Multicanonical Recursions\textsuperscript{1}

Bernd A. Berg\textsuperscript{2,3}

(berg@hep.fsu.edu)

Abstract

The problem of calculating multicanonical parameters recursively is discussed. I describe in
detail a computational implementation which has worked reasonably well in practice.

\textsuperscript{1}This research was partially funded by the Department of Energy under contracts DE-FG05-87ER40319
and DE-FC05-85ER2500.

\textsuperscript{2}Department of Physics, The Florida State University, Tallahassee, FL 32306, USA.

\textsuperscript{3}Supercomputer Computations Research Institute, Tallahassee, FL 32306, USA.
1 Introduction

Recently Monte Carlo (MC) sampling with respect to unconventional ensembles has received some attention [1–20]. In the multicanonical ensemble [1, 3] one samples configurations such that exact reconstruction of canonical expectation values becomes feasible for a desired temperature range. This requires a broad energy distribution, and leaves innovative freedom concerning the optimal shape [7]. Considerable practical experience exists only for the uniform energy distribution, where one samples such that:

(a) The energy density is flat in a desired range

\[ P(E) = \text{const} \quad \text{for} \quad E_{\text{min}} \leq E \leq E_{\text{max}}. \] (1)

(b) Each configuration of fixed energy \( E \) appears with the same likelihood.

It should be noted that condition (b) is non-trivial. A simple algorithm [21] exists to achieve (a), but which give up (b). Exact connection to the canonical ensemble is then lost. Such algorithms are interesting for hard optimization problems, but unsuitable for canonical statistical physics. The present paper focuses on achieving (a) and (b).

The average computer time \( \tau \), measured in updates, which it takes to proceed from \( E_{\text{min}} \) to \( E_{\text{max}} \) \textit{and back} has been named “tunneling time” [1, 2]. It should be noted that the method overcomes free energy barriers actually not by a tunneling process, but through moving along valleys, which are connected to the disordered phase. Once an updating scheme is given, like standard Metropolis, it is an interesting theoretical question to find the weight factors which minimize the tunneling time. It is by no means clear that this will be the uniform choice (1), on which the present paper is focused.

Multicanonical and related sampling has allowed considerable gains in situations with “supercritical” slowing down. Such are:

(a) First order transitions [1, 3], for a recent review see [20].
(b) Systems with conflicting constraints, such as spin glasses \[2, 4, 17, 18\] or proteins \[15, 16\].

To achieve a flat energy distribution, the appropriate unnormalized weight factor \(w(E)\) is the inverse spectral density \(w(E) = n^{-1}(E)\), just like the weight factor for canonical MC simulations is the Boltzmann factor \(w^B(E) = \exp(-\beta E)\). Now, the spectral density is a–priori unknown. Otherwise we would have solved the problem in the first place. Presumably, reluctance about simulations with an a–priori unknown weight factor is the main reason why the earlier umbrella sampling \[22\] never became popular in statistical physics.

For first order phase transitions the problem of the a–priori unknown weight factor is rather elegantly overcome by means of finite size scaling (FSS) methods \[1, 9, 10, 12, 20\]. A sufficiently accurate estimate is obtained by extrapolation from the already simulated smaller lattices. The smallest lattices allow still for efficient canonical simulations.

For systems with conflicting constraints the situation is less satisfactory. For instance for spin glasses one has to perform the additional average over quenched random variables (which are the exchange coupling constants). Different choices of these random variables define different realizations of the same system. For the Edward–Anderson Ising spin glass it turned out \[2, 17\] that, even for identical lattice sizes, different realizations need different weight factors. Each system requires a new estimate of the weight factors with no a–priori information available. To achieve this, a recursion\(^{23}\) was introduced by Celik and the author \[2\]. However, details of the recursion (see section 3) may need considerable attention by hand. This attention is possible when only a few lattices are simulated, but impractical when hundreds or even thousands of different realizations have to be handled. This renders it inconvenient for more complicated situations, like the 3d Edwards–Anderson Ising (EAI) spin glass.

Consequently, the recursion actually used in Ref.\[17\], where multicanonical simulations were performed for more then 1,500 different realizations of the EAI model, differed from the one described in \[2\]. The main purpose of this article is to describe this particular
approach. In each recursion step the statistical information from all previous runs is used directly for estimating the multicanonical parameters as well as for noise reduction. Further, the recursion turned out to be robust. Little attention by "hand" was needed. However, no claim is made that it is in any sense optimal (actually the author is considering various improvements). It is supposed to be a reasonable starting point to provide a running code quickly.

