

Matching Kasteleyn cities for spin glass ground states

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As spin glass materials have extremely slow dynamics, devious numerical methods are needed to study low-temperature states. A simple and fast optimization version of the classical Kasteleyn treatment of the Ising model is described and applied to two-dimensional Ising spin glasses. The algorithm combines the Pfaffian and matching approaches to directly strip droplet excitations from an excited state. Extended ground states in Ising spin glasses on a torus, which are optimized over all boundary conditions, are used to compute precise values for ground state energy densities.

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The Ising spin glass is a model for disordered magnetic alloys which captures the complexity of materials with frozen randomness and competing interactions, including frustration, extremely slow dynamics, and intricate memory effects.¹ The spins in the model are coupled by random choices of ferromagnetic or antiferromagnetic bonds, leading to a complex free-energy landscape. There are at least two theoretical approaches,² including the droplet and replica-symmetry-breaking pictures, used to describe the nonequilibrium dynamics and low-free-energy structure of the spin glass phase space. As these theoretical approaches differ significantly and exact results for spin glasses are rare,³ computational work has been essential for computing scaling exponents and as a qualitative check of theoretical pictures.⁴

The history of the relationship between the physical analysis and the mathematics of numerical approaches to spin glasses is long and rich. In general, characterizing the complex free-energy landscape of disordered materials is challenging. Direct Monte Carlo simulations are hindered by the same high free-energy barriers that inhibit equilibration in the physical system. It is expected^{1,2} that times t satisfying $\ln(t) \sim L^\psi$ are required to equilibrate systems of size L , where $\psi \geq \theta$ and θ determines the energy scale $\Delta E(\ell)$ of excitations or domain walls on length scale ℓ , $\Delta E \sim \ell^\theta$. To replicate the many decades of experimental time scales and to develop a better understanding of disordered systems for $t \rightarrow \infty$, algorithms for either accelerating the approach to equilibrium or finding ground states in spin glasses have been developed. Many of these techniques (which are often generally applicable to disordered materials) are inspired by, or have inspired, approaches for combinatorial optimization problems. Parallel tempering, genetic algorithms, and extremal optimization are examples of heuristic algorithms to find close approximations to equilibrated and ground state configurations.⁶ Exact general algorithms such as transfer matrix methods⁷ and branch-and-cut methods⁸ require times that are exponential in powers of the system size, though extensive development has led to computing ground states in three-dimensional Ising spin glasses with up to 12^3 spins.⁸

We have found a simple algorithm for studying two-dimensional (2D) Ising spin glasses that combines use of the classical Kasteleyn city⁹ and application of a standard combinatorial optimization algorithm. Besides solving the problem on planar graphs and linking together these methods, we

use this algorithm to study “extended” ground states, which optimize the energy over choices of periodic or antiperiodic boundary conditions, as well as the spin configuration. This approach dramatically improves the treatment of boundary-free samples, so that the finite-size effects are greatly reduced. We have used this algorithm to determine very precisely the energy of the Ising spin glass in the large-volume limit.

The Edwards-Anderson Hamiltonian that is used for Ising spin glasses is $\mathcal{H}(\{s_{ij}\}) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$, where the couplings J_{ij} between nearest neighbor pairs of spins $\langle ij \rangle$ are independent identically distributed variables, fixed in a given sample, and the s_i are Ising spin variables, $s_i = \pm 1$, with L^d sites i on a d -dimensional lattice. The distribution for J_{ij} is generally taken either to be Gaussian or bimodal (the “ $\pm J$ ” case). Barahona¹⁰ has shown that computing the ground state energy of a 3D spin glass (or even two coupled 2D layers) is an NP-hard problem.⁵ This implies that, if the ground state of the 3D spin glass could be efficiently computed, i.e., found in a time polynomial in L , many outstanding computational problems that are believed to require worst-case exponential time to solve, such as the traveling salesperson problem, could also be solved in time polynomial in the size of the problem. Improvements in 3D spin glass calculations therefore focus on reducing the numerical constants in the exponent for the expected solution time.

The two-dimensional Ising spin glass (2DISG) is a case where exact algorithms have allowed for study of the ground state and density of states. These approaches have used two methods: the dimer-Pfaffian method (Pfaffian method) and matching to minimize frustration.

