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Geometrical phase transitions

Wolfhard Janke, Adriaan M.J. Schakel *

Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

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Abstract

The geometrical approach to phase transitions is illustrated by simulating the high-temperature representation of the Ising model on a square lattice.
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1. Prelude

The geometrical approach to phase transitions is an exciting research topic in contemporary physics. The approach is patterned after percolation theory which describes clusters of randomly occupied sites or bonds on a lattice [1]. The fractal structure of these geometrical objects and whether or not a cluster spans the lattice are central topics addressed by percolation theory. By lumping together with a certain temperature-dependent probability neighboring spins in the same spin state, spin models such as the q-state Potts models can be mapped onto percolation theory [2]. The resulting Fortuin–Kasteleyn spin clusters percolate at the critical temperature, while their percolation exponents coincide with the thermal ones. In this way, a purely geometrical description of the phase transition in these models was achieved.

Percolation theory is generic and transparent at the same time, making it easy to adapt for the description of other geometrical objects such as lines and domain walls. Typical line objects featuring in phase transitions are, for example, (i) vortex lines in superfluids with a spontaneously broken global U(1) symmetry or in gauge theories, and (ii) worldlines in Bose–Einstein condensates:

(i) Because of topological constraints, vortices in a superfluid cannot terminate inside the system and generally form closed loops. Whereas in the broken-symmetry phase only a few small vortex loops are present, loops of all sizes appear at the critical point. A typical configuration then has one very large vortex loop and many smaller ones. In other words, *the*

* Corresponding author.
E-mail addresses: janke@itp.uni-leipzig.de (W. Janke), schakel@itp.uni-leipzig.de (A.M.J. Schakel).

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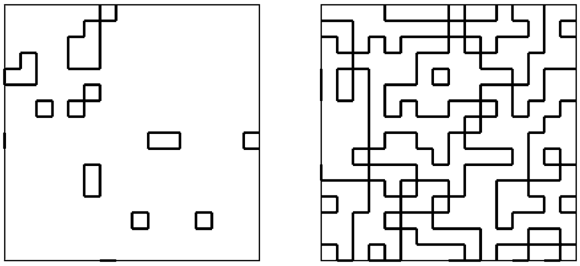

Fig. 1. Typical HT graph configurations generated on a 16×16 square lattice with periodic boundary conditions in the high- (left panel) and low-temperature (right panel) phase.

superfluid is pierced through and through with vortex line [3]. This vortex proliferation is in complete analogy to the presence of a spanning cluster at the percolation threshold in percolation phenomena. The disordering effect of the proliferating vortices destroys superfluidity in a superfluid, and often leads to charge confinement in gauge theories (both Abelian and non-Abelian).

(ii) Boson worldlines at finite temperature form closed loops in imaginary time. Feynman's theory of Bose–Einstein condensation asserts that upon lowering the temperature, small loops describing single particles hook up to form larger exchange rings, so that the particles become indistinguishable [4]. At the critical temperature, again as in percolation phenomena, worldlines proliferate and loops of arbitrary size appear, signaling the onset of Bose–Einstein condensation. The fractal structure of these worldlines encode the thermal critical exponents of the phase transition [5].

In this contribution, we report numerical results on the geometrical approach to the Ising model on a square lattice [6]. We consider the high-temperature (HT) representation of the model which, as is common for HT or strong-coupling representations, can be represented by closed graphs on the lattice. We do not enumerate all possible graphs to a given order, as is usually done in HT series expansions [7], but instead generate HT graphs by means of a Metropolis plaquette update [8] and study their fractal structure (see Fig. 1). In the high-temperature phase, large graphs are exponentially suppressed. Upon lowering the temperature, graphs of increasing size are generated, cumulating in a proliferation of graphs at the critical point. From the percolation strength P_∞ (defined as the number of bonds per site in the largest graph) and the average graph size χ_G, the fractal dimension of the graphs is extracted through finite-size scaling. Our numerical results are in good agreement with the analytic prediction by Duplantier and Saleur [9], which was derived using the Coulomb gas map.

2. Order and entropy

Central in the geometrical description of phase transitions is the distribution l_n of the geometrical objects under consideration,

$$l_n \propto n^{-\tau} \mathrm{e}^{-\theta n}, \tag{1}$$

giving the average number density of objects of size n present. The distribution consists of two parts. The second is a Boltzmann factor which exponentially suppresses large objects. The suppression coefficient θ vanishes with an exponent $1/\sigma$ when the critical temperature T_c is approached, $\theta \propto |T_c - T|^{1/\sigma}$. At criticality, only the first factor survives and the distribution becomes algebraic: $l_n(T_c) \propto n^{-\tau}$. This factor, giving the number of ways an object of given size n can be implemented on the lattice, measures the configurational entropy. The exponent τ is related to the fractal dimension D of the objects via $\tau = d/D + 1$ as in percolation theory, where d is the space dimension. The algebraic behavior of the distribution implies that objects of arbitrary size appear. Together with the exponent σ, the so-called Fisher exponent τ determines the critical exponents through scaling relations. Note that only two independent exponents are needed to determine the entire set of thermal critical exponents. In the geometrical approach, this is reflected by the two parts comprising the distribution, with both having their own distinct physical meaning.