The paper is organized as follows: In section 2 generalized Ising models and related preliminaries are introduced. Mainly for pedagogical reasons I focus on them for examples of this paper. It is clear that generalization to other systems is straightforward, although possibly tedious for continuous systems. In section 3 I introduce the multicanonical method, and discuss the recursions given in the literature [2, 13]. Section 4 describes the recursion which I invented for the simulations of [17], and section 5 illustrates its performance. Summary and conclusions follow. The appendix gives and explains a corresponding program listing.

2 Generalized Ising Models

Let us consider a $d$–dimensional hypercubic lattice of volume $V = N = L^d$ with periodic boundary conditions. Spins $s_i = \pm 1$ are located at the $N$ sites, and exchange interactions $J_{ik} = \pm 1$ at the $dN$ links of the lattice. The energy of generalized Ising models is given by

$$E = -\sum_{ik} J_{ik} s_i s_j,$$

(2)

where the sum is over the nearest neighbors. For $J_{ik} \equiv 1$ the standard Ising ferromagnet (IF) is recovered. When the $J_{ik}$ are quenched random variables, one obtains the EAI spin glass. I confine the subsequent discussion to these two situations, although there are other cases of interest [24]. Let us further restrict the EAI spin glass to the situation $\sum_{<ik>} J_{ik} = 0$.

The partition function may be written as

$$Z(\beta) = \sum_E n(E)e^{-\beta E},$$

(3)
where $n(E)$ is the spectral density \cite{25}, more precisely the number of configurations (or states) with energy $E$. As the system has $2^N$ different states, this implies the normalization

$$\sum_{E} n(E) = 2^N.$$  \hspace{1cm} (4)

The lowest possible energy is $-dN$, reached when each link contributes $J_{ik}s_is_k = 1$. For the IF this is achieved with either all spins up (+1) or all spins down (−1). For a generic configuration the possible energy increments under the flip of a single spin are

$$\Delta E = 0, \pm 4, ..., \pm d.$$  \hspace{1cm} (5)

Consequently $n(E)$ may take non-zero values for

$$E = -dN, -dN + 4, ..., 0, ..., dN - 4, dN.$$  \hspace{1cm} (6)

For instance for the IF $n(-dN) = 2$, $n(-dN + 4) = 0$, ..., and $n(-dN + 4d) = N$. For a typical EAI spin glass configuration the groundstate energy $E_{\text{min}}$ is considerably larger than $-dN$.

## 3 Multicanonical Sampling

In the pedagogical review \cite{5} I emphasized that the inverse spectral density is the appropriate weight factor to obtain a flat energy density

$$w(E) = n^{-1}(E) = e^{-\beta(E)E + \alpha(E)}.$$  \hspace{1cm} (7)

Here $\beta(E), \alpha(E)$ is the multicanonical parameterization \cite{1, 2, 27}. Its rationale is to relate to the temperature. It should be noted that MC calculations are insensitive to an over-all independent factor, i.e. against replacing $w(E)$ by $cw(E)$. In the following I will exploit this property from time to time, and not trace back the corresponding multiplicative or additive constants. If necessary they may be obtained by introducing a convenient normalization.

The spectral density may be written as

$$n(E) = e^{S(E)},$$  \hspace{1cm} (8)
where $S(E)$ is the microcanonical entropy $^{25}$. The thermodynamical relation for the inverse temperature ($\beta = T^{-1}$, where my Boltzmann constant convention is $k = 1$) is

$$\beta = \frac{\partial S}{\partial E}. \quad (9)$$

For models with discrete energy values this may be translated into

$$\beta(E) = \frac{S(E + \epsilon) - S(E)}{\epsilon}, \quad (10)$$

where $\epsilon$ is the smallest possible energy increment such that $n(E + \epsilon)$ and $n(E)$ are both non-zero. i.e. typically we have $\epsilon = 4$ for the model of section 2 (special care is needed for the IF close to its groundstate). Note that equation (10) is in part convention. Other valid options would be $\beta(E) = [S(E) - S(E - \epsilon)]/\epsilon$ or $\beta(E) = [S(E + \epsilon) - S(E - \epsilon)]/(2\epsilon)$. For consistency with $^{2, 3}$ I stay with (10).

