Exact Ground States of Two-Dimensional $\pm J$ Ising Spin Glasses

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Abstract

In this paper we study the problem of finding an exact ground state of a two-dimensional $\pm J$ Ising spin glass on a square lattice with nearest neighbor interactions and periodic boundary conditions when there is a concentration p of negative bonds, with p ranging between 0.1 and 0.9. With our exact algorithm we can determine ground states of grids of sizes up to 50×50 in a moderate amount of computation time (up to one hour each) for several values of p. For the ground state energy of an infinite spin glass system with $p = 0.5$ we estimate $E_{0.5}^{\infty} = -1.4015 \pm 0.0008$.

We report on extensive computational tests based on more than 22 000 experiments.

Keywords: branch and cut, Ising spin glasses, exact ground states

1 Introduction

The last twenty years have witnessed a great deal of work on spin glasses [BY86, MPV88]. Nevertheless, the description of the phase transition and the nature of the ordered state remains controversial [BT91, Gro95a]. The starting point for most theoretical work is the Edwards-Anderson (EA) model, whose Hamiltonian is

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

where the J_{ij} are random interactions and the spins lie on a regular lattice. An important case is the short-range model with Ising spins σ_i.

A widely studied model is the $\pm J$ Ising spin glass in which the sign of each bond is random but its magnitude is fixed. In two dimensions, the $\pm J$ spin glass with nearest-neighbor interactions enters its spin glass phase only at zero temperature [MB80].

In our paper we deal with two-dimensional models at zero temperature. We consider Ising spins $\sigma_i = \pm 1$ on an $L \times L$ lattice with periodic boundary conditions and nearest neighbor interactions. In this case, the total energy of the spin system is given by the Hamiltonian (1), with the sum restricted to pairs of nearest neighbor spins. Our goal is to compute an exact ground state configuration of spin glasses when there is a concentration p of negative bonds. As p is increased from zero, one can observe a critical concentration p_c which marks the phase transition between ferro- and paramagnetism. Different publications give estimates for p_c that lie between 0.09 and 0.16, see Bendisch [Ben94].