The partition function for Ising models with arbitrary couplings can be solved for either open or toroidal boundary conditions by using techniques developed for the pure Ising model,⁹ i.e., computing and summing Pfaffians, antisymmetric combinations of ordered statistical weights, from $L^2 \times L^2$ sparse matrices. The ground state energy can be computed¹¹ in $O(L^5)$ time for discrete-valued disorder; the spectrum is discrete and bounded by a power of L . Note that the Pfaffian method uses perfect matchings (dimer coverings) on a decorated lattice and requires a sum over four combinations of odd and even constraints on these matchings on a torus.

The fastest ground state algorithms for the 2DISG map

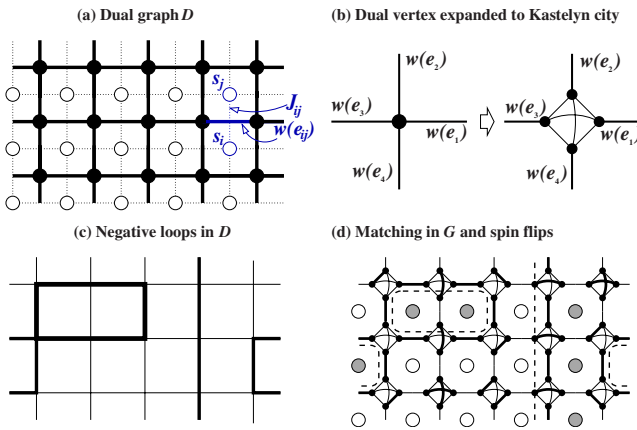


FIG. 1. (Color online) An outline of the steps that convert a spin and bond configuration first to the dual weighted lattice D and then to the weighted graph G , in order to compute the extended ground state. (a) The original spin system, here with initial spins $s_i=1$ indicated by white circles, and bond configuration J_{ij} (dashed lines) determine edge weights $w_{ij}=J_{ij}s_i s_j$ (taking the initial BCs to be periodic) in the dual graph D (solid vertices and edges), with periodic boundary conditions. (b) The vertices in D are replaced by Kasteleyn cities (light lines have zero weight in G). (c) An example set S of negative weight loops in D is shown, with two simple loops and one winding loop. (d) Heavy lines indicate the minimum-weight perfect matching M for G (light lines are free edges and solid circles are vertices in G). The negative weight loops S (heavy dashed lines) are found by clipping out the Kasteleyn cities and keeping the remaining edges. Finally, spins are assigned by scanning across the sample: each time an odd number of loops is crossed, the spins are flipped (gray circles indicate $s_i=-1$). In this case, the inconsistency at the right side is corrected by changing horizontal boundary conditions from periodic to antiperiodic.

the Ising spin glass problem to the weighted perfect matching problem, a common problem in combinatorial optimization. Given a graph $G=(V,E)$, with vertices V and edges E , with a weight function $w:E\rightarrow\mathbb{R}$, the problem is to select a perfect matching, a subset of edges $M\subset E$ where every vertex in V belongs to a single edge $e\in E$, such that the total weight $w(M)=\sum_{e\in M}w_e$ is minimal. The solution can be found in time polynomial in the number of edges.⁵ Matching is the core routine in two mappings for finding 2DISG ground states. The mapping by Bieche *et al.*¹² uses a graph where the vertex set V contains the frustrated plaquettes (primitive polygons p with $\prod_{\langle ij\rangle\in p}J_{ij}<0$). The edges connect points in V within some distance r_{\max} . This algorithm is exact as $r_{\max}\rightarrow\infty$, but it works for a large fraction of cases even with small values of r_{\max} , especially for $\pm J$ disorder. Barahona's mapping¹⁰ replaces each plaquette with a subgraph that is connected to neighboring subgraphs by dual bonds, with each dual bond crossing one edge in G [see Fig. 1(a)]. The subgraph edges have zero weight and the dual edges that cross bonds of strength J_{ij} have weight $w_{ij}=|J_{ij}|$; the subgraph comes in two types, assigned according to the frustration of the plaquette. These algorithms have been extremely useful, e.g., in studying domain walls and the nature of the ground state as $L\rightarrow\infty$.^{13,14} Note that the graphs used are derived from the (sample-dependent) plaquette frustrations;

this is not the case with our algorithm, where the graph is independent of the J_{ij} , so its implementation is simpler.

