Computer Physics Communications 121–122 (1999) 176–179

Computer Physics Communications

www.elsevier.nl/locate/cpc

Multi-overlap simulations of free-energy barriers in the 3D Edwards–Anderson Ising spin glass

Wolfhard Janke [a,b,1], Bernd A. Berg [c], Alain Billoire [d]

[a] *Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, D-04109 Leipzig, Germany*
[b] *Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany*
[c] *Department of Physics and Supercomputer Computations, Research Institute, The Florida State University, Tallahassee, FL 32306, USA*
[d] *Service de Physique Théorique de Saclay, F-91191 Gif-sur-Yvette, France*

Abstract

We report large-scale simulations of the three-dimensional Edwards–Anderson Ising spin-glass model using the multi-overlap Monte Carlo algorithm. We present our results in the spin-glass phase on free-energy barriers and the non-trivial finite-size scaling behavior of the Parisi order-parameter distribution.

Spin-glass systems [1] are simple models of disordered materials such as, e.g., $(Fe_{0.15}Ni_{0.85})_{75}P_{16}B_6Al_3$ [2], with randomly distributed, competing interactions. Analytical solutions are only known in the mean-field limit which corresponds to infinite dimensionality or, equivalently, infinite-range interactions. For the physical case of short-ranged spin glasses in three dimensions this may serve as a guideline, but for quantitative predictions we have to rely either on numerical methods such as Monte Carlo (MC) simulations or high-temperature series expansions [3]. The prototype model is the Edwards–Anderson Ising (EAI) spin glass whose energy is given by

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

where the sum is over nearest-neighbor lattice sites, the spins s_i and s_k take values ± 1, and the exchange coupling constants J_{ik} are quenched, random variables. One popular choice is the bimodal distribution where $J_{ik} = \pm 1$, with equal probability. Each fixed assignment of the J_{ik} defines a realization of the system, and all physical results from simulations must be sampled over all possible realizations of the couplings.

Due to the competing interactions the phase space of spin glasses is highly non-trivial with many thermodynamic states separated by free-energy barriers. Canonical MC simulations are hence extremely difficult to perform. Refined update schemes such as multicanonical sampling [4], simulated and parallel tempering simulations [5] target at this problem, but the performance has remained below early expectation. One of the (many) problems of spin-glass simulations is that no explicit order parameter exists which allows us to exhibit the barriers. Usually one considers an implicit parametrization, the Parisi overlap parameter [1]

$$q = \frac{1}{N}\sum_{i=1}^{N} s_i^1 s_i^2, \tag{2}$$

which allows to visualize at least some of the barriers. The spins s_i^1 and s_i^2 correspond to two independent copies (replica) of the same realization (defined by its

[1] E-mail: wolfhard.janke@itp.uni-leipzig.de.

0010-4655/99/$ – see front matter
PII: S0010-4655(99)00306-9

couplings J_{ik}), each with its own time evolution in the MC process (realized by different threads of pseudo-random numbers). An important question is whether the degenerate thermodynamic states are separated by infinite barriers in q or whether this is just an artifact of mean-field theory.

In Ref. [6] two of the authors introduced a so-called "multi-overlap" method which, in contrast to the methods of Refs. [4,5] which aim at *avoiding* the rare-event regions associated with the free-energy barriers, focuses directly on *enhancing* the probability for sampling these rare-event regions. The basic observation, closely related to multicanonical methods [7], is that one does still control canonical expectation values at temperature β^{-1} when one simulates with the unphysical weight function

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

where the two replica are coupled through the function $S(q)$. In our large-scale simulations of the 3D EAI model [8] we determine $S(q)$ recursively such that the q-histogram $H(q)$ becomes uniform ("multi-overlap"). For each realization $i = 1, 2, \ldots$ the canonical probability density $P_i(q)$ is calculated (the dependence of $P_i(q)$ on lattice size and temperature is implicit). The multi-overlap algorithm is thus particularly designed for simulations of the interesting region below the freezing temperature where $P_i(q)$ does exhibit quite different shapes ranging from a simple peak at $q = 0$ over a double-peak to involved structures with several minima and maxima, for figures see [8].

In our study of the 3D EAI model we therefore focus on simulations at $\beta = 1 > \beta_c \approx 0.9$ [9]. We investigated lattices of size $N = L^3$ with $L = 4$, 6, 8, and 12, simulating 2×4096 different realizations for the smaller systems (drawing the J_{ik} in the first set with the pseudo-random number generator RANMAR [10] and in the second set with RANLUX [11]) and 2×512 for $L = 12$ (with RANMAR completed and with RANLUX in progress). In the simulations themselves we always employed the RANMAR generator due to CPU time considerations. For each realization the simulation consisted of three steps:

(1) Construction of the weight function (3), using an improved variant of the accumulative iteration scheme discussed in Ref. [12] that was stopped after at least 10 tunneling events of the form $(q = 0) \to (q = \pm 1)$ and back occurred (4–20 tunneling events for $L = 12$).
(2) An equilibration run for given fixed weight factors.
(3) A series of production runs for given fixed weight factors. In the production run data taking was concluded after at least 20 tunneling events occurred. By using an adaptive data compression procedure we made sure that for each realization a total of 65 536 measurements were recorded.

