complex social networks to fragmentation transitions in atomic nuclei. The present issue discusses a cross section of the current research on phase transitions and critical phenomena in condensed-matter physics, with a focus on soft and hard matter systems as well as the most important methods used for studying such problems.

The study of phase transitions is by now a quite mature subject. Early notions akin to modern ideas of phase transitions are already present in ancient Greek philosophical texts, for instance in Aristotle's theory of the elements. Still, it was only in the late 18th and early 19th century that the advent of the steam engine necessitated a profound theoretical description. This clarified the conversion of heat from and to mechanical work, helped establish an abstract notion of energy, and finally resulted in the formulation of the laws of thermodynamics. The evaporation and condensation of water in the steam engine are prototypic examples of first-order phase transitions. As the temperature or pressure are increased, this system eventually reaches a critical point at which liquid and vapor become indistinguishable. The transition is no longer discontinuous but becomes continuous there. The character of this special point was

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only fully understood with the introduction of the renormalization group by Kadanoff and Wilson about 50 years ago, which explains scaling and universality and now serves as a complete fundamental theory of critical phenomena.

While the foundations of the subject hence stand firm, there are many aspects of the theory which have only recently been worked out or are still under dispute, and which are hence at the centre of very active current research efforts. These include the effect of confinement that is relevant in biological systems such as proteins in the cell or in thin films of magnetic materials. In the former case entropic effects become relevant, while in the latter case the dimensional crossover from films to fully three-dimensional structures matters. To the extent that such confinement is still macroscopic or mesoscopic, its effects in the vicinity of phase transitions are described by the theory of finite-size scaling, which is by now well developed both for first-order and for second-order phase transitions. For sufficiently small systems, on the other hand, such as (bio-)polymers or fluids in nano-pores it is often no longer useful to describe them in terms of an idealized thermodynamic limit as they are of an intrinsic finite size that is constitutive of their particular nature. This applies, for instance, to a protein defined by a specific length and sequence of amino-acids. In these cases, the established notions of phase transitions as non-analyticities in the free energy no longer apply and the different thermodynamic ensembles remain distinct. The required thermodynamic theory for small systems has been the subject of much recent research.

The classic theoretical frameworks such as Landau theory, the renormalization group and approaches for first-order transitions are essentially focused on the behavior in thermal equilibrium, with the exception of the phenomenon of metastability at first-order transitions and related problems. In nature, however, equilibrium does not exist, and it is merely an idealized state towards which a system might or might not develop. Relaxation towards an equilibrium state occurs for instance for quenches from one phase to another, and the underlying kinetic description of phase transitions has been developed more recently. In driven systems, on the other hand, no relaxation to equilibrium can be expected, but non-equilibrium steady states can occur and as control parameters are varied the system might undergo transitions between different non-equilibrium phases. Examples are directed percolation and epidemic spreading. Such behavior is understood by an analysis of the associated master equations, but also by a suitable generalization of the equilibrium approaches, such as the scale invariance found for critical systems to the time domain.

The behavior of systems with disorder has puzzled the community for decades. One class of systems is characterized by quenched impurities that do not fluctuate on the physically relevant time scales. Here, systems with weak, non-frustrating disorder are comparatively well understood: first-order transitions are softened by the disorder, continuous transitions acquire new critical exponents if the disorder is relevant. For frustrating disorder as it is found in spin glasses and random-field models, the situation is less clear, and significant disputes about the nature of the transitions and the ordered phases remain. A second class is formed by systems with self-induced disorder, such as in structural glasses, gels and jammed states of matter. Here, even the question of whether an equilibrium phase transition occurs is only recently coming significantly closer to a definite answer.

While most of these problems live in the domain of classical physics, a lot of interest is now focused on the behavior of systems that are inherently quantum in nature. In equilibrium this includes quantum phase transitions that occur at zero temperature, but dynamical transitions following quantum quenches are now widely studied too. Investigations of such phenomena are fuelled by the wide availability of experimental realizations in the form of cold atoms on optical lattices that allow for the direct observation of many phenomena relating to phase transitions in (quantum)

spin systems. The approach to equilibrium and the questions of the relation between system and bath are particularly natural subjects for the quantum case.

While progress up until the late sixties and early seventies of the 20th century was achieved in an interplay of experimental and analytical work only, the possibility of also performing numerical studies to understand phase transitions and critical phenomena has dramatically changed the landscape of research in the field. It is now a combination of analytical and numerical work that determines the theoretical understanding of such systems. While the classic renormalization group (RG) with its core approach of the ϵ expansion has found manifold extensions in more modern techniques such as conformal field theory, stochastic Loewner evolution or functional RG, simulation methods have evolved from the basic single-particle Metropolis updates and NVE ensemble simulations of particle systems to encompass generalized ensembles, collective moves, the sampling of rare events and transition states and methods suitable for massively parallel architectures.

