A dedicated algorithm for calculating ground states for the triangular random bond Ising model

O. Melchert, A. K. Hartmann

Institut für Physik, Universität Oldenburg, Carl-von-Ossietzky Straße 9–11, 26111 Oldenburg, Germany

Abstract

In the presented article we present an algorithm for the computation of ground state spin configurations for the 2*d* random bond Ising model on planar triangular lattice graphs. Therefore, it is explained how the respective ground state problem can be mapped to an auxiliary minimum-weight perfect matching problem, solvable in polynomial time. Consequently, the ground state properties as well as minimum-energy domain wall (MEDW) excitations for very large 2*d* systems, e.g. lattice graphs with up to $N = 384\times384$ spins, can be analyzed very fast.

Here, 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 magnetization and MEDW excitation energy and we contrast our numerical results with previous simulations and presumably exact results.

Keywords: Random bond Ising model, Negative-weight percolation, Groundstate phase transitions

1. Introduction

Triggered by the exchange of ideas between computer science and theoretical physics in the past decades, it was realized that several basic problems in the context of disordered systems relate to "easy" optimization problems. These are problems where the solution time is polynomial in the size of the problem description. As a result, many disordered systems can now be analyzed numerically exact through computer simulations by using fast combinatorial optimization algorithms [1, 2, 3]. E.g., ground state (GS) spin configurations for the random-field Ising magnet (in any dimension *d*) can be obtained by computing the maximum flow for an auxiliary network problem [2]. Another example is the 2*d* Ising spin glass (ISG), where the lattice can be embedded in a plane. For this model, the problem of finding a GS spin configuration for a given realization of the nearest neighbor couplings can be mapped to an appropriate minimum-weight perfect-matching (MWPM) problem [2, 4]. Finally, the MWPM problem can be solved in polynomial time by means of exact combinatorial optimization algorithms [5]. Thus, the planar 2*d* ISG can be studied directly at zero temperature without equilibration problems and within polynomial time. Hence, very large systems can be considered, giving very precise and reliable estimates for the observables. Actually, there are different approaches that allow for an exact computation of GSs for the planar 2*d* ISG [6, 7, 8]. Albeit all of these approaches rely on the computation of MWPMs on an auxiliary graph, they differ regarding the subtleties of the mapping to the respective auxiliary problem. The most efficient of these approaches (see Ref. [8]) is based on the Kasteleyn treatment of the Ising model [9], which previously was also used to obtain extended ground states for the 2*d* ISG with fully periodic boundary conditions [10].

Here, we introduce a dedicated algorithm that yields exact GS spin configurations for the 2*d* random-bond Ising model (RBIM) on planar triangular lattice graphs. As the previous approaches, the algorithm presented here requires to solve an associated MWPM problem. The corresponding mapping uses a relation between perfect matchings and paths on a graph [11, 12]. In effect, these paths can be used to partition the graph into domains of up and down spins that comprise a GS spin configuration, see Fig. 1. Consequently, the GS properties as well as minimum-energy domain wall (MEDW) excitations, see Fig. 1, can be analyzed very fast. The presented algorithm enables us to study large systems, while allowing for an appropriate disorder average within a reasonable amount of computing time. In this regard, it requires to compute a MWPM for an auxiliary graph with $O(N)$ edges only (wherein N is the number of spins on the lattice). However, note that the algorithm presented here is asymptotically not faster than the algorithm presented in Refs. [8, 10], but it highlights the algorithmic relation between the GS problem for spin glasses and the recently proposed negative-weight percolation (NWP) problem [13].

In the presented article, we investigate the critical behavior of the $T = 0$ ferromagnet (FM) to spin-glass (SG) transition for the 2*d* RBIM, signaled by a breakdown of the magnetization, using finite-size scaling (FSS) analyses of the MEDW excitation energy. In this regard, we obtain a highly precise estimate of the critical point for the triangular lattice geometry and we

Email addresses: oliver.melchert@uni-oldenburg.de (O. Melchert), alexander.hartmann@uni-oldenburg.de (A. K. Hartmann)