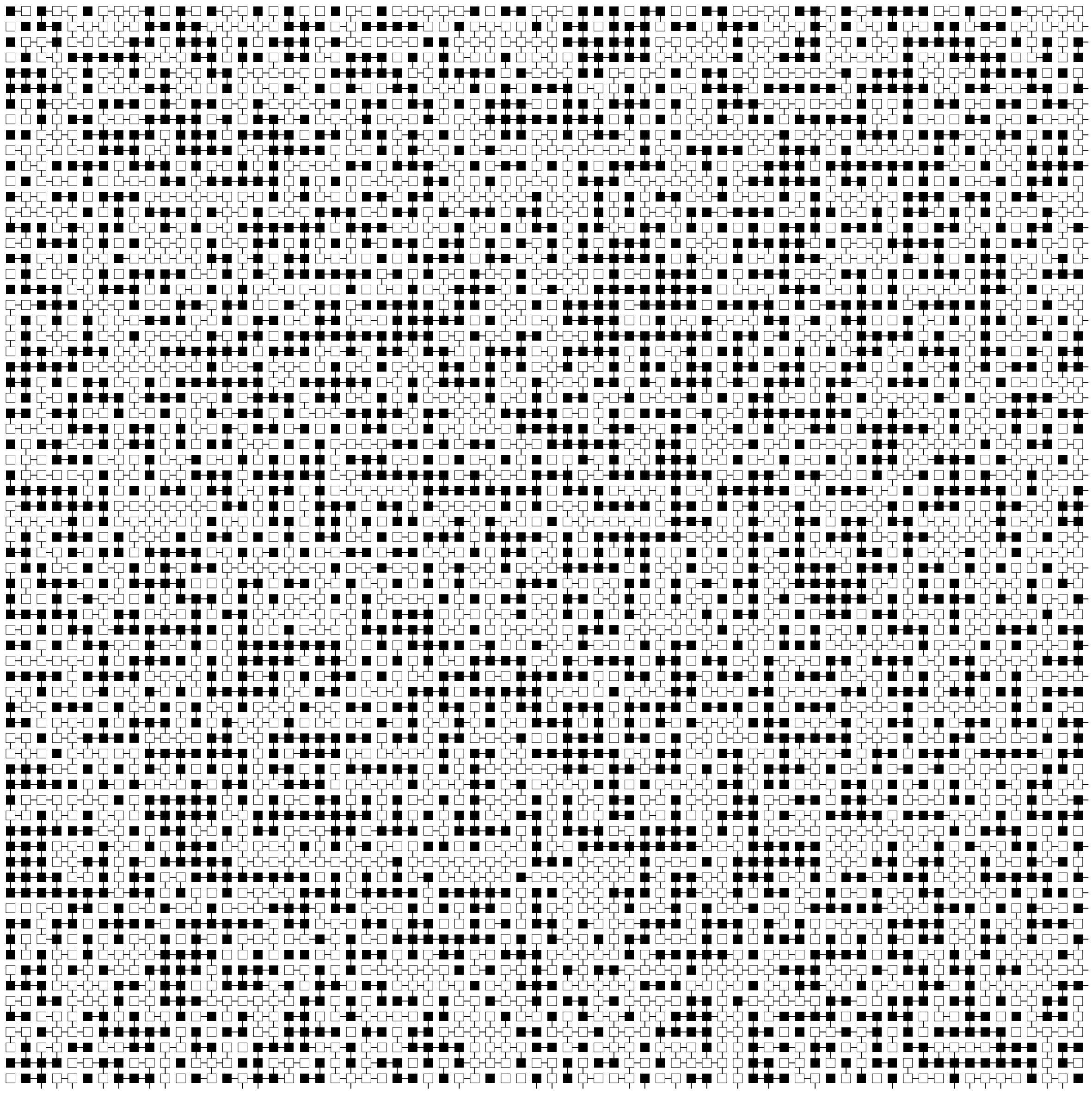
Since there are no partition functions in closed form that, given all interactions between the spins, yield a ground state, the only way to compute a ground state is using a numerical algorithm. However, the total number of states is $2^{L \times L}$, and so it is impossible, from a computational point of view, to find a ground state by just enumerating all possible states and computing the energy for each of them (unless L is small enough). In fact, Barahona [Bar81] found a polynomial-time algorithm; however, his algorithm is also of high complexity and was never implemented to the best of our knowledge.

Ground state energies at $p = 0.5$ have been calculated by several authors. Unfortunately, most of the methods proposed in the literature do not find the exact ground state but an approximation for it. Such methods usually use Monte Carlo simulation [WS88], evolutionary [Gro95a, Gro95b] and genetic algorithms [SB94, SHJ94]; in [BP91] a Gauge-invariant method is proposed. In [SK93] an exact integer method is proposed to find ground states for small systems.

The Branch and Cut method we proposed and described in [BGJR88] which computes an exact ground state by finding a cut of maximum weight in a weighted graph is able to solve large samples. It is the same method we used to find ground states for two-dimensional Ising spin glasses with periodic boundary conditions and nearest neighbor interactions based on a Gaussian bond distribution and an exterior magnetic field [DDJ+95]. With our method we can compute exact ground states of $\pm J$ Ising spin glasses on square lattices of size up to $L = 50$ within one hour and up to $L = 70$ within a day of computation time. We used $p \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$. Because of the moderate computation time, we can give results based on more than 22 000 samples.

In the following section, we discuss the results we obtained for two-dimensional systems.

2 Computational experiments



```
Size          : 70 x 70, 4900 spins
Energy        : -1.406530612245
Magnetization : 0.010612244898
Spins up      : 2424
CPU-Time      : 952:26.03
```

Figure 1: Ground state of a sample with $L = 70$. Positive couplings are drawn as solid lines.

Our computational experiments were carried out on a SUN SPARCstation 10. The complete computer code, except the linear programming routines, was written by us;

to solve the linear programs we used the CPLEX Callable Library [CPL93].