Once $\beta(E)$ is given, $\alpha(E)$ may be determined recursively. The equality of $e^{-S(E)}$ and $e^{-\beta(E)E + \alpha(E)}$ implies

$$S(E) - S(E - \epsilon) = \beta(E)E - \beta(E - \epsilon)(E - \epsilon) - \alpha(E) + \alpha(E - \epsilon).$$

Using (10) to eliminate the term $\epsilon \beta(E - \epsilon)$, we find for $\alpha(E)$ the recursion relation

$$\alpha(E - \epsilon) = \alpha(E) + [\beta(E - \epsilon) - \beta(E)]E, \quad \alpha(E_{\text{max}}) = 0. \quad (11)$$

Here $\alpha(E_{\text{max}}) = 0$ is a choice of the over-all multiplicative constant, needed to start off the recursion.

To perform a multicanonical simulation, we do not need to know the exact weight factor (7). Instead, a working estimate $\overline{w}(E)$ of $w(E)$ is sufficient, such that the sampled energy histogram $H(E)$ is approximately flat in the desired energy range (1). In the subsequent discussion I use the notation $\overline{n}(E), \overline{S}(E), \overline{\beta}(E), \overline{\alpha}(E)$ for estimators of the corresponding quantities $n(E), S(E), \beta(E)$ and $\alpha(E)$.

The technical feasibility of multicanonical sampling depends on the existence of efficient methods to obtain an acceptable estimate $\overline{w}(E)$. Computational resources and concurrent
numerical options determine how much computer time one will consider acceptable for the
calculation of $\overline{w}(E)$. Typically it should be less or at most of the order of the CPU time
spent on the subsequent multicanonical sampling (with then fixed parameters). It seems
that different workers in the field have tried various approaches. I am only familiar with two
of them.

(a) Approaches which work in one or two steps \cite{1, 9, 12}. Employing FSS a reasonable
good approximation $\overline{w}^{(1)}(E)$ is obtained by extrapolation from previously simulated,
smaller lattices. With $\overline{w}^{(1)}(E)$ a first multicanonical simulation is carried out. Its
results give an improved estimate $\overline{w}^{(2)}(E)$ with which additional simulations may be
done. This approach works well for first order phase transitions, but failed badly for
some disordered systems.

b) Recursive calculations $\overline{w}^n(E) \rightarrow \overline{w}^{n+1}(E)$ have been employed. They are subject of the
following subsection.

3.1 Recursive multicanonical calculations

Let $H^n(E)$ be the unnormalized histogram obtained from a (short) multicanonical simulation
with $\overline{w}^n(E)$. At energy values for which $H^n(E)$ is reliable, the new estimate is

$$\overline{w}^{n+1}(E) = \frac{\overline{w}^n(E)}{H^n(E)}. \quad (12)$$

Clearly (12) fails for energy values for which $H^n(E) = 0$, and also values like $H^n(E) = 1$
or 2 are of course statistically unreliable. Worse, even large values like $H^n(E) = 10^6$ may
still not give reliable estimates. Namely, situations can be encountered where the integrated
autocorrelation time is of the same order of magnitude or even larger. Before I come to
a more thorough discussion of this problem, I would like to discuss two approaches in the
literature.

To be definite, let us assume that the starting point for the recursion is

$$\overline{w}^0(E) \equiv 1. \quad (13)$$
In general this is a reasonable choice, which will allow us to recover the normalization (4) when desired. For some practical applications other choices, like a canonical simulation at a certain temperature, may be more convenient.