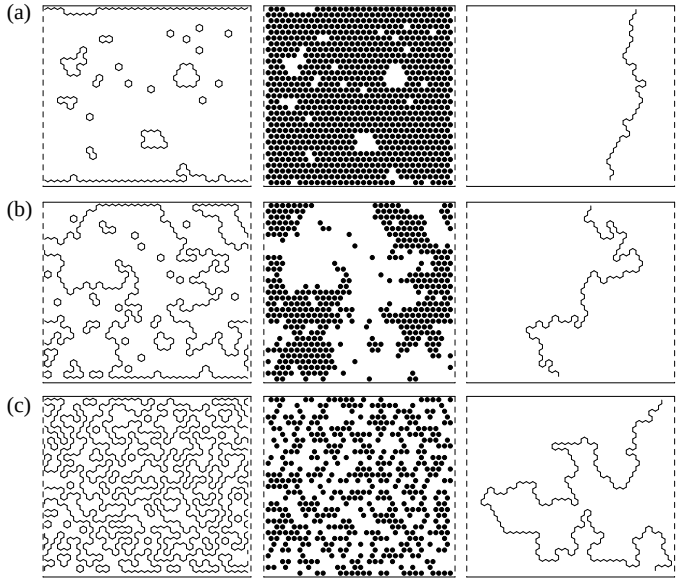

Figure 1: Samples of a $\pm J$ random bond Ising spin system on a triangular lattice of side length $L = 32$. The samples are taken at three different values of the disorder parameter p. (a) $p = 0.15$ characterized by a ferromagnetic GS, (b) $p = 0.2$ characterized by a GS with SG order and (c) $p = 0.5$, i.e. the canonical $\pm J$ ISG. In the figure, periodic BCs are indicated by the dashed vertical lines. From left to right: (Left) Transition graph that describes the difference between a ferromagnetic reference spin configuration and the GS spin configuration, (center) corresponding GS, (right) MEDW excitation relative to the GS.

verify the critical exponents obtained earlier for the RBIM on the planar square lattice [14, 15]. Finally, we contrast our numerical results with previous simulations and presumably exact results [16].

The remainder of the presented article is organized as follows. In section 2, we introduce the model in more detail and we outline the algorithm used to compute the GS spin configurations. In section 3, we present the results of our numerical simulations and in section 4 we conclude with a summary.

2. Model and Algorithm

In the presented article we perform GS calculations for the $2d$ RBIM, where the respective model consists of $N = L \times L$ Ising spins $\sigma = (\sigma_1, \ldots, \sigma_N)$, where $\sigma_i = \pm 1$, located on the sites of a planar triangular lattice graph. Therein, the energy of a given spin configuration is measured by the Edwards-Anderson Hamiltonian

$$H(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\, \sigma_i \sigma_j, \tag{1}$$

where the sum runs over all pairs of nearest-neighbor spins (on the triangular lattice) with periodic boundary conditions (BCs) in the x-direction and free BCs in the y-direction. In the above energy function, the bonds J_{ij} are quenched random variables drawn from the disorder distribution

$$P(J) \;=\; p\,\delta(J+1) \;+\; (1-p)\,\delta(J-1). \tag{2}$$

Therein, one realization of the disorder consists of a random fraction p of antiferromagnetic bonds ($J = -1$) that prefer an antiparallel alignment of the coupled spins, and a fraction $(1-p)$ of ferromagnetic bonds ($J = 1$) in favor of parallel aligned spins. In general, the competitive nature of these interactions gives rise to frustration. A plaquette, i.e. an elementary triangle on the lattice, is said to be frustrated if it is bordered by an odd number of antiferromagnetic bonds. In effect, frustration rules out a GS (i.e. a minimizer σ_{GS} of Eq. 1) in which all the bonds are satisfied. As limiting cases one can identify the Ising ferromagnet at $p = 0$ and the canonical $\pm J$ ISG at $p = 1/2$. Hence, as a function of the disorder parameter p we expect to find a ferromagnetic phase (spin-glass phase) for $p < p_c$ ($p > p_c$), wherein p_c denotes the critical point at which the $T = 0$ FM-SG transition takes place. For the ISG with a bimodal disorder distribution the GS is highly degenerate and the average number of such GSs increases exponentially with N [17, 18]. Apart from the GSs, we here also aim to characterize the energetic properties of MEDW excitations. A domain wall is an interface that spans the system in the direction with thee free BCs. Now, the MEDW is such an interface with an excitation energy δE that is minimal among all possible domain walls. Due to the extensive degeneracy of the GSs, the "lattice-path" associated with a MEDW is not unique. I.e., there are many DWs with minimal excitation energy. Albeit the geometric properties of a MEDW are not unique, its excitation energy is unique. MEDWs for three different values of the disorder parameter p are illustrated in Fig. 1.