Our experiments were done on $\pm J$ Ising spin glasses on $L \times L$ square lattices with a concentration p of negative bonds, for a range of values of L up to 50. Indeed we can solve lattices of bigger size, say 70×70, but the running times for these systems are so high, that we cannot run a sufficiently large number of these systems to get statistically stable results. One out of the eight 70×70 samples we solved is shown in Figure 1. To find this optimal configuration the program needed a little less than 16 hours. An electronic version of each sample is available from the authors. Send an e-mail to: **diehl@informatik.uni-koeln.de**.

At the beginning we considered L up to 40 and p equals to $0.1, 0.3, 0.5, 0.7$ and 0.9. Note that, when L is not too small, the value of the ground state energy per spin for $p = 0.1$ is very close to the value for $p = 0.9$; the same holds also for the cases $p = 0.3$ and $p = 0.7$ (see Figure 2).

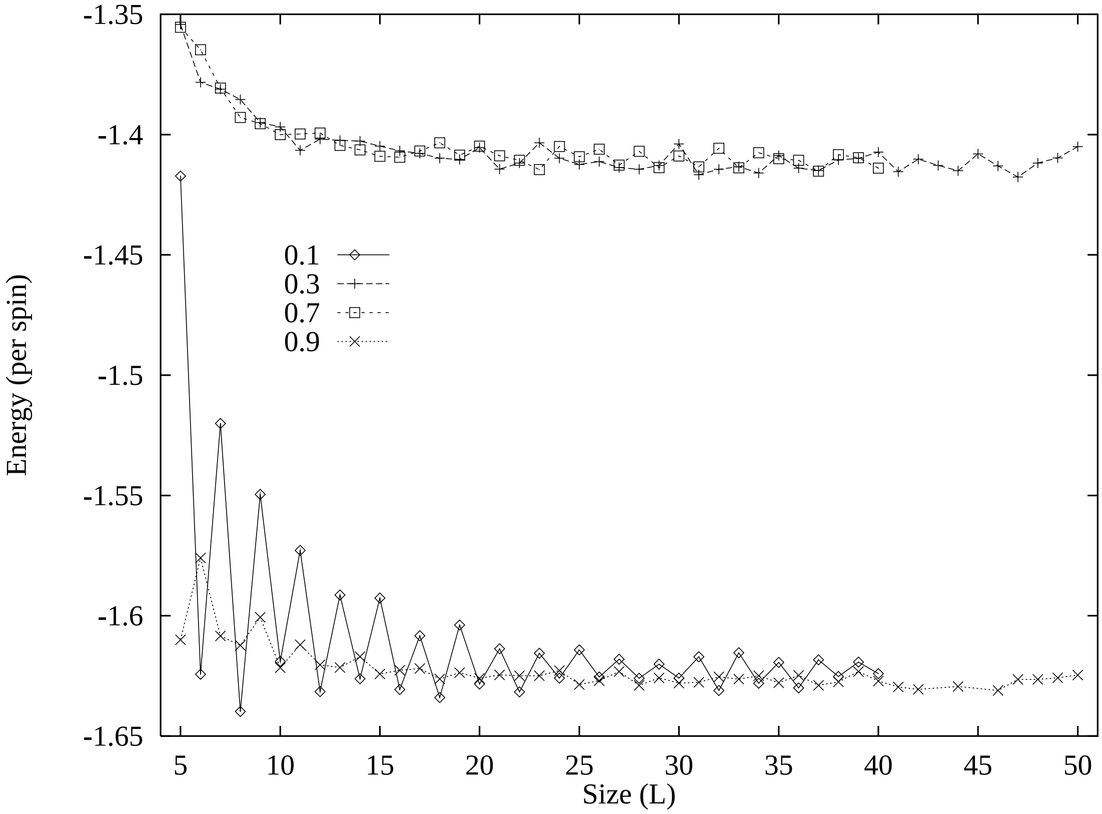


Figure 2: Ground State Energy for Different Concentration.

