Determining Energy Barriers by Iterated Optimization: The Two-Dimensional Ising Spin Glass.

C. Amoruso and A.K. Hartmann

Institut für Theoretische Physik, Universität Göttingen, Tammannstrasse 1, 37077 Göttingen, Germany

M.A. Moore

School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, U.K.

Energy barriers determine the dynamics in many physical systems like structural glasses, disordered spin systems or proteins. Here we present an approach, which is based on subdividing the configuration space in a hierarchical manner, leading to upper and lower bounds for the energy barrier separating two configurations. The fundamental operation is to perform a constrained energy optimization, where the degree of constraintness increases with the level in the hierarchy.

As application, we consider Ising spin glasses, where the energy barrier which needs to be surmounted in order to flip a compact region of spins of linear dimension \( L \) are expected to scale as \( L^\psi \). The exponent \( \psi \) is very hard to estimate from experimental and simulation studies. By using the new approach, applying efficient combinatorial matching algorithms, we are able to give the first non-trivial numerical bounds \( 0.25 < \psi < 0.54 \) for the two-dimensional Ising spin glass.

PACS numbers: 75.10.Nr, 75.40.Mg, 02.10.Jf

A unifying concept in the physics of disordered systems is the notion of energy landscapes. The dynamics of these systems is determined by (free) energy barriers. Prominent examples include spin glasses [1], structural glasses [2] and folding of proteins [3]. The barrier problem is also related to theoretical computer science, because it belongs [4] to the fundamental class of nondeterministic polynomial (NP) hard problems [5], hence all known algorithms determining lowest barriers take a time growing exponentially with system size.

In this paper, we will present a hierarchical approach to calculate minimum barriers, which is based on the application of combinatorial optimization algorithms [6]. As application, we apply it to the prototypical two-dimensional Ising spin glass, where the value of the barrier-height exponent could not be determined so far.

In the droplet [7] or scaling theory of Ising spin glasses the low-energy excitations are compact droplets. The creation of a droplet (a region of reversed spins) results in the formation of a domain wall around the reversed spins and the energy of the droplet scales as \( L^\theta \) where \( L \) is the linear extension of the droplet. The system orders at low temperatures only if \( \theta > 0 \). The domain wall is fractal and has size \( L^{d_S} \), with \( d-1 \leq d_S \leq d \). The dynamics of the system are controlled by the height of the barriers which have to be crossed to create such droplets. It is generally assumed that the barrier to be surmounted to create a droplet of linear extent \( L \) has an energy which scales as \( L^\psi \) where \( \theta \leq \psi \leq d-1 \) for dimension \( d \). The argument for these inequalities goes as follow: the barrier must be at least as large as the energy required to create the domain, hence \( \theta \leq \psi \). The upper limit is due to the fact that the barrier must be lower than the energy of the same number of reversed spins. While for a directed polymer in a random system it was shown that \( \psi = \theta \), for Ising spin glasses \( \psi \) appears to be an independent exponent.

While many numerical studies have been done to calculate the exponent \( \theta \), we are aware of only one direct numerical estimate of \( \psi \) in two dimension [8]. It was equal to the upper bound i.e, \( \psi = d - 1 \), but only small systems were studied \( (L \leq 6) \). As mentioned, the barrier problem is NP hard and it has been difficult even to find good approximate algorithms for barriers. This is presumably the reason for the paucity of studies of this exponent. Recently Drossel and Moore instead of attempting to calculate the barrier exactly, placed bounds on its energy [9]. They showed that for the hierarchical (i.e. Berker) lattice there exists a lower bound on \( \psi \) which is the same as the upper bound \( d - 1 \) and hence they concluded that \( \psi = d - 1 \). In the same spirit as their work, we will also obtain upper and lower bounds on the energy of the barriers but for the more physically relevant case of the square lattice. Rather than study droplets, we will consider the computationally simpler (but equivalent) task of determining upper and lower bounds for the barrier separating the two ground states (GSs) related by a flip of all spins. The algorithm is based on subdividing the configuration space in a hierarchical manner and performing constrained energy optimizations, where the degree of constraintness increases with the level in the hierarchy. This approach can be applied in general to obtain minimum barrier for many problems, but for the convenience of the reader, we formulate it here for the case of the two-dimensional Ising spin glass.