We now give a brief description of the algorithm that we use to compute the GSs. Therefore, we first set a reference spin configuration σ_R. The most convenient choice is a maximally polarized, i.e. ferromagnetic, configuration $\sigma_R = (+1, \ldots, +1)$. Then, we construct a weighted dual of the spin lattice as shown in Fig. 2(a). Since the spin lattice considered here has a triangular geometry, the corresponding dual graph possesses a honeycomb geometry. Note, that we introduced $4L$ extra nodes on top and at the bottom of the dual in order to account for the free BCs along that direction and to maintain the honeycomb structure of the respective graph. This means, a triangular spin lattice of size $L \times L$ is transformed to a honeycomb lattice with an over all number of $(2L) \times (L+1)$ nodes. Further note that adjacent extra nodes are connected by edges e that carry a weight $\omega(e) = 0$. Hence, the topological dual graph associated to the triangular spin lattice is modified to some extend. All other edges e on the dual graph get an edge-weight $\omega(e) \equiv J_{ij}\sigma_{R,i}\sigma_{R,j}$. Therein, e is assumed to cross a bond J_{ij} on the spin lattice, where J_{ij} couples the two spins $\sigma_{R,i/j}$, see Fig. 2(a). Consequently, the edge weight on the weighted dual is positive (negative), if the corresponding bond on the spin lattice is satisfied (broken) with respect to σ_R. A pivotal observation is, that there exists an equivalence between clusters of adjacent spins on the spin lattice that might be flipped in order to decrease the configurational energy of σ_R and negative-weighted loops (i.e. closed paths) on the weighted dual graph. In this regard, if a loop with negative weight on the dual is found, the cluster of spins surrounded by this loop can be flipped so as to decrease the configurational energy of σ_R. Finally, to obtain a GS spin configuration one needs to find a minimum-weight set of negative-weighted loops on the dual graph (see discussion below). This

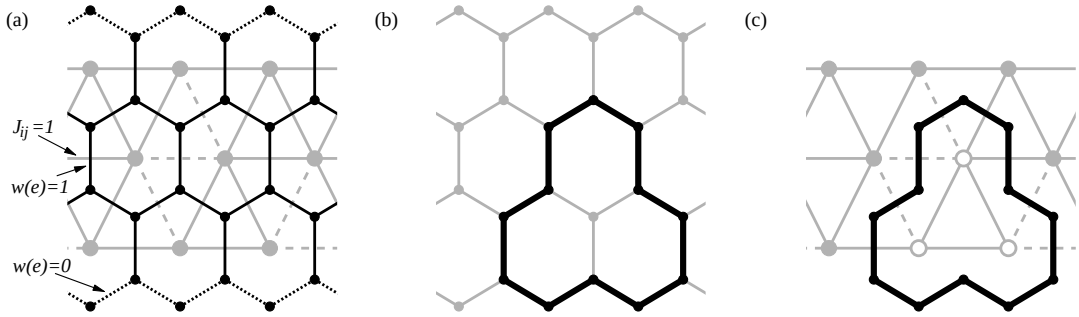

Figure 2: Illustration of the computation of the transition graph that allows to determine a GS spin configuration on a planar triangular RBIM. The figure illustrates a sample system of side length $L = 3$ and periodic BCs in the horizontal direction. (a) Mapping of the original lattice G (grey edges, triangular geometry), where a solid (dashed) line indicates a ferromagnetic (antiferromagnetic) bond, to the weighted dual graph G_D (black edges, honeycomb geometry). Note that additional edges (dotted lines) where introduced to account for the open boundary conditions in the respective direction. These edges carry zero weight. (b) Minimum weight set of loops (bold black edges) on G_D as obtained from a mapping to the NWP problem (not shown here, see Ref. [13]). (c) Loop on the dual surrounding a cluster of spins on the spin lattice. If the orientation of the spins is chosen as explained in the text, this procedure yields a GS spin configuration. In the figure, spin orientations are distinguished by gray filled and non-filled circles.

set of loops comprises the transition graph for the given realization of the disorder, as illustrated in Fig. 2(b). Since initially a ferromagnetic reference configuration was chosen, the GS is obtained if the orientation of the spins on the spin lattice is chosen such, that (i) spins within a cluster are aligned in the same direction and (ii) spins in adjacent clusters are aligned in opposite directions. The resulting GS is indicated in Fig. 2(c), see also Fig. 1.

