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by

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Overlap Barrier Calculations for Spin Glasses¹

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Abstract. A novel method for numerical spin glass investigations is described: Simulations of two replica at fixed temperature, weighted such that a broad distribution of the Parisi overlap parameter q is achieved. Canonical expectation values for the entire q -range (multi-overlap) follow by re-weighting and allow a calculation of spin glass tunneling barriers.

1. Introduction

We focus on the 3d Edwards-Anderson Ising (EAI) spin glass on a simple cubic lattice. It is widely considered to be the simplest model to exhibit realistic spin glass behavior. The energy is given by

$$E = - \sum_{\langle ik \rangle} J_{ik} s_i s_k \quad , \quad (1)$$

where the sum is over nearest-neighbour sites. The Ising spins s_i and s_k as well as the exchange coupling constants J_{ik} take values ± 1 . A realization is defined by a fixed assignment of the exchange coupling constants J_{ik} .

The intuitive picture for spin glasses and other systems with conflicting constraints, for reviews see [1, 2, 3], is that there exist a large number of degenerate thermodynamic states with the same macroscopic properties but with different microscopic configurations. These states are separated by free-energy barriers in phase space, caused by disorder and frustration. However, one difficulty of the theory of spin glasses is to give a precise meaning to this classification: No explicit order parameter exists which allows to exhibit the barriers. The way out of this dilemma appears to use an implicit parametrization, the Parisi overlap parameter q , which allows to visualize at least some of the encountered barriers. For the model at hand q is defined by

$$q = \frac{1}{N} \sum_{i=1}^N s_i^1 s_i^2 \quad . \quad (2)$$

Here N denotes the number of spins, the spins s_i^1 correspond to the first and the spins s_i^2 to the second replica (of the same realization). Calculations of these barriers in q are of major interest: For instance, it is unclear whether the degenerate thermodynamic states are separated by infinite barriers or whether this is just an artifact of mean-field theory.

Here I focus on Monte Carlo calculations. One question which ought to be addressed before attempting such a numerical approach is: "What are suitable weight factors for the problem at hand?" The weight factor of canonical Monte Carlo (MC) simulations is

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$\exp(-\beta E)$, where E is the energy of the configuration to be updated and β is the inverse temperature in natural units. However, by their very definition free energy barriers are suppressed by canonical weight factors. Fortunately, it became widely recognized in recent years that MC simulations with a-priori unknown weight factors, like for instance the inverse spectral density $1/n(E)$, are also feasible and deserve to be considered, see Ref.[4, 5] for recent reviews. An example are temperature-driven first-order phase transitions, controlled by the energy. The multicanonical method defines energy dependent weight factors to enhance configurations needed to estimate the interfacial tension. The multimagnetical method [6] does the same for magnetic field-driven first-order transitions, controlled by the magnetization. Along this line we have introduced a novel approach [7], which performs weighting in the Parisi overlap parameter (2).

2. Multi- q Simulations

Our [7] observation is that one does still control canonical expectation values at temperature β^{-1} when one simulates with a weight function

$$w(q) = \exp \left[\beta \sum_{\langle ik \rangle} J_{ik} (s_i^1 s_k^1 + s_i^2 s_k^2) + S(q) \right] \quad , \quad (3)$$

This is obvious for $S(q) = 0$, and a non-trivial $S(q)$ can be mapped onto this situation by re-weighting. In particular, when $S(q)$ is chosen such that the histogram $H(q)$ becomes uniform in q , the interpretation of $S(q)$ is that of a microcanonical entropy for the overlap parameter.