This is not surprising, since a (random) spin glass with concentration p of negative interactions becomes (a random) one with a concentration $1 - p$ when all couplings are multiplied by -1. The following holds (and is proven in the appendix):

Proposition 1 *The ground state energies of a spin glass system with a concentration p of negative interactions and the corresponding one with all couplings multiplied by -1 (concentration $(1-p)$ of negative interactions), are exactly the same if L is even and differ by at most $4L$ if L is odd.*

In other words, the deviations in the energy per spin are of order $O(1/L)$, i.e., negligible for bigger sizes, however these differences are noticeable for smaller samples.

Hence, for L greater than 40 we just considered values of p equal to $0.3, 0.5$, and 0.9. For each L between 5 and 50, we did $\lceil 20\,000/L^2 \rceil$ runs, for every value of p. Figure 2 shows the averages for the ground state energy for the different values of p except for $p = 0.5$. When L is small the ground state energy values for $p = 0.1$ and $p = 0.9$ show a very different behaviour depending on whether L is odd or even; these differences are not as high for the other values of p. For $p = 0.1$ (or $p = 0.9$) and $p = 0.3$ (or $p = 0.7$) we estimate the ground state energies for infinite systems as $E^{\infty}_{0.1,0.9} \approx -1.62$ and $E^{\infty}_{0.3,0.7} \approx -1.41$, respectively.

In Figure 3 we show the ground state energies with $p = 0.5$, which is the "classical" $\pm J$-spin glass. To make especially the values for bigger lattices more accurate, we computed another 2000 ground states for the $p = 0.5$ case.

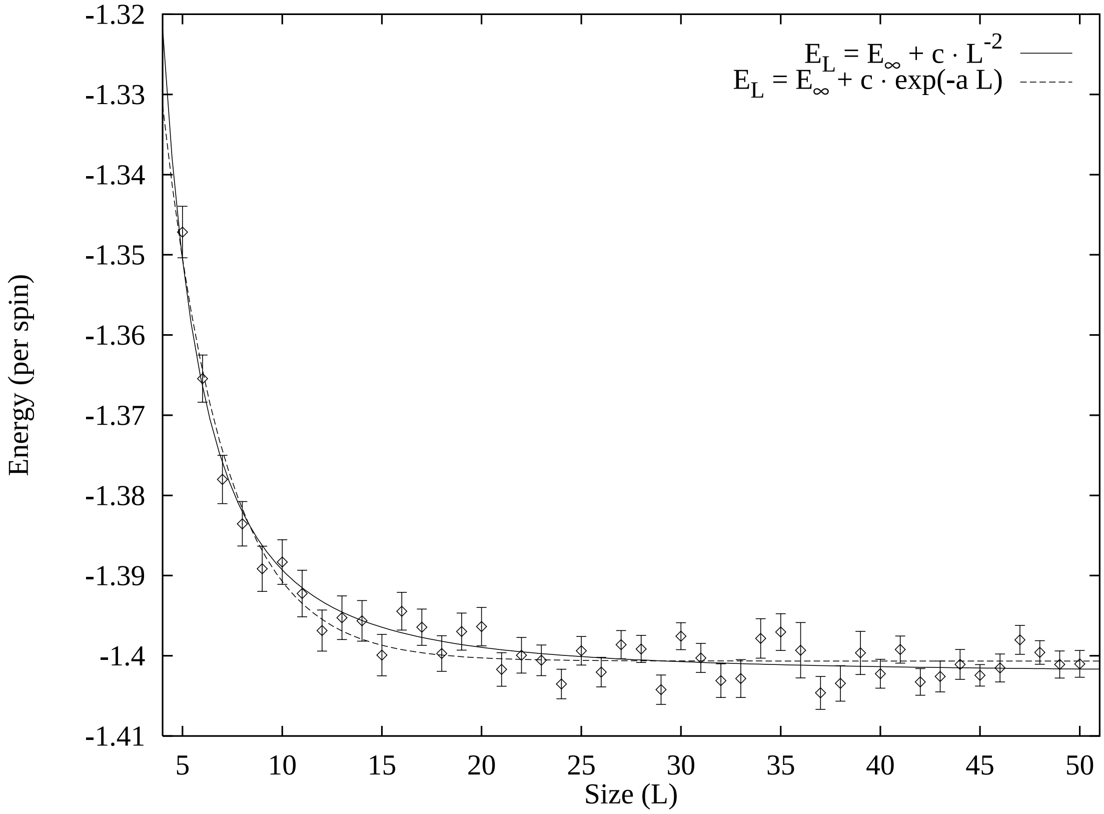


Figure 3: Ground State Energy for $p = 0.5$.