The thus created data allows us to calculate a number of physically interesting quantities. In particular accurate determinations of the canonical potential barriers in q are possible which in Ref. [6] are defined as

$$B_i = \prod_{q=-1}^{-\Delta q} \max\left[1, P_i(q)/P_i(q+\Delta q)\right], \qquad (4)$$

where Δq is the step-size in q. Our definition generalizes from the simpler double-peak situation at first-order phase transitions (where $B_i = P_i^{\max}/P_i^{\min}$ with $P_i^{\max}$ and $P_i^{\min}$ being the absolute maximum and minimum, respectively) to the more involved situation of spin glasses where several minima and maxima occur. Graphically, the distributions of our values for the B_i are presented in Fig. 1. It comes as a surprise that the finite-size dependence of the distributions is very weak. This indicates that at least some essential features of mean-field theory are violated in three dimen-

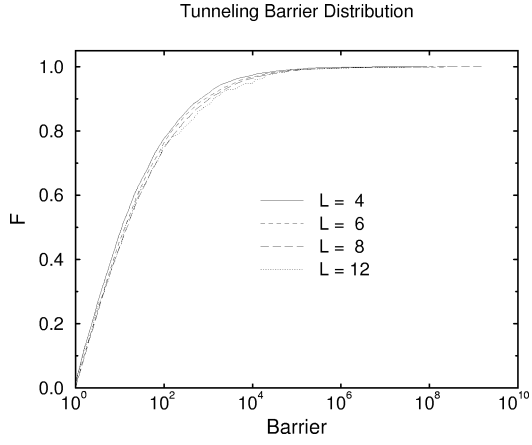

Fig. 1. Integrated probability density F of canonical tunneling barrier heights at $\beta = 1$.

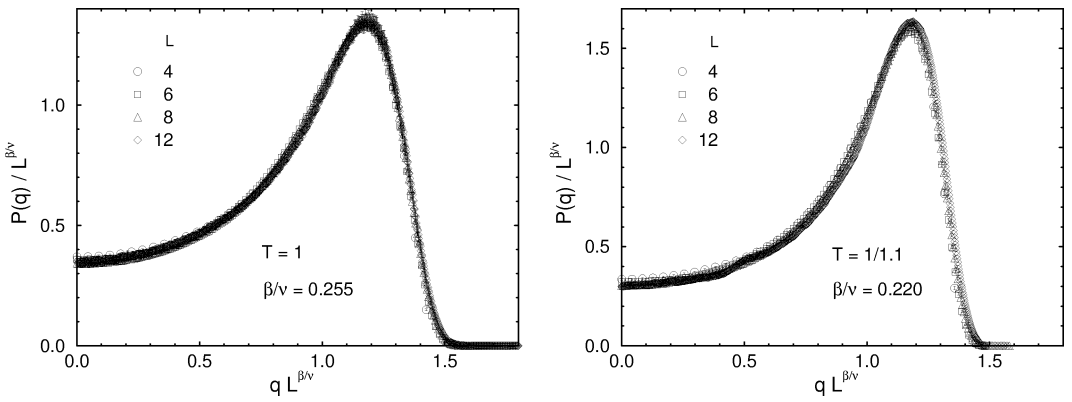

Fig. 2. Finite-size scaling plots for $P(q)$ at $T = 1$ and $T = 1/1.1$.

sions, or that larger lattices are required in order to observe the mean-field behavior.

Even though less detailed than the barrier data the averaged canonical probability densities $P(q) = [P_i(q)]_{\mathrm{av}}$ also contain important information on the system. Close to the freezing temperature T_{c} one expects that the probability densities $P(q)$ for different lattice sizes satisfy the finite-size scaling relation

$$P(q) = L^{\beta/\nu}\hat{P}\big(L^{\beta/\nu}q, L/\xi\big), \tag{5}$$

$$\xi \propto |T - T_{\mathrm{c}}|^{-\nu}, \tag{6}$$

where $\hat{P}$ is a scaling function, and β and ν are the critical exponents of the order parameter and correlation length, respectively. Right at T_{c} the second argument of $\hat{P}$ vanishes and when plotting $L^{-\beta/\nu}P(q)$ versus $L^{\beta/\nu}q$ the data for different lattice sizes should fall onto a common master curve. By employing standard techniques to reweight the simulation data at $T = 1$ to $T_{\mathrm{c}} \approx 1/0.9$ such a data collapse was already observed in our exploratory study [6], in agreement with results in Ref. [9]. It should be remarked, however, that extreme care is needed when estimating the reliable reweighting range for disordered systems. We suspect that this is the reason why the data of the present large-scale simulation still show good scaling behavior at T_{c} for the smaller system sizes but deviations for the $L = 12$ curve [8].