In the paper by Celik and myself [3] equation (12) was stated in the multicanonical notation (7). It reads then (note $\epsilon = 4$ in Ref.[3])

$$\overline{\beta}^{n+1}(E) = \overline{\beta}^n(E) + \epsilon^{-1} \ln[H^n(E + \epsilon)/H^n(E)].$$

(14a)

The function $\overline{\alpha}^{n+1}(E)$ is then determined by equation (11). In addition to (14a) specific rules were given about how to exclude unreliable histogram entries. Namely,

$$\overline{\beta}^{n+1}(E) = \begin{cases} \overline{\beta}^n(E) & \text{for } E \geq E^n_{\text{median}}; \\ \overline{\beta}^{n+1}(E_{\text{cut-off}}) & \text{for } E < E^n_{\text{cut-off}}. \end{cases}$$

(14b)

Here $E^n_{\text{median}}$ is the median of the $n^{th}$ energy distribution, and $E^n_{\text{cut-off}} < E^n_{\text{median}}$ is an energy cut–off, such that in simulation $n$ the temperature is kept constant for $E < E^n_{\text{cut-off}}$. Further, note that the starting condition (13) becomes $\overline{\beta}^0(E) \equiv 0$, $\overline{\alpha}^0(E) \equiv 0$.

Lee [13] states his recursion in two parts:

$$\overline{S}^{n+1}(E) = \overline{S}^n(E) + \ln H^n(E) \quad \text{for } H^n(E) \geq 1,$$

(15a)

and

$$\overline{S}^{n+1}(E) = \overline{S}^n(E) \quad \text{for } H^n(E) = 0,$$

(15b)

The first part is obviously equation (12), as follows from $\overline{w}^n(E) = \exp[-\overline{S}^n(E)]$. The identity [14] of (15a) and (14a) follows from (10). Obviously (15a) is a convenient intermediate step to derive (14a). The second part (15b) is a specific prescription about how to handle $H^n(E) = 0$. The other unreliable $H^n(E)$ are included into the recursion (12). Let us note the following:

(a) Besides from minor notational differences, it is uniquely determined how to handle the reliable part of the data. One should note that the equivalent equations (12), (14a) and (15a) are all non–local in the sense that ultimately histogram entries over the entire
sampled range will determine the transitions amplitudes from one energy to the next. It may be a little surprising that equation (14a) looks less local than equation (12) or (15a). This is entirely irrelevant, because the weight factors are only auxiliary quantities to determine (for instance by detailed balance) the decisive transition probabilities \( w[E \rightarrow E'] \). The transition probabilities relate different energies. \( W = (w[E \rightarrow E']) \) forms a (sparse) matrix, and its eigenvector with eigenvalue one is finally supposed to become the spectral density, \textit{i.e.} determines the weight factors. This diagonalization (implicitly carried out by the MC simulation) is a non-local process. This non-locality may induce certain instabilities. For instance, if inaccurate weight factors somewhere in the energy range create a region of attraction, all CPU time in the next run may be wasted on iterating on an irrelevant energy region.

(b) As the recursion (12) and (15a) stand, the statistical accuracy of estimate \( n + 1 \) is entirely determined by MC simulation \( n \). With increasing \( n \) the covered energy range gets larger and larger. One needs longer and longer simulations just to regain the previously reached statistical accuracy (on the appropriate energy subrange). It is possible, but tedious, to combine the statistics of simulations \( n, n - 1, ..., 1, 0 \). The gain is not quite as dramatic as one may superficially expect, because simulation \( n + 1 \) does still explore the entire energy range, just for the purpose to explore an additional increment of the desired energy range.

(c) Note that the median rule of (14b) freezes estimates on some part of the already covered energy range. One should improve on it by using subsequent statistics when available. In \cite{2} it was suggested to combine the median rule with upper bounds on the energy, such that the energy range gets reasonably restricted. However, it is then difficult to ensure ergodicity.

(d) A central difficulty of the recursion is the handling of energy regions for which reliable statistical information is not yet available. I elaborate on this now.
Lee’s proposal (15b) looks attractive because of its simplicity. It works for the very small systems considered in his paper, but for many realistic situations it will lead to an unacceptable slowing down. The reason is that (15b) is equivalent to simulating with a constant weight factor (7). Now, at low temperatures one typically encounters
\[ n(E - \epsilon) / n(E) \sim V^{-1}. \] (16)

Therefore, for a not yet covered energy range \( E \leq E_0 \) one will need of order \( V \) attempts just to achieve once the transition \( E_0 \rightarrow E_0 - \epsilon \).