The error bars show the probable error $\sigma/\sqrt{N_L}$, where N_L is the number of computed ground states. With a fitting function of the form $E_v(L) = E_v^\infty + cL^{-2}$, we found $E_v^\infty = -1.4022 \pm 0.0003$, with a function of the form $E_e(L) = E_e^\infty + c\exp(-aL)$ we get $E_e^\infty = -1.4007 \pm 0.0003$. Both results agree with the result given in [Gro95b]. Note that L^2 is the volume of the system, see [Pál96] for a brief discussion about both fitting functions.

In Figure 4 the average CPU-times are shown. For better orientation there is also the graph of a function proportional to L^6 drawn as a straight line. Up to $L = 50$ the CPU-time can be approximated by this polynomial, for bigger systems the variance is very high. It is not surprising that the running time can be bounded by a polynomial (in this size range), since branching was nearly never necessary (99.53% of the samples were solved in the root node), so the program behaves mostly like a cutting plane algorithm with polynomial time separation routines.

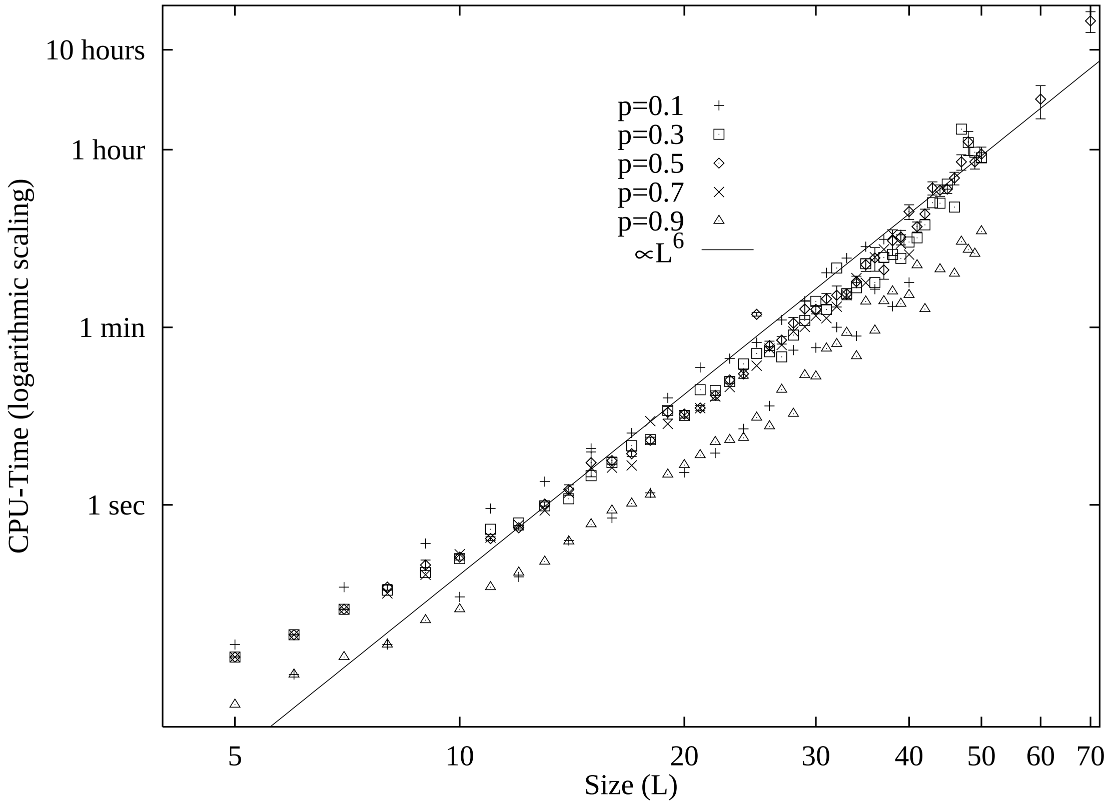


Figure 4: CPU-Time over System Size

In [BT91], Barahona and Titan reported their computational results on $\pm J$ spin glass systems where they published a certain 50×50 instance which took them about 17 hours CPU-time on a MIPS M-120 workstation using CPLEX as an LP-solver. We solved this one in 11 minutes.

Gropengiesser (see [Gro95b]) used biologically motivated algorithms for spin glasses with $p = 0.5$. He approximated ground states up to grid sizes of 24×24 which took about 350 seconds on a iPSC860 processor. Our program needed 17 seconds on the average to find an exact ground state for this sample size.

3 Conclusions