While the scaling property of $P(q)$ at T_{c} was expected, it came as another surprise that also in the broken phase at $T = 1 \approx 0.88T_{\mathrm{c}}$ a relatively good data collapse was observed [6]. This can be understood by assuming an unusually large correlation length, $\xi \gg L$. With our simulation set-up, this scaling conjecture in the broken phase can be tested most reliably at the simulation point $T = 1$, since then no temperature reweighting is involved. By adjusting the only free parameter, $\beta/\nu = 0.255$, we obtain the finite-size scaling plot in Fig. 2 which shows a clear data collapse onto a single master curve for all considered lattice sizes. Moreover, if we reweight our data down to the even lower temperature $T = 1/1.1 \approx 0.80T_{\mathrm{c}}$, we still find a very good data collapse, see Fig. 2. At $T = 1/1.2 \approx 0.73T_{\mathrm{c}}$ the smaller lattices behave similarly, but here it is again questionable whether we are still within the reliable reweighting range for the $L = 12$ curve.

In conclusion, we have performed a high-statistics simulation of the 3D EAI model at $\beta = 1$. The use of q-dependent (multi-overlap) weight factors in the simulations allows us to obtain precise results for free-energy barriers in q. Using slight modifications of the method will allow us to extend our investigation into various interesting directions, like an improved study of the thermodynamic limit at and below the freezing point, a study of the 4D EAI model, the influence of a magnetic field, etc.

Acknowledgements

W.J. thanks K. Binder for useful discussions and acknowledges support from the DFG through a Heisenberg Fellowship. The numerical simulations were per-

formed on T3E computers of CEA Grenoble, ZIB Berlin, and HLRZ Jülich. This research was partially funded by DOE under Contracts No. DE-FG02-97ER41022 and DE-FG05-85ER2500.

References

[1] K. Binder, A.P. Young, Rev. Mod. Phys. 58 (1986) 810;
M. Mézard, G. Parisi, M.A. Virasoro, Spin Glass Theory and Beyond (World Scientific, Singapore, 1987);
K.H. Fischer, J.A. Hertz, Spin Glasses (Cambridge University Press, Cambridge, 1991).
[2] P. Granberg, P. Svedlindh, P. Nordblad, L. Lundgren, H.S. Chen, Phys. Rev. B 35 (1987) 2075.
[3] B. Lobe, W. Janke, K. Binder, Mainz preprint (May 1998); to appear in Europ. Phys. J. B.
[4] B.A. Berg, T. Celik, Phys. Rev. Lett. 69 (1992) 2292;
B.A. Berg, U. Hansmann, T. Celik, Phys. Rev. B 50 (1994) 16444.
[5] W. Kerler, P. Rehberg, Phys. Rev. E 50 (1994) 4220;
K. Hukusima, K. Nemoto, J. Phys. Soc. Japan 65 (1996) 1604;
E. Marinari, G. Parisi, J.J. Ruiz-Lorenzo, in: Spin Glasses and Random Fields, P. Young (Ed.) (World Scientific, Singapore, 1997) 59.
[6] B.A. Berg, W. Janke, Phys. Rev. Lett. 80 (1998) 4771.
[7] B.A. Berg, in: Multiscale Phenomena and Their Simulation, F. Karsch, B. Monien, H. Satz (Eds.) (World Scientific, Singapore, 1997) 137–146;
W. Janke, in: Classical and Quantum Dynamics in Condensed Phase Simulations, B. Berne, G. Ciccotti, D. Coker (Eds.) (World Scientific, Singapore, 1998) 195–210.
[8] W. Janke, B.A. Berg, A. Billoire, Ann. Phys. (Leipzig) (1998) in press;
B.A. Berg, A. Billoire, W. Janke, in preparation.
[9] N. Kawashima, A.P. Young, Phys. Rev. B 53 (1996) R484.
[10] G. Marsaglia, A. Zaman, W.W. Tsang, Stat. Prob. Lett. 8 (1990) 35.
[11] M.L. Lüscher, Comp. Phys. Commun. 79 (1994) 100;
F. James, Comp. Phys. Commun. 79 (1994) 111.
[12] B.A. Berg, J. Stat. Phys. 82 (1996) 323.