Here, for the $2d$ RBIM on a planar triangular lattice, where the dual has a honeycomb geometry, the minimum weight set of loops on the weighted dual can be obtained by means of a mapping to the NWP problem, as explained in [13]. In brief, the NWP statement consists in the task to find a minimum-weight set of nonintersecting negative-weighted loops for a given weighted graph. Therefore, it considers a minimum-weight perfect matching problem on an associated auxiliary graph with $O(N)$ edges (provided that the input graph has $O(N)$ edges, as it is the case here), from which the set of loops can be deduced. Note that the mapping to the NWP problem yields the correct transition graph only for this particular lattice setup, since any two-coloring of the spin lattice (i.e. assignment of up/down spin orientations) can be composed by loops on the dual that do not intersect. That means, each site on the dual is an end-node of either 0 or 2 loop segments, as e.g. in Fig. 2(b). In contrast, two-colorings of the spins on a square lattice might involve loops on the dual that involve figure-8 twists. That means, each site on the dual is end-node of either 0, 2 or 4 loop segments. For the latter problem, a different mapping [8] was used recently to obtain exact GSs for $2d$ ISGs on a square lattice with free BCs in at least one direction within polynomial time. This mapping was further used to compute "extended" GSs for the $2d$ ISG with fully periodic BCs [10].

Now, the interpretation of the $T = 0$ FM-SG transition in terms of the NWP problem reads as follows: For small values of p, there are only few bonds on the spin lattice that are not satisfied by the reference spin configuration. Accordingly, there are only few small loops that comprise the transition graph. For all nonzero values of p, a sufficiently large lattice will feature at least some small loops that surround an elementary plaquette on the dual. These small loops correspond to local "manipulations" of the order-parameter (i.e. the magnetization), only. Hence, in the thermodynamic limit, the GS has still ferromagnetic order (see Fig. 1(a)). However, if the value of p increases and exceeds a critical value p_c, large loops appear that have a linear extension of the order of the system size and eventually span the system along the direction with the periodic boundary conditions. These loops represent global manipulations of the order-parameter, that, in the thermodynamic limit, destroy the ferromagnetic order of the GS (see Figs. 1(b),(c)).

Once we obtained a GS spin configuration in this manner, we compute a MEDW by means of a similar mapping, thoroughly explained in Ref. [19]. In the following we will use the procedure outlined above to obtain GSs and to investigate MEDWs for the RBIM introduced above.

3. Results

As pointed out above, at small values of p there exists an ordered ferromagnetic phase, while for large values of p a spin-glass ordered phase appears. A proper order parameter to characterize the respective FM-SG transition is the magnetization per spin $m_L = |\sum_i \sigma_i|/L^2$ for a system of linear extend L. Below, we perform a finite-size scaling analysis (FSS) in order to locate the critical point p_c and to estimate the critical exponents

Table 1: Critical exponents for the $2d$ RBIM. From left to right: Problem setup (SQ=square lattice, TR=triangular lattice), critical exponent of the correlation length ν, order parameter exponent β, and exponents ϕ_1 and ψ_1 that characterize the scaling of the MEDW excitation energy. The figures for SQ-a are taken from Ref. [15]. The figures for SQ-b are taken from Ref. [14].

Setup	ν	β	ϕ_1	ψ_1
SQ-a	1.49(7)	0.097(6)	0.67(3)	0.17(2)
SQ-b	1.55(1)	0.09(1)	0.75(5)	0.12(5)
TR	1.47(6)	0.086(5)	0.68(8)	0.15(2)