The rule \( \beta^{n+1} = \beta^{n+1}(E_{\text{cut-off}}) \) for \( E < E_{\text{cut-off}} \) from (14b) achieves a far better performance for this situation. Assume that \( \beta(E) \) is monotonically increasing towards lower energies (exceptions are first order phase transitions). A canonical simulation with \( \beta^{n+1}(E_{\text{cut-off}}) \) will have its maximum energy density at \( E = E_{\text{cut-off}} \), because its first derivative with respect to the energy is zero there. The width of its energy distribution is of order \( \sqrt{V} \). Consequently, there will be no weight factor problem associated with proceeding towards lower energies. In practice one has to use estimators \( \overline{\beta}^{n+1}(E) \). One would like to chose \( E_{\text{cut-off}} \) as low as possible, but one encounters noise problem when the cut-off energy is shifted too far towards the edge of the reliably covered energy range. With some experience a good “pick” for \( E_{\text{cut-off}} \) can be achieved by just inspecting the function \( \overline{\beta}^{n+1}(E) \). Alternatively, one may use a fit \( \overline{\beta}_{\text{max}}^{n+1} \) from several energy values instead of \( \overline{\beta}^{n+1}(E_{\text{cut-off}}) \), or even fit the continuation of the entire function \( \overline{\beta}^{n+1}(E) \) for \( E < E_{\text{cut-off}} \) (with the penalty of spurious instabilities). In any case, in energy regions where (16) holds, one expects a performance increase by at least a volume factor over using (15b). On the other hand, it is precisely this part of the recursion (14) which required annoying attention by hand. This experience can, of course, set rule out the possible existence of some more perfect fitting procedure, to estimate \( \overline{\beta}^{n+1}(E) \) towards lower energies.

How the recursion (14) slows down with volume depends thus on the details of its implementation. Typically, one has to cover a macroscopic energy range, \( i.e. E_{\text{max}} - E_{\text{min}} \sim V \). The optimal slowing down of a single multicanonical simulation on this range is \( \sim V^2 \), cor-
responding to a random walk in the energy $[1]$. Of order $V^{0.5}$ simulations are needed to iterate from an initial canonical distribution up to covering the entire energy range multicanonically. This leads to an optimal slowing down $\sim V^{2.5}$ for the recursion. That this is not an overestimate follows from the fact that the slowing down of a multicanonical simulation on half the energy range still scales with $V^2$, and it still takes of order $V^{0.5}$ simulations to iterate from half the range to the full range.

4 Accumulative Recursion

I now introduce a recursion which calculates $\beta^{n+1}(E)$ on the basis of the statistics accumulated in all previous runs $n, n-1, ..., 1$. For this purpose let us first re–write (14a) as

$$\beta^{n+1}(E) = \epsilon^{-1} \ln[H^n(E + \epsilon)/H^n_{\beta}(E)],$$

(17)

where

$$H^n_{\beta}(E) = H^n(E)e^{-\beta^n(E)\epsilon}.$$  

(18)

Equation (17) still holds when $H^n(E)$ and $H^n_{\beta}(E)$ are replaced by non–zero linear combinations $\hat{H}^n(E)$ and $\hat{H}^n_{\beta}(E)$:

$$\hat{H}^n(E) = \sum_{m=0}^{n} W^m(E)H^m(E),$$  

(19a)

$$\hat{H}^n_{\beta}(E) = \sum_{m=0}^{n} W^m(E)H^m_{\beta}(E).$$  

(19b)

The accumulated statistics can be presented by suitable choice of the weight factors $W^m(E)$. The optimal choice is not clear, as it may depend non-trivially on the dynamics. In practice

$$W^m(E) = \frac{\min[H^m(E + \epsilon), H^m(E)]}{\max[H^m(E + \epsilon), H^m(E)]}$$  

(20)

has worked well. It relies on the conservative assumption that each contribution to the estimate

$$\beta^{n+1}(E) = \epsilon^{-1} \ln[\hat{H}^n(E + \epsilon)/\hat{H}^n_{\beta}(E)]$$  

(21)
will be as good as its weakest part. This equation is supplemented by
\[ \overline{\beta}^{n+1}(E) = \overline{\beta}^{n+1}(E + \epsilon) \] (22)
for the case that either \( \hat{H}^n(E + \epsilon) \) or \( \hat{H}^n_{\beta}(E) \) has insufficient statistics. To provide some feeling for the estimator (21) let me discuss two special cases.