Matching algorithms have been used for planar graphs. The case of the torus, with periodic boundary conditions in both directions, has not been addressed in very large systems, as Pfaffian methods are much slower (and, in practice, mean-time exponential run-time algorithms are still commonly used). Studies of smaller toroidal systems with Gaussian disorder have used the branch-and-cut algorithm¹³ or the transfer matrix; such studies confirm that the finite-size corrections vanish much more quickly in toroidal geometries rather than planar geometries. It would therefore be useful to have a fast algorithm for finding information about the ground states for the 2DISG on the torus.

We have developed an approach that is not limited to planar graphs; it also provides significant information about the ground state on the torus. One component of this approach is a ground state algorithm that combines a representation from the Pfaffian method with matching. The other component is applying this algorithm on the torus to find an extended ground state: the minimum-energy state over all spin configurations and over the set of four boundary conditions (BCs). That is, we find the extended state $(\{s_i^0\}, \sigma_h^0, \sigma_v^0)$ which minimizes $\mathcal{H}^*=-\sum_{\langle ij\rangle}J_{ij}s_i s_j \sigma_{ij}$, with $\sigma_{ij}=1$ except on one vertical column of horizontal bonds, where $\sigma_{ij}=\sigma_v$, and on one horizontal row of vertical bonds, where $\sigma_{ij}=\sigma_h$ and σ_h and σ_v take values $\sigma_{h,v}=\pm 1$. The extended ground state on the torus is the minimum-energy state over the four possible combinations of BCs given by choosing (anti)periodic BCs for each direction. The standard ground state for given BCs is therefore exactly found for $\frac{1}{4}$ of the samples. Note that, in general, when all $\sigma_{ij}=1$, $\mathcal{H}^*=\mathcal{H}$, so the extended ground state is equal to the standard ground state (this is always the case for planar graphs, so the algorithm finds ground states of planar graphs without modification). The extended ground state on the torus is also of interest in its own right. For example, it can be used as an edge-free background for studying equilibration and droplets¹⁵ and to rapidly compute the energy density for large samples.

We first give an overview of our algorithm. A spin and bond configuration is used to define a weighted dual lattice D , which in turn is mapped to a weighted graph G . A minimum-weight perfect matching for G is computed and used to identify a set of negative weight loops in D with the most negative total weight. These loops are exactly the excitations of the current configuration relative to an extended ground state. The configuration is thus set to the ground state by flipping the spins “within” each loop. This method can be applied to any planar graph by supplying the appropriate boundary conditions (i.e., in the same way as the Bieche *et al.* and Barahona algorithms).

A more detailed description of the method for the $L\times L$ toroidal square lattice starts with a list of the inputs: an initial configuration $c=(\{s_i\}, \sigma_h, \sigma_v)$ and couplings J_{ij} . The dual lattice $D=(V,E)$ has edges $e_{ij}\in E$ (e_{ij} crosses the bond $\langle ij\rangle$ in the original lattice) connecting neighboring plaquettes (these make up V) on the original spin lattice; it also is an $L\times L$ torus. Given c , weights w_c for edges in E are set by $w_c(e_{ij})=J_{ij}s_i s_j \sigma_{ij}$; see Fig. 1(a). The value of the extended Hamil-

tonian is then $\mathcal{H}^*(c) = -w_c(E) \equiv -\sum_{e_{ij} \in E} w_c(e_{ij})$.

To minimize \mathcal{H}^* , we find the extremal (i.e., minimum total weight) set of negative weight loops in the dual graph D by computing a minimal-weight perfect matching M on a related graph G . In the case of a square lattice, we form G by replacing each vertex in D by a ‘‘Kasteleyn city’’ subgraph, a complete graph with four nodes [see Fig. 1(b)]; such mappings exist for any lattice. Weights for edges in G are zero on city edges and are given by $w_c(e_{ij})$ on edges e_{ij} kept from D (cf. the Barahona algorithm, which instead uses $|w(e_{ij})|$, which is independent of c ; frustration is incorporated via the use of two distinct graph decorations). Matchings in G can be mapped to sets of loops in D : one simply contracts out the Kasteleyn cities from M to arrive at a set of loops made of edges $S \subseteq E$ [see Figs. 1(c) and 1(d)]. The Kasteleyn cities enforce the constraint that an even number of edges in S meet at each dual vertex (i.e., S is a collection of Eulerian subgraphs of D).