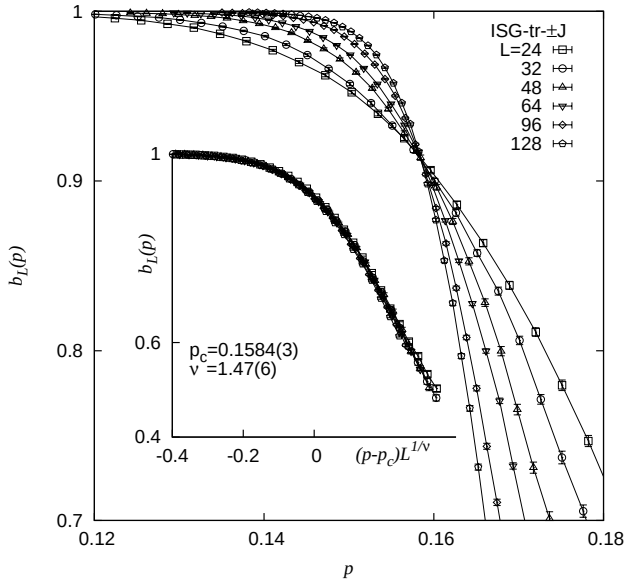

Figure 3: Results of the finite-size scaling analysis for the binder parameter $b_L(p)$, considering different system sizes L. The main plot shows the unscaled data close to the critical point and the insets illustrate the data collapse obtained after rescaling the raw data using the scaling assumption discussed in the text and scaling parameters as listed in Tab. 1.

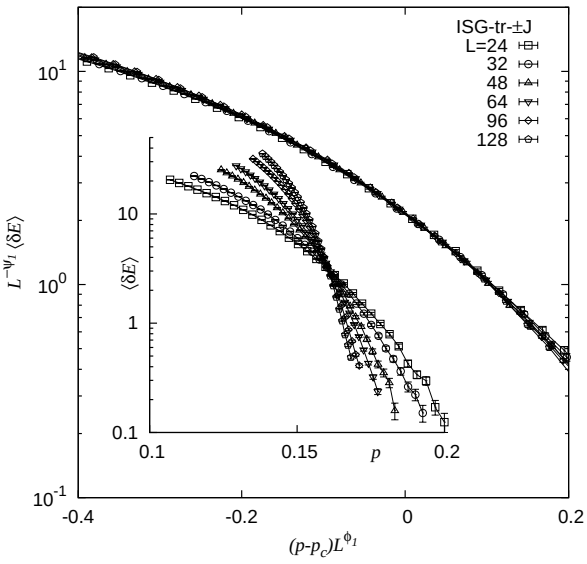

Figure 4: Results of the finite-size scaling analysis for the average MEDW energy $\langle\delta E\rangle$. The main plot shows the data collapse after rescaling the raw data using the scaling parameters listed in Tab. 1 and the inset illustrates the unscaled data close to the critical point.

that describe the scaling behavior of the magnetization in the vicinity of the critical point. Therefore, we first consider the Binder parameter [20]

$$b_L = \frac{1}{2}\left(3 - \frac{\langle m_L^4\rangle}{\langle m_L^2\rangle^2}\right) \tag{3}$$

associated with the magnetization. It is expected to scale as $b_L(p) \sim f_1[(p - p_c)L^{1/\nu}]$, wherein $f_1[\cdot]$ signifies a size-independent scaling function and ν denotes the critical exponent that describes the divergence of the correlation length as the critical point is approached. Here, we simulated triangular systems of side length $L = 24$ through 128 at various values of the disorder parameter p. Observables are averaged over 64 000 samples for the largest systems and we used the data collapse generated by the scaling assumption above to obtain $p_c = 0.1584(3)$ and $\nu = 1.47(6)$ with a quality $S = 0.94$ of the data collapse [21, 22], see Fig. 3. In general, the above scaling relation holds best near the critical point and one can expect that there are corrections to scaling off criticality. As a remedy, we restricted the latter scaling analysis to the interval $[-0.3, +0.3]$, enclosing the critical point on the rescaled abscissa.

Further, the order parameter of the transition is expected to scale according to the scaling relation $\langle m_L(p)\rangle \sim L^{-\beta/\nu} f_2[(p - p_c)L^{1/\nu}]$, where $f_2[\cdot]$ denotes a size-independent function, and where the order-parameter exponent β can be obtained after fixing ν and p_c to the values obtained from the analysis of the Binder parameter. The best data collapse ($S = 1.01$) was obtained for the choice $\beta = 0.086(5)$ (not shown).

Moreover, an analysis of the average MEDW excitation energy $\langle\delta E\rangle$ according to the scaling assumption $\langle\delta E\rangle \sim L^{\psi_1} f_3[(p - p_c)L^{\phi_1}]$, see Ref. [23], yields the critical point $p_c = 0.1586(2)$, in agreement with the above estimate obtained using the Binder parameter. The critical exponents ψ_1 and ϕ_1 are listed in Tab. 1. Therein, we restricted the scaling analysis to the interval $[-0.1, +0.1]$ and obtained a best data collapse with $S = 1.63$.