(a) When the desired, flat distribution is already reached, the weight factors (20) equal 1 up to statistical fluctuations. Let us ignore fluctuations for the moment. Then \( \hat{H}^{n-1}(E + \epsilon) = \hat{H}^{n-1}(E) \) holds before the \( n^{th} \) run, which uses \( \overline{\beta}^n(E) \) as defined by equation (21). In the \( n^{th} \) recursion \( H^n(E+\epsilon) = H^n(E) \) is obtained by assumption. This leads to \( \hat{H}^n(E + \epsilon) = \hat{H}^{n-1} + H^n(E + \epsilon) \) and \( \hat{H}^n_{\beta}(E) = \hat{H}^{n-1}_{\beta} + H^n(E) \exp(-\overline{\beta}^n \epsilon) \). Equations (19), (21) yield \( \overline{\beta}^{n+1}(E) = \overline{\beta}^n(E) \), i.e. the \( \beta(E) \) function is a fixed point when the sampled distribution is flat.

(b) Consider the first recursion, carried out with \( \overline{\beta}^0(E) \equiv 0 \). The sampling results will be \( H^0(E + \epsilon)/H^0(E) = n(E + \epsilon)/n(E) \), again up to statistical fluctuations. Recursion (21) yields \( \overline{\beta}^1(E) = \epsilon^{-1} \ln[n(E + \epsilon)/n(E)] \), which is already the final multicanonical answer due to the fact that we have neglected statistical fluctuations. Quite generally it can be shown that the desired multicanonical function \( \beta(E) \) is an attractive fixed point of the recursion.

In practice there may be severe statistical fluctuations due to only few, correlated entries in \( H^n(E + \epsilon) \), \( H^n(E) \) or both. If the number of entries in both arrays is small, but approximately equal (\( W^n(E) \approx 1 \)), equations (19) guarantee that increase from \( \hat{H}^{n-1} \rightarrow \hat{H}^n \) is in proportion the the generated statistics (assuming similar autocorrelation time in runs \( n - 1, n - 2, \ldots \)). If the number of entries is only small in either \( H^n(E + \epsilon) \) or \( H^n(E) \), the weight factor (20) correct for the asymmetry. The larger statistics is reduced to the smaller one, and the smaller even more suppressed. As the ratio \( \hat{H}^n(E + \epsilon)/\hat{H}(E) \) determines the estimate \( \overline{\beta}^n(E) \), it is clear that a large statistical fluctuations in either the numerator or the denominator is sufficient to destroy the entire estimate. The weight factor prevents this.
The obvious advantage of equation (21) over recursion versions of section 3 is that the accumulative statistics of all runs is used to reduce statistical fluctuations. In [17] we have not supplemented the present recursion by a median restrictions of the type (14b), although this might lead to further improvements. Without such restrictions, typically the recursion leads quickly to rather high $\bar{\beta}$ values, and works its way back from the corresponding low energy values through the entire energy range. Occasionally this has led to “hang–up” situations, for which a simple “retreat” strategy has turned out to be sufficient. For the case of generalized Ising model, the appendix gives and explains an actual program listing, which was used for the numerical illustrations of the next section. A generalization of my recursion to non–flat distributions, like for instance those proposed in [7] would be straightforward.

5 Numerical Tests

I confine myself to reporting results for the 3d IF and the 3d EAI spin glass. Similar tests have been performed for the 2d IF and are in progress for the 2d EAI spin glass as well as for fully frustrated Ising models [29]. To keep the relation to the program listing in the appendix close, I shall use

$$I_A = \frac{1}{4} (-E + dN), \quad \text{(with } N = L^d)$$

(23)

instead of the energy, defined by (2). The rationale of $I_A$ is its range:

$$I_A = 0, 1, 2, ..., dN/2$$

(24)

in typical increments of 1. For comparison, we had $-dN \leq E \leq dN$ in typical increments of 4. Consequently, for the purposes of programing $I_A$ is far more convenient. Functions of $E$ are now interpreted as functions of $I_A$ in the obvious way, i.e. $\beta(E) = \beta[E(I_A)] \to \beta(I_A)$, and so on.
5.1 Three dimensional Ising ferromagnet

The first few terms of the low temperature expansion on a finite (but sufficiently large) lattice collected in table 1. The present computer program is unsuitable to cope with \( n(I_A) = 0 \) for \( I_A = (3N/2) - 1, (3N/2) - 2 \) and \( (3N/2) - 4 \). I just bypass\(^{28}\) the problem by restricting the updating to the range \( I_A \leq N_{\text{max}} = (3N/2) - 5 \). Proposals with \( I_A > N_{\text{max}} \) are simply rejected.