In this paper, we investigated exact ground state computations for $\pm J$ Ising spin glasses on 2-dimensional square lattices with nearest neighbor interactions and periodic boundary conditions. For the ground state energy of an infinite spin glass system with $p = 0.5$ we estimate $E^{\infty}_{0.5} = -1.4015 \pm 0.0008$. Since our approach is applicable also to three-dimensional systems, we plan to investigate them in the future.

Appendix: Proof of Proposition 1

In the proof we will use a result proven in [DR94]. For an edge weighted graph $G = (V, E, w)$ with node set V, edge set E and weight w_e for each $e \in E$ and a subset $D \subseteq E$, let $w(D) := \sum_{e \in D} w_e$ and for a subset $S \subseteq V$ let $\delta(S) := \{(u, v) \in E \mid u \in S, v \notin S\}$ denote the cut induced by S.

Theorem 1 ([DR94]) *Let $G = (V, E, w)$ be an arbitrary weighted graph; let $\delta(S)$ denote an arbitrary cut of G. The weighted graph $G_{\delta(S)} = (V, E, w')$ is the graph that is obtained by switching the weights of the graph G along the cut $\delta(S)$ i.e.,*

$$w'_e = \begin{cases} -w_e & \text{if } e \in \delta(S) \\ w_e & \text{if } e \notin \delta(S) \end{cases}$$

If W_G is the weight of a maximum cut in G, then the weight $W_{G_{\delta(S)}}$ of a maximum cut in $G_{\delta(S)}$ is given by

$$W_{G_{\delta(S)}} = W_G - w(\delta(S)).$$

Theorem 2 *Let $G = (V, E, w)$ be a toroidal grid graph with $L \times L$ nodes and weights $w_e = \pm 1$ on the edges. Let $G' = (V, E, w')$ be the graph that is obtained by multiplying the weight of every edge in G by -1. The weight $W_{G'}$ of a maximum cut in G' is given by*

$$W_{G'} = \begin{cases} W_G - w(E) & & \text{if } L \text{ is even} \\ W_G - w(E) + \Delta & \text{with } |\Delta| \le 2L & \text{if } L \text{ is odd} \end{cases}$$

Proof.

L is even

Since E is a cut in G the graph G' can be obtained by switching along E. Applying Theorem (1) directly results in

$$W_{G'} = W_G - w(E)$$

L is odd

Consider the graph $\tilde{G} = (\tilde{V}, \tilde{E}, \tilde{w})$ which is obtained from G by adding one row and one column of nodes and edges (see Figure 5).