Right at the critical point p_c we performed additional simulations for spin lattices of up to 384×384 spins (and 3.6×10^4 samples), i.e. weighted dual graphs of up to 768×385 nodes. Upon analysis of the data we obtain the estimate $\beta = 0.097(8)$ from the scaling behavior of the magnetization, see Fig. 5(a). We allowed for small deviations from a pure power-law scaling using a scaling assumption of the form $\langle m\rangle \sim (L + \Delta L)^{-\beta/\nu}$, wherein $\Delta L = O(1)$. Considering the scaling of the average MEDW excitation energy $\langle\delta E\rangle$ and using a similar scaling assumption as above, we found $\psi_1 = 0.15(1)$, see Fig. 5(b). Both these exponents agree within error bars with those obtained earlier, see Tab. 1. As pointed out above, for the ISG with bimodal disorder, there a numerous MEDWs that differ regarding their geometric properties. However, here we also analyze the average length $\langle\ell\rangle$ of the particular MEDWs obtained within the simulations, see Fig. 5(b). Therefore, we considered a scaling according to the form $\langle\ell\rangle \sim (L + \Delta L)^{d_f}$, wherein d_f signifies the fractal dimension of the MEDWs at p_c. We obtained $d_f = 1.222(1)$ (and $\Delta L = O(1)$), which is in agreement with the value $d_f = 1.222(1)$ found earlier for the $T = 0$ FM-SG transition for the RBIM on a $2d$ square lattice, see Ref. [15].

4. Conclusions

In the presented article we have illustrated how GSs for the $2d$ RBIM on planar triangular lattice graphs can be computed by a mapping to the NWP problem. I.e., the problem of finding a GS spin configuration for a planar $2d$ triangular RBIM is

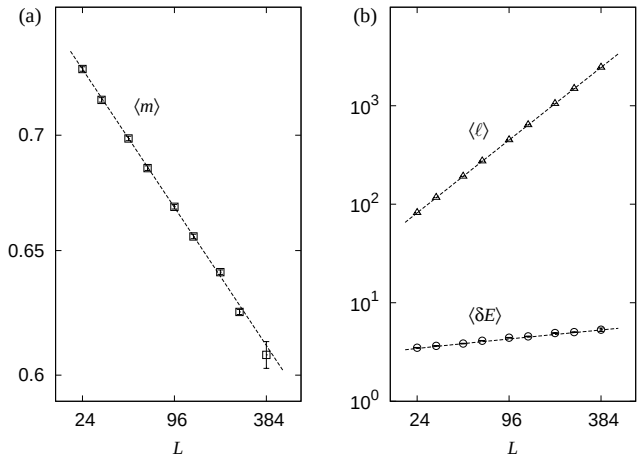

Figure 5: Results of the finite-size scaling analysis at the critical point, where the $T = 0$ FM-SG transition occurs. (a) Scaling behavior of the magnetization $\langle m \rangle$, and, (b) scaling of the average MEDW length $\langle \ell \rangle$ and the MEDW excitation energy $\langle \delta E \rangle$.

equivalent to the NWP problem on a properly weighted corresponding dual graph that exhibits a honeycomb structure. Using this approach, we have investigated GSs and MEDW excitations for the respective lattice structure. Therein, a disorder parameter could be used to distinguish a ferromagnetic and a spin-glass ordered phase. We characterized the corresponding $T = 0$ FM-SG transition by means of a FSS analysis of the magnetization and the MEDW excitation energy.

In this regard, we found that the values of the critical exponents obtained here agree within errorbars with those obtained earlier for the $2d$ RBIM on a planar square lattice by considering a Gaussian bond distribution with ferromagnetic bias [15] or a bimodal bond distribution [14], as listed in Tab. 1.

Hence, the results for the triangular lattice structure obtained here highlights the universality of the $T = 0$ FM-SG transition. Further, note that p_c and ν found here agree well with the values $p_c = 0.1583(6)$ and $\nu = 1.47(9)$ that characterize the negative-weight percolation of loops on $2d$ lattice graphs with a honeycomb geometry and fully periodic boundary conditions [13]. Finally, the location of the critical point obtained here via FSS analysis is close to the theoretical prediction $p_{c,tr} = 0.15$, that was obtained for systems with fully periodic boundary conditions using the adjoined problem approach [24, 16].