The model consists of \( N = L^2 \) spins \( S_i = \pm 1 \) on a square lattice with periodic boundary conditions in the x-direction.
direction and free boundary conditions in the $y$ direction. The Hamiltonian is

$$H = - \sum_{\langle ij \rangle} J_{ij} s_i s_j,$$

where the sum runs over all pairs of nearest neighbors $\langle ij \rangle$ and the $J_{ij}$ are the quenched random spin couplings. We will consider a Gaussian distribution of couplings with zero mean and unit width. We define the barrier to be the energy required to invert all spins in the GS within the context of single spin flip dynamics, as in \[8\]. Each trajectory of reversal is characterized by the highest maximum in the trajectory having energy $\delta E_{\text{max}}$, in excess of the GS energy, so that $E_B = \min(\delta E_{\text{max}})$, where the minimum has to be computed over all the possible trajectories.

Thus the first task is to compute the GS $\{\sigma^0\}$ of the spin glass; in general already this problem is NP hard, but for planar graphs it can be mapped on to the minimum-weight perfect matching problem, which is solvable in polynomial time. The algorithms for minimum-weight perfect matchings \[10, 11\] are among the most complicated algorithms for polynomial problems but the LEDA library offers a very efficient implementation \[12\].

We will now show how is it possible to extract bounds on $E_B$. In general, a lower bound on the energy barriers can be obtained, if one considers a sequence of constraints fixing some degrees of freedom leading from one configuration to the other and calculating the GS under each constraint. Here, we force a domain wall, which separates spins having orientation $\{\sigma^0\}$ from spin having orientation $\{-\sigma^0\}$, through constraining successive bonds along the x-axis. Thus, for each realization of the bonds $J_{ij}$, a GS is first calculated with free boundary conditions in both directions. Then “hard” bonds \[13\] are introduced, i.e. bonds with a high value of the absolute strength, compatible with the relative GS orientation of the adjacent spins, in a line which runs from the left border to the right border. Next the sign of exactly one hard bond on this line is inverted and the GS of the new realization is computed. The minimum of these $L$ energies is the domain wall associated with the exponent $\theta$. The maximum can be associated with a lower bound on $\psi$, because one is calculating the minimum with the highest energy in the sequence from putting the hard bonds at successive places on the x-axis. The true barrier height is associated with flipping one spin at a time and one might have to climb an even higher barrier to reach the maximum domain wall energy starting from the domain wall of minimum energy. We will next explain how to place an upper bound on the barrier height before discussing the results of the numerical work.

The basic idea of the general algorithm is to continue the constrained minimization in a hierarchical manner, i.e. one introduces additional constraints between all adjacent pairs of constrained GSs obtained above. This is continued recursively, until the level of changes of single degrees is reached. Hence, one obtains a path in configuration space where the maximum energy configuration yields an upper bound for the minimum energy barrier. I.e. For the spin glass we do this by introducing hard bonds along the line corresponding to the maximum spacing between two “adjacent” domain walls (either in the $x$ or the $y$ direction) and by forcing the first domain wall through each of these bonds, see Fig. \[1\]. This procedure is repeated iteratively until two consecutive domain walls differ only by a unique sequence of spin flips. Of course, since we are minimizing over a restricted set of paths, there could be some lower path over the energy landscape, hence our result will be an upper bound on the energy barrier. However, since the upper bound makes an attempt to estimate the energy needed to move the domain wall to successive places along the x-axis by a sequence of single spin flips, we believe the true value of $\psi$ is likely to be nearer the upper bound than the lower bound.

\[ \text{FIG. 1: Example showing how the domain wall is shifted. In (a) the black and the gray area represent the domain walls created by changing the sign of two consecutive hard bonds in the top (thick) line. The maximum distance between the two domain walls is determined and hard bonds are introduced along this line (thick line at the middle). Then the sign of each of these bonds is inverted exactly once (wiggled segment) and the new GS is calculated, so that the domain wall is forced to pass through them. In (b) the grey area now represents the configuration obtained when changing the sign of the leftmost hard bond and calculating the new GS. Again hard bonds are introduced along the line of maximum distance and the new GS (c) is computed for the realization in which the leftmost hard bond is inverted, as in (a). Now the distance between the two domain walls is at most one spin, so this spin is now flipped (yielding one step of the whole sequence) and the resulting configuration is shown in (d).} \]
For each flipped spin the energy of the configuration is calculated, and at the end the maximum among the \(N\) energies is considered. In this way we give an explicit rule to build a sequence of spin-flip taking one from the GS configuration \(\{\sigma^0\}\) to \(\{-\sigma^0\}\). An example of the corresponding energy landscape sampled by this sequence is shown in Fig. 2.