The average graph size χ_G is given in terms of the graph distribution l_n as [1] $\chi_G = \sum'_n n^2 l_n / \sum'_n n l_n$, where the prime on the sum indicates that the largest graph in each measurement is omitted. At the critical temperature, the percolation strength P_∞ and χ_G obey the finite-size scaling relations $P_\infty \sim L^{-\beta_G/\nu}$, $\chi_G \sim L^{\gamma_G/\nu}$, with the graph exponents [1] $\beta_G = (\tau_G - 2)/\sigma_G$, $\gamma_G = (3 - \tau_G)/\sigma_G$, and ν the correlation length exponent, which for the 2D Ising model takes the value

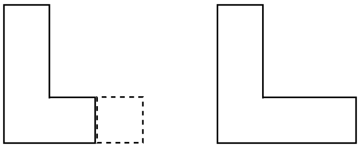

Fig. 2. Metropolis plaquette update at work. *Left panel*: Existing HT graph with the plaquette proposed for updating indicated by the broken square. *Right panel*: New graph after the proposal is accepted.

$\nu = 1$. Measurement of these two observables using different lattice sizes gives the two exponents β_G, γ_G from which in turn the graph distribution exponents τ_G and σ_G can be extracted.

3. Plaquette update

The well-known HT representation of the Ising model on a square lattice reads:

$$Z = (\cosh\beta)^{2N} 2^N \sum_{\{\Gamma_O\}} v^n, \tag{2}$$

where $\{\Gamma_O\}$ denotes the set of *closed* graphs specified by n occupied bonds, N is the total number of sites, and $v = \tanh\beta$, with β the inverse temperature. The closed graphs are generated by means of a Metropolis plaquette algorithm, where a proposed plaquette update resulting in n' occupied bonds is accepted with probability $p_{HT} = \min(1, v^{n'-n})$, with n denoting the number of occupied bonds before the update [8]. Reflecting the Z_2 symmetry of the Ising model, all bonds of an accepted plaquette are changed, i.e. those that were occupied become unoccupied and *vice versa* (see Fig. 2). By the famous Kramers–Wannier duality, the HT graphs form Peierls domain walls between spin clusters of opposite orientation on the dual lattice, and in the infinite-volume limit the plaquette update is equivalent to a single spin update on that lattice [6].

4. Results

To determine whether the HT graphs proliferate precisely at the critical temperature, we measure the so-called spanning probability P_S as function of β for different lattice sizes. Giving the probability for the presence of a graph spanning the lattice, P_S tends to zero for small β, while it tends to unity for large β. This observable has no scaling dimension and plays the role of the Binder cumulant in standard thermodynamic studies, so that the crossing point of the curves obtained for different lattice sizes marks the proliferation temperature of the infinite system. Within the achieved accuracy, we found that the measured curves cross at the thermal critical point, implying that the HT graphs (domain walls) lose their line tension θ and proliferate precisely at the Curie point (see Fig. 3). For the graph exponents we found [6] $\beta_G = 0.626(7)$, $\gamma_G = 0.740(4)$, leading to $\sigma_G = 0.732(6)$, $\tau_G = 2.458(5)$ in perfect agreement with the exact values $\sigma_G = 8/11 = 0.7273\ldots$, $\tau_G = 27/11 = 2.4546\ldots$, and the predicted fractal dimension [9] $D_G = 11/8$ of the HT graphs. From the HT graph exponents all the thermal critical exponents can be obtained, so that these graphs encode the critical behavior.

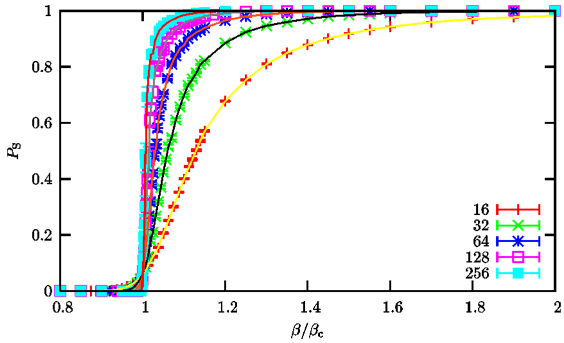

Fig. 3. Probability P_S for the presence of a spanning graph as function of the inverse temperature β measured for lattice sizes $L = 16, 32, 64, 128, 256$. Within the achieved accuracy, the curves cross at the thermal critical point $\beta = \beta_c$.

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