Acknowledgment

We are grateful to B. Ahrens for a critical reading of the manuscript. OM acknowledges financial support from the VolkswagenStiftung (Germany) within the program "Nachwuchsgruppen an Universitäten". The simulations were performed at the GOLEM I cluster for scientific computing at the University of Oldenburg (Germany).

References

[1] S. Bastea, A. Burkov, C. Moukarzel, P. M. Duxbury, Combinatorial optimization methods in disordered systems, Comp. Phys. Comm. 121-122 (1999) 199. Proceedings of the Europhysics Conference on Computational Physics CCP 1998.

[2] A. K. Hartmann, H. Rieger, Optimization Algorithms in Physics, Wiley-VCH, Weinheim, 2001.

[3] H. Rieger, Application of exact combinatorial optimization algorithms to the physics of disordered systems, Comp. Phys. Comm. 147 (2002) 702.

[4] A. K. Hartmann, Domain walls, droplets and barriers in two-dimensional ising spin glasses, in: J. W (Ed.), Rugged Free Energy Landscapes, Springer, Berlin, 2007, pp. 67 – 106.

[5] W. Cook, A. Rohe, Computing minimum-weight perfect matchings, INFORMS J. Computing 11 (1999) 138–148.

[6] I. Bieche, R. Maynard, R. Rammal, J. P. Uhry, On the ground states of the frustration model of a spin glass by a matching method of graph theory, J. Phys. A: Math. Gen. 13 (1980) 2553–2576.

[7] F. Barahona, On the computational complexity of Ising spin glass models, J. Phys. A: Math. Gen. 15 (1982) 3241–3253.

[8] G. Pardella, F. Liers, Exact ground states of large two-dimensional planar Ising spin glasses, Phys. Rev. E 78 (2008) 056705.

[9] P. W. Kasteleyn, Dimer Statistics and Phase Transitions, J. Math. Phys. 4 (1963) 287–293.

[10] C. K. Thomas, A. A. Middleton, Matching Kasteleyn cities for spin glass ground states, Phys. Rev. B 76 (2007) 220406.

[11] R. K. Ahuja, T. L. Magnanti, J. B. Orlin, Network Flows: Theory, Algorithms, and Applications, Prentice Hall, 1993.

[12] O. Melchert, PhD thesis, not published, 2009.

[13] O. Melchert, A. K. Hartmann, Negative-weight percolation, New. J. Phys. 10 (2008) 043039.

[14] C. Amoruso, A. K. Hartmann, Domain-wall energies and magnetization of the two-dimensional random-bond Ising model, Phys. Rev. B 70 (2004) 134425. Note that the value of $\beta = 0.9(1)$ is a misprint and should read $\beta = 0.09(1)$.

[15] O. Melchert, A. K. Hartmann, Scaling behavior of domain walls at the $T = 0$ ferromagnet to spin-glass transition, Phys. Rev. B 79 (2009) 184402.

[16] J. Bendisch, Groundstate threshold in triangular anisotropic ±J Ising models, Physica A 245 (1997) 560 – 574.

[17] L. Saul, M. Kardar, The $2d$ $\pm J$ Ising spin glass: exact partition functions in polynomial time, Nucl. Phys. B 432 (1994) 641.

[18] J. W. Landry, S. N. Coppersmith, Ground states of two-dimensional $\pm J$ Edwards-Anderson spin glasses, Phys. Rev. B 65 (2002) 134404.

[19] O. Melchert, A. K. Hartmann, Fractal dimension of domain walls in two-dimensional Ising spin glasses, Phys. Rev. B 76 (2007) 174411.

[20] K. Binder, Finite size scaling analysis of ising model block distribution functions, Z. Phys. B 43 (1981) 119.

[21] J. Houdayer, A. K. Hartmann, Low-temperature behavior of two-dimensional Gaussian Ising spin glasses, Phys. Rev. **B** 70 (2004) 014418. S measures the mean square distance of the scaled data to the master curve in units of standart errors.

[22] O. Melchert, autoScale.py - A program for automatic finite-size scaling analyses: A user's guide, Preprint: arXiv:0910.5403v1 (2009).

[23] N. Kawashima, H. Rieger, Finite-size scaling analysis of exact ground states for $\pm J$ spin glass models in two dimensions, Europhys. Lett. 39 (1997) 85–90.

[24] J. Bendisch, Groundstate threshold pc in ising frustration systems on 2d regular lattices, Physica A 202 (1994) 48 – 67.