In our investigation we enforced the constraint $\sum_{\langle ik \rangle} J_{ik} = 0$ by picking half of the J_{ik} at random and assigning them the value $+1$, whereas the others are fixed at -1 . Simulations were performed on $V = L^3$ lattices at $\beta = 1$, in the region below the freezing temperature at $\beta_c \approx 0.9$, see [8, 9] for up-to-date determinations. All calculations were done on a cluster of Alpha workstations at FSU. We simulated 512 different realizations for $L = 4, 6$, and 8 , and 33 for $L = 12$. For all of them tunneling between the extrema $q = \pm 1$ was achieved. Initially in each run, a working estimate of the weight function (3) had to be obtained. Using a variant of the recursion explained in [10] this has turned out to be remarkably easy and took less than 25% of the CPU time spent. Each production run of data taking was concluded after at least twenty tunneling event of the form

$$(q = 0) \rightarrow (q = \pm 1) \text{ and back} \quad (4)$$

were recorded. Figure 1 depicts fits of the thus defined tunneling time τ , *i.e.* of the average number of sweeps it took to sample one tunneling event. An exponential fit has an unacceptable low goodness of fit Q , see [11] for the definition of this quantity. The power law fit is better (although not yet in the desired range $Q > 0.05$) and yields $z = 2.42 \pm 0.03$ for the autocorrelation exponent z . Although this slowing down is far off from the multicanonical optimum $z = 1$ [4], the improvement versus canonical simulations is huge, as we shall show. For a quantitative investigation we first generalize the definition of an interface barrier as used in studies of first order phase transitions, *e.g.* ref.[6]. Let $P_i(q)$ be the canonical probability densities of q , where $i = 1, \dots, n$ labels the different

Figure 1: Tunneling time versus lattice size on a double log scale.

realizations (additional dependence on lattice size and temperature is implicit). We define the corresponding potential barrier by

$$B_i = \prod_{q=-1}^{-\Delta q} \max [1, P_i(q)/P_i(q + \Delta q)] , \quad (5)$$

where Δq is the stepsize in q . For the double-peak situations of first-order phase transitions [6] equation (5) becomes $B_i = P_i^{\max}/P_i^{\min}$, where $P_i^{\max}$ is the absolute maximum and $P_i^{\min}$ is the absolute minimum (for ferromagnets at $q = 0$) of the probability density $P_i(q)$. Our definition generalizes to the situation where several minima and maxima occur due to disorder and frustration. When evaluating (5) from numerical data for $P_i(q)$ some care is needed to avoid contributions from statistical fluctuations of $P_i(q)$.

For the largest barriers (5) found in our simulations figure 2 gives the canonical and multi- q probability densities of the corresponding realizations. Where the multi- q probability densities stay flat around $P_i^{\text{muq}}(q) = 1$, the canonical $P_i^{\text{can}}(0)$ -values are suppressed by five to almost eight orders of magnitude. For the two $L = 4$ and for the $L = 6$ realization depicted we have performed canonical simulations to determine the improvement factor R_i , defined as ratio of the corresponding tunneling times. We find

$$R_{324} = 4,800, \quad R_{162} = 31,000 \text{ for } L = 4 \quad \text{and} \quad R_{459} = 12,800 \text{ for } L = 6 .$$

For $L = 6$ the statistics is rather bad as it relies on only five canonical tunneling events, which to produce took already several days on an Alpha 500 MHz processor. For the same realization the multi- q algorithm needs about 125 seconds for twenty tunneling events. As expected, R_i scales with the barrier B_i . Using this, we can estimate improvements factors

Figure 2: Probability densities for the realizations with the largest barriers (5) for each lattice size.

for the drawn $L = 8$ and $L = 12$ realizations, which do not allow for canonical tunneling anymore. To produce twenty canonical tunnelings would take us about 100 years for the $L = 8$ and 1000 years for the $L = 12$ lattice. These numbers ought to be compared with or actual runtime of 55 minutes for the $L = 8$ and 21 hours for the $L = 12$ lattice.

3. Conclusions

Multi-overlap simulations allow, for the first time, to study q -barriers in some details. An initial physical analysis is given in ref.[7] and, surprisingly, the typical median barrier show almost no finite size dependenc. This cast doubts on the apparently accepted opinion that these barriers a primiarly responsible for the breakdown of canonical ergodicity for this spin glass.

Using parallel computers and slight modifications of our method (like narrowing the q -range, including a magnetic field, etc.) will allow to extend our investigation into various interesting directions, like an improved study of the thermodynamic limit at and below the transition point (more realizations and larger lattice sizes), or ϵ -physics [12].

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