To prove the correctness of the algorithm, we first show that the weight of the loops that relate two configurations is proportional to the energy difference between the configurations. For an extended spin configuration c , let $b_{ij}(c) = s_i s_j \sigma_{ij}$. When comparing two extended configurations c and c' , call S the set of bonds in which $b_{ij}(c) = -b_{ij}(c')$ [note that $b_{ij}(c) = \pm b_{ij}(c')$ always]. Since in S , $b_{ij}(c) = -b_{ij}(c')$ and in $E \setminus S$, $b_{ij}(c) = b_{ij}(c')$, we have that

$$\begin{aligned} \mathcal{H}^*(c) - \mathcal{H}^*(c') &= -\sum_{\langle ij \rangle} J_{ij} b_{ij}(c) + \sum_{\langle ij \rangle} J_{ij} b_{ij}(c') \\ &= -\sum_{e_{ij} \in S} J_{ij} b_{ij}(c) - \sum_{e_{ij} \in E \setminus S} J_{ij} b_{ij}(c) \\ &\quad + \sum_{e_{ij} \in S} J_{ij} b_{ij}(c') + \sum_{e_{ij} \in E \setminus S} J_{ij} b_{ij}(c') \\ &= -2 \sum_{e_{ij} \in S} J_{ij} b_{ij}(c) \\ &= -2 \sum_{e_{ij} \in S} w(e_{ij}(c)), \end{aligned} \quad (1)$$

so that the energy difference between configurations is given by twice the weight of S .

The proof that the minimum-weight even-degree subgraph always finds the ground state, then, is as follows. Assume, for the sake of contradiction, that there exists some extended spin configuration c^0 with a lower total energy than the c' returned by our algorithm from initial configuration c . Call S the set of bonds for which $b_{ij}(c) = -b_{ij}(c')$, and S^0 the set of bonds for which $b_{ij}(c) = -b_{ij}(c^0)$. Since $\mathcal{H}^*(c^0) < \mathcal{H}^*(c')$, the energy difference $\mathcal{H}^*(c) - \mathcal{H}^*(c^0) > \mathcal{H}^*(c) - \mathcal{H}^*(c')$ gives $2\sum_{e_{ij} \in S^0} w_c(e_{ij}) < 2\sum_{e_{ij} \in S} w_c(e_{ij})$, which means S^0 is an even-degree subgraph of D with a more negative weight than S , in contradiction with the assumption that S is the extremal-weight even-degree subgraph of D .

Note that Kasteleyn cities are often described on the original lattice, where loops represent a high-temperature expansion, but here on the dual lattice these loops contain clusters in a low-temperature expansion. The terms that contribute to

the Pfaffian⁹ are products of statistical weights $\pm e^{-\beta J_{ij}}$ over edges in loops in D and statistical weights of unit norm from the Kasteleyn cities. The dominant term in the Pfaffian that maximizes the norm of such a product minimizes the sums of the w_{ij} consistent with a perfect matching in the graph G . Least-weight paths on graphs with negative weights have been used to find domain walls in 2D spin glasses.¹⁶ We note that there has been at least one mention of using matching on the torus,¹⁷ where one of the four ground states was found using the Bieche *et al.* algorithm, but the utility of the extended ground state has been made apparent and proven by this algorithmic framework.

This algorithm is simple to implement (given a standard matching algorithm) and fast. On a 3.2 GHz Pentium IV processor, the extended ground state for a 100^2 square lattice on a torus is computed in 0.8 s for Gaussian disorder, where we use BLOSSOM IV (Ref. 18) for the matching routine. The mean solution time scales approximately as $L^{3.5}$ through toroidal lattices of size 400^2 . On toroidal graphs with $L \leq 128$, our algorithm, which finds exact ground states, is at least three times as fast as our implementation of the Bieche *et al.* algorithm. Note that the Bieche *et al.* algorithm does not find the exact optimal state in all cases—in this case 1.5% of the samples (when $r_{\max} = 8$). Because the structure of the graph used in the Barahona algorithm is similar in structure to that of our algorithm, the two algorithms have similar performance, with the Barahona algorithm using slightly less time (about 20%) and more memory (about 20%).