One has to be careful to exclude the domain walls which are not crossing the system and for which the width \(L\) is not an appropriate measure of their scale. Those configurations can appear in the first steps of the algorithm described above because of the use of free boundary conditions. Fortunately most of the domain walls do span the system. We have restricted our analysis to those configurations.

![FIG. 2: An example of the energy landscape explored by our algorithm for \(L = 14\); the exponent \(\psi\) is associated with the scaling of the maximum energy found in the sequence.](image)

We applied our method for system sizes in the range \(8 < L < 40\), and for each \(L\) used 1000 independent realizations of the bonds \(J_{ij}\). The two quantities \(\Delta E_{\text{min}}\) (the lower bound) and \(\Delta E_{\text{max}}\) (the upper bound) as a function of system size are shown in Fig. 3. Both quantities can be fitted by an algebraic function \(\sim L^{\psi}\), where \(\psi_{\text{tw}} = 0.25 \pm 0.01\) and \(\psi_{\text{up}} = 0.54 \pm 0.01\). There could of course be a procedure to obtain a better path in configuration space, yielding a barrier which grows more slowly than \(L^{0.54}\). However this is to our knowledge the only numerical estimate of the energy barriers exponent giving an upper bound different from the trivial one \(d - 1\).

There are many experimental estimate of \(\psi\) in the literature, and there is disagreement as to its value. Dekker et al. reported experimental verification of activated dynamics in a \(d = 2\) system obtaining \(\psi = 0.9\). Schins et al. find \(\psi = 1.0 \pm 0.1\) by studying aging via the low-frequency ac susceptibility giving credence to the claim that \(\psi\) is equal to its upper bound. However, Dupius et al. extracted \(0.3 < \psi < 0.7\) in \(d = 2\) and \(\psi \sim 1.1\) in \(d = 3\). The numerical study of Gawron et al. gave \(\psi = 0.9 \pm 0.1\) in 2 dimension, while that of Berthier and Bouchaud had \(\psi \sim 1.0\) and \(\psi \sim 2.3\) in 3 and 4 dimensions respectively. We remark that our optimization algorithms do not suffer from equilibration problems, they are exact and they allow the study of large systems at least in two dimensions. Besides, by iteratively applying our matching algorithm, we are producing large scale changes to the domain wall, which is how \(\psi\) can become less than \(d - 1\). (We have studied the barrier associated with a straight domain wall and found that the expected linear behavior is approached by \(L \sim 40\)).

In Figs. 4 and 5 the rescaled probability distributions of the barriers heights corresponding to both the lower and upper bounds which we have found, averaged over the disorder, is shown for different sizes \(L\): in both cases it seems to approach a fixed shape in the thermodynamical limit (although the approach to a scaling collapse is faster for the upper bound).

Notice that both these distributions have long tails indicating the existence of some very large barriers, which implies that some spin configurations could be very long-lived.

We also investigated geometrical properties of the domain walls corresponding to the energy barriers. The numerical estimate of the energy barriers exponent giving an upper bound different from the trivial one \(d - 1\).
from the European Community via the DYGLAGE-MEM, High-Level Scientific Conferences (HLSC) and the “Existence” programs.

 boundaries of the low-energy excitations are fractal with an average length along the perimeter of order $P \sim L^{d_S}$, with $d - 1 \leq d_S \leq d$. We have computed the fractal dimension of the domain wall $d_S$ corresponding to the configuration of maximum energy. We have found the interesting result that $d_S = 1.27 \pm 0.01$, which is the same value for domain walls of minimum energy.