The study of phase transitions and critical phenomena is thus a well established, but by no means a complete and hence closed field of research. Against the backdrop of a well-established theory there is a wealth of exciting new developments. These are the focus of the present issue. It was not possible to represent the full breadth of such developments in the articles to follow, but the selection of papers will still allow the interested reader to get an idea of important recent developments in the field, with a focus on the advancement of the methodological machinery and on applications in soft and hard matter physics.

The first series of papers revolves around the history and methodological developments in the field. The issue is opened by a translation and commentary by Sauer of the seminal 1933 paper by Ehrenfest setting out his famous classification of phase transitions [1]. Turning to simulation methods, Berg [2] reviews the history of generalized ensemble techniques with a focus on Markov chain Monte Carlo simulations. Hartmann [3] applies such reweighting methods and importance sampling to the estimation of rare events in random graphs to reveal the large deviation behavior of observables. While cluster updates for short-ranged interactions are standard textbook knowledge, this is less the case for methods for systems with long-ranged interactions. Flores-Sola et al. review the available approaches and propose a new single-cluster update for spin systems with power-law interactions [4]. A recent new addition in the simulational toolbox that is particularly well suited for massively parallel architectures, population annealing, is discussed by Barash et al. [5] with applications to the simulation of first-order phase transitions. Moving away from equilibrium applications, Henkel [6] gives a tutorial introduction to dynamical scaling and its consequence in the theory of local scale invariance with applications in ageing.

A second series of papers concerns the statistical physics of polymers. For proteins, the physics of folding is a subject of sustained interest. Irbäck et al. [7] review experiments and simulations for the problem of folding in the presence of molecular crowders, where intelligently designed coarse-grained models are required to see the relevant behavior with present-day computational resources. Suitable techniques for determining the folded ground state are discussed for the HP lattice model of proteins by Günther et al. [8], focusing on the thermal cycling approach. Polymer-colloid mixtures in confinement are the topic of the review by Usatenko et al. [9], which discusses the effects of polymer topology as well as different confining potentials, such as slits, with a focus on the field-theoretic treatment of such problems. Single chains of polymers are studied in the papers by Ivanov et al. [10], Zierenberg et al. [11] and Shakirov et al. [13]. Ivanov et al. report on simulations of poly(3-hexylthiophene) (P3HT), comparing the results of three different effective models for the system. Zierenberg et al. focus on the effects of grafting two flexible polymers to a surface at nearby points, finding a continuous binding transition due to a reduction

of translational entropy. The conceptual difficulties relating to the analysis of finite systems with thermodynamic methods are discussed in the contribution by Shakirov et al. [13], who consider single-chain phase transitions of polymers and analyze Monte Carlo data using Boltzmann as well as Gibbs entropies and taking into account the full microcanonical energy. The dynamics of polymer melts are the subject of the article by Hsu et al. [12]. The authors report on extensive molecular dynamics simulations, extracting the scaling behavior of the autocorrelation function through a Rouse mode analysis. Finally, Landsgesell et al. [14] compare the reaction ensemble method and the constant pH approach for the simulation of weak polyelectrolytes, illustrating their findings for a coarse-grained bead-spring model.

The final section of this issue comprises papers dealing with lattice systems. One of the most widely discussed and arguably the simplest model system for phase transitions is the percolation problem. Adler et al. [15] review the history of percolation as a model for phase transitions and discuss contemporary applications, in particular from an educational perspective, but also including realizations of bootstrap percolation in condensed matter physics. While finite-size scaling at first-order phase transitions seemed to have been well understood, it recently turned out that for models with highly degenerate ordered phases the established theory requires modification. These effects are discussed by Johnston et al. [16] for the case of the gonihedric Ising model. The kinetics of phase ordering for the Ising model are studied by Das et al. [17], who report on their finding of different domain growth, ageing and persistence for quenches to temperatures above or below the roughening transition of the three-dimensional Ising model. Turning to systems with continuous degrees of freedom, Selke et al. [18] present results on an anisotropic XY model in a field, revealing surprisingly rich phase diagrams in two and three dimensions with lines of first- and second-order transitions and a bicritical point. A classical example of tricriticality is provided by the Blume-Capel or spin-1 Ising model that is reviewed for two dimensions in the contribution by Zierenberg et al. [19]. The phase diagram of the model is mapped out with Monte Carlo simulations, carefully studying the finite-size scaling, in particular in the region of first-order transitions. The final article by Chatelain [20] is dedicated to the physics of disordered systems, discussing the behavior of the Potts model on a disordered substrate with long-ranged correlations. With a stability analysis of the correlated percolation fixed point it is shown that for this problem the asymptotic regime is inaccessible to numerical simulations.

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