On a torus, we use this algorithm to exactly solve for the extended ground state, which is closely related to, but different than, finding the ground state of the spin glass for given BCs. The ground state energies for the four possible BCs differ by $O(L^\theta)$, which is the energy of a system-spanning domain wall. The extended ground state, the minimum of the four, therefore has at most an energy difference of $O(L^\theta)$ from that for specified BCs.

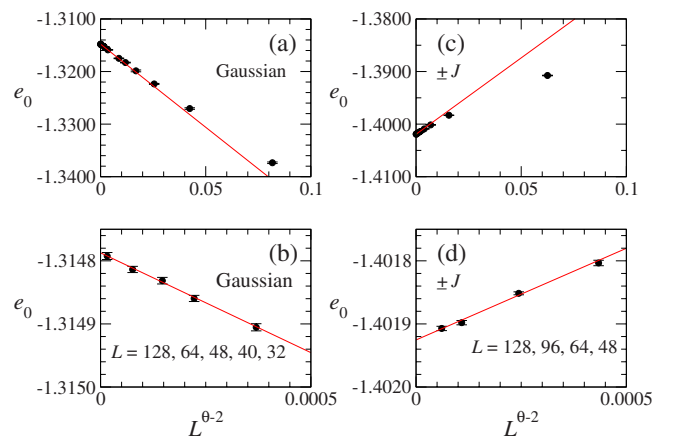


FIG. 2. (Color online) Extended ground state energy density $e_0(L)$ for the 2D Ising spin glass on a torus vs scaled system size $L^{\theta-2}$. Two scales for each disorder type are used, to show the linear fit at large L and the higher-order corrections at small L . (a),(b) Assuming $\theta \approx -0.28$ for Gaussian disorder gives $e_0(\infty) = -1.314\,788(4)$. (c),(d) A similar plot using $\theta = 0$ for discrete values of $J_{ij} = \pm 1$ gives $e_0^\pm(\infty) = -1.401\,925(3)$.

This $O(L^\theta)$ difference is the same order as the expected finite-size correction to the ground state energy in a periodic system, so the extended ground state is useful for studying energy densities. We computed the sample average of the extended ground state energy \mathcal{H}_0^* , using at least 5×10^6 samples for $L \leq 64$ and at least 10^6 samples for sizes $128 \geq L > 64$, both for Gaussian disorder ($J_{ij}^2=1$, $J_{ij}=0$) and for the $\pm J$ model, $J_{ij}=\pm 1$ with equal probability. We then plotted the sample average of the ground state energy density, $e_0(L)=\overline{\mathcal{H}_0^*}L^{-2}$, vs $L^{\theta-2}$, which will give a straight line where the leading finite-size correction dominates. For Gaussian disorder, we find a linear fit to be very good for $L \geq 32$, as shown in Figs. 2(a) and 2(c), for a wide range of $\theta \approx -0.28(4)$ (θ is not precisely determined by this method; see a summary of results in Ref. 13) and a highly precise estimate $e_0 = -1.314\,788(4)$ (cf., e.g., $e_0 = -1.314\,79(2)$ from Ref. 13). Taking $\theta=0$ for the $\pm J$ data also gives a good fit, with $e_0^\pm = -1.401\,925(3)$ (cf. $e_0^\pm = -1.401\,93(2)$ from Ref. 19; finite-size effects in our $L=48$ samples are less than those for $L=1800$ samples with open BCs). The extra precision results from the rapid convergence to the thermodynamic limit in boundary-free samples, which can be solved much faster than standard periodic samples solved using branch-and-cut techniques.

In conclusion, we have linked together Pfaffian and matching methods to develop a fast algorithm for finding extended ground states in the two-dimensional Ising spin glass on a torus or standard ground states on planar graphs. For many purposes, the extended ground states on a torus are as useful as ground states that are computed for a fixed choice of periodic and antiperiodic boundary conditions, as we show by precisely computing ground state energy densities. In the Pfaffian method for computing the partition function Z using the dual lattice (i.e., low-temperature expansion), the dominant term in any of the four Pfaffians used to compute Z is due to this extended ground state; the partition function for a specified BC combination is found by carefully canceling out configurations with other boundary conditions in the sum. Our method therefore is a combinatorial method, based on matching, for finding the term that dominates the contributing Pfaffians at low temperature.

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