To conclude we have introduced a hierarchical algorithm to compute upper and lower bounds on energy barriers in disordered systems. Applying the algorithm to two-dimensional Ising spin glasses, we find that the minimum barrier energy is bounded above by the scale $L^{0.54}$ and below by $L^{0.24}$. Our numerical upper bound is significantly less than the rigorous upper bound (and the value for the hierarchical lattice), $d - 1$. Hence, we suspect that $\psi$ is an entirely non-trivial exponent. At the present time there seems no theoretical approach which might explain a non-trivial value of $\psi$.

The authors have obtained financial support from the VolkswagenStiftung (Germany) within the program “Nachwuchsgruppen an Universitäten”, from the Paderborn Center for Parallel Computing in Germany, and see also http://www.algorithmic-solutions.de

FIG. 5: Rescaled probability distribution of the upper bound for the barriers heights corresponding to $\psi = 0.54$

FIG. 6: The perimeter (length) of the surface of the domain wall corresponding to the upper bound (maximum) energy. Data are fitted very well by a power law $P \sim L^{d_S}$, with $d - 1 \leq d_S \leq d$. We have computed the fractal dimension of the domain wall $d_S$ corresponding to the configuration of maximum energy. We have found the interesting result that $d_S = 1.27 \pm 0.01$, which is the same value for domain walls of minimum energy.

[1] Reviews on spin glasses can be found in: K. Binder and A.P. Young, Rev. Mod. Phys. 58, 801 (1986); M. Mezard, G. Parisi, and M.A. Virasoro, Spin glass theory and beyond, (World Scientific, Singapore 1987); K.H. Fisher and J.A. Hertz, Spin Glasses, (Cambridge University Press, Cambridge 1991); A.P. Young (ed.), Spin glasses and random fields, (World Scientific, Singapore 1998).

[2] Reviews on glasses can be found in C.A. Angell, Science 267, 1924 (1995); P.G. DeBenedetti, Metastable liquids, (Princeton University Press, 1996); S. Franz, S.C. Glotzer, and S. Sastry (eds.), Unifying Concepts in Glass Physics, J. Phys. Cond. Matt. 12, 6295-6682 (2000)

[3] T.E. Creighton (ed.), Protein folding, (Freemann, New York 1992).

[4] A.A. Middleton, Phys. Rev. E 59, 2571 (1999).

[5] M. R. Garey and D. S. Johnson, Computers and intractability (Freeman, San Francisco, 1979)

[6] A. K. Hartmann and H. Rieger, Optimization Algorithms in Physics, (Wiley-VCH, Berlin 2001).

[7] D.S. Fisher and D.A.Huse, Phys. Rev. B 38, 273 and 386 (1988).

[8] T.R. Gawron, M. Cieplak and J.R. Banavar J. Phys. A:Math. Gen. 24 L127 (1991)

[9] B. Drossel and M.A. Moore, Phys. Rev. B 70, 064412 (2004).

[10] W.J. Cook, W.H. Cunningham, W.R. Pulleyblank, and A. Schrijver, Combinatorial Optimization, (John Wiley & Sons, New York 1998).

[11] B. Korte and J. Vygen, Combinatorial Optimization - Theory and Algorithms, (Springer, Heidelberg 2000).

[12] K. Mehlhorn and St. Nähler, The LEDA Platform of Combinatorial and Geometric Computing (Cambridge University Press, Cambridge 1999).

[13] A.K. Hartmann and M.A. Moore, Phys. Rev. Lett. 90, 127201 (2003).

[14] I. Biche, R. Maynard, R. Rammal, and J.P. Uhry, J. Phys. A 13, 2553 (1980); F. Barahona, R. Maynard, R. Rammal, and J.P. Uhry, J. Phys. A 15, 673 (1982); U. Derigs and A. Metz, Math. Prog. 50, 113 (1991).

[15] C. Dekker, A.F.M. Arts and H.W de Wijn, and A.J. van Duynenfieldt and J.A. Mydosh, Phys. Rev. Lett. 61, 1780 (1988)

[16] A.G. Schins, E.M. Dons, A.F.M.Arts, H.W. de Wijn, E. Vincent, L.Leylekian and J. Hamman, Phys. Rev B 48, 16524 (1993)

[17] V.Dupuis, E. Vincent, J.P. Bouchaud, J.Hamman, A. Ito and H. Aurga Katorim, Phys Rev B 48, 174204 (2002)

[18] L. Berthier and J-P. Bouchaud Phys. Rev. B 66, 054404 (2002)