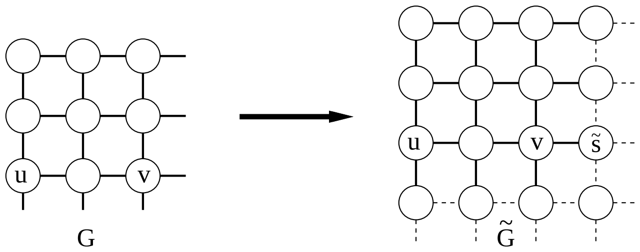


Figure 5: Converting G into $\tilde{G}$ and S into $\tilde{S}$

All new edges have weight 0. Because $\tilde{G}$ is again a toroidal grid graph with an even $\tilde{L}$ now, Theorem (1) can be applied to the graphs $\tilde{G}$ and $\tilde{G}'$ obtained from $\tilde{G}$ by multiplying all edge weights by -1. So we have

$$W_{\tilde{G}'} = W_{\tilde{G}} - w(E) \tag{2}$$

because $\tilde{w}(\tilde{E}) = w(E)$.

We can easily extend any $S \subseteq V$ to $\tilde{S}$ where $S \subseteq \tilde{S} \subseteq \tilde{V}$ in order to obtain a cut in $\tilde{G}$ of the same weight $\tilde{w}(\delta(\tilde{S})) = w(\delta(S))$ as the cut in G induced by S. Namely, let $\tilde{s} \in \tilde{V} \setminus V$ be adjacent to the nodes u and v, where $u, v \in V$. (All but one node in $\tilde{V} \setminus V$ are of that kind.) Let $\tilde{e} = (v, \tilde{s}) \in \tilde{E} \setminus E$, $\tilde{e}' = (u, \tilde{s}) \in \tilde{E} \setminus E$ and $e = (u, v) \in E$, such that $\tilde{w}(\tilde{e}) = w(e)$ and $\tilde{w}(\tilde{e}') = 0$. Then let $\tilde{s} \in \tilde{S}$ if and only if $u \in S$, because then the edge $\tilde{e}$ is in the cut $\delta(\tilde{S})$ if and only if $e \in \delta(S)$. The same reasoning applies to G' and $\tilde{G}'$, so we have

$$W_G \leq W_{\tilde{G}} \text{ and } W_{G'} \leq W_{\tilde{G}'} \tag{3}$$

Let $\delta(\tilde{S})$ with $\tilde{S} \subseteq \tilde{V}$ be a cut of maximum weight in $\tilde{G}$, i.e., $W_{\tilde{G}} = \tilde{w}(\delta(\tilde{S}))$. Then we can restrict $\tilde{S}$ to $S = \tilde{S} \cap V$ in order to obtain a cut $\delta(S)$ in G whose weight is at least $W_{\tilde{G}} - 2L$ because there are $2L$ edges in E that are connected to nodes in $\tilde{V} \setminus V$ and the edges connecting only nodes in $\tilde{V} \setminus V$ have all weight zero by construction. Since the value of this cut in G is in turn a lower bound for the value of an optimal cut in G, we obtain

$$W_G \geq W_{\tilde{G}} - 2L \text{ and } W_{G'} \geq W_{\tilde{G}'} - 2L \tag{4}$$

because the same holds for G' and $\tilde{G}'$.

Combining (2), (3), and (4) we have

$$\begin{aligned} W_G - w(E) - 2L &\overset{(3)}{\leq} W_{\tilde{G}} - w(E) - 2L \overset{(2)}{=} W_{\tilde{G}'} - 2L \\ &\overset{(4)}{\leq} W_{G'} \\ &\overset{(3)}{\leq} W_{\tilde{G}'} \overset{(2)}{=} W_{\tilde{G}} - w(E) \\ &\overset{(4)}{\leq} W_G - w(E) + 2L \end{aligned}$$

q.e.d.

Since the energies of configurations in spin glass systems represented by graphs $G = (V, E, w)$ and $G' = (V, E, w')$ are given by

$$E = -2W_G + w(E) \text{ and } E' = -2W_{G'} + w'(E)$$

respectively (see [DDJ+95]), and

$$w'(E) = -w(E)$$

the ground state energies of a spin glass system with concentration p of negative interaction and the corresponding one with all couplings multiplied by -1 (concentration $(1-p)$), are exactly the same if L is even and differ by at most $4L$ if L is odd. So the energy per spin difference is at most $\frac{4L}{L^2} = \frac{4}{L}$ for odd L.

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