We want to calculate multicanonical parameters for the temperature range infinity down to zero. Simulations with \( \beta \equiv 0 \) are peaked around \( I_A = N_{\text{min}} = 3N/4 \). We therefore fix the function \( \beta \) to \( \beta(I_A) = 0 \) for \( I_A \leq N_{\text{min}} \), and never change it there. For \( I_A > N_{\text{min}} \) we perform the multicanonical recursion of section 4. The covered range of lattices was \( 4 \leq L \leq 16 \). In a first set of runs the recursion was applied until the system tunneled at least 60 times. The (expected) experience from these runs is that the recursion remained stable after the first tunneling. The tunneling time \( \tau_{\text{tun}} \) is then measured after the first tunneling has occurred, while continuing to update the parameters. Table 2 collects the measured tunneling times \( \tau \), and states on how many tunneling events \( n_\tau \) the estimates actually rely.

By \( \tau_0 \) I denote the time (as always in updates) it takes until the first tunneling has taken place. This is essentially the time our recursion needs to provide a reliable estimate of the multicanonical parameters, and it will therefore be called recursion time in the following. Two estimates, \( \tau_{0}^a \) and \( \tau_{0}^b \), are given in table 2. They differ by the number of sweeps performed before the multicanonical parameters are updated (\( i.e. \) the subroutine \texttt{UPMUCA} of the appendix is called). A sweep is defined by updating \( N = L^d \) spins. For \( \tau_{0}^a \) \texttt{UPMUCA} was called every 120 sweeps, whereas for \( \tau_{0}^b \) it was called every \( N \) sweeps. Respectively, this amounts to letting the numbers of intermediate updates grow in proportion to the volume and to the volume squared. Within the (still large) statistical errors there is no difference noticeable.

The values \( n_{\tau_0} \) and \( n_{\tau_0}^b \) are the numbers of \( \beta(I_A) \equiv 0 \) re–starts on which the respective estimates rely. As the average CPU time needed per recursion is substantially higher than...
the average tunneling time $\tau$, I have limited the $\tau_0$ analysis to $L \leq 12$. The given error bars are somewhat unreliable as the obtained distributions have long tails towards large $\tau_0$ values. A large statistics is needed to get into the region where the central limit theorem provides a good approximation. My typical number of $n_{\tau_0} = 126$ events is a bit at the low edge. Figure 1 employs a log–scale for $\tau_0$ to show the histograms for $\tau_0^b$. The distributions for the tunneling times $\tau$ themselves, are more reasonably, Poisson like, behaved.

Figure 2 shows the increase of $\tau$ and $\tau_0^b$ with volume on a log–log scale. The straight lines correspond to the fits $\tau = cV^\delta$ and $\tau_0^b = c_0V^{\delta_0}$. The results for the fit parameters are

$$\ln(c) = -0.53 \pm 0.16, \quad \delta = 2.249 \pm 0.021, \quad (Q = 0.18)$$

and

$$\ln(c_0) = -1.24 \pm 0.17, \quad \delta_0 = 2.931 \pm 0.023, \quad (Q = 0.70),$$

where $Q$ is the goodness of fit \cite{34}. It should be remembered that the lower bounds are $\delta = 2$ \cite{34} and $\delta_0 = 2.5$ (see section 3).

To demonstrate that after a few tunneling events the multicanonical parameters are indeed already useful, I have also measured a tunneling time $\tau_1$, obtained by fixing the multicanonical parameters after the first four tunneling events. Table 2 contain also the corresponding estimates $\tau_1$. Within the statistical errors, there is no difference with the estimates $\tau$.

### 5.2 Three dimensional Edwards–Anderson Ising spin glass

First I present some results from the extensive investigation \cite{17}, which are not contained in this reference. For fixed lattice size $L$ tunneling times $\tau$ are found to vary greatly for different $J_{ik}$ realizations. For each lattice size figure 3 connects the tunneling times, sorted in decreasing order. For $L = 4 − 8$ there are 512 different realizations per lattice. For $L = 12$ there are only seven realizations, depicted at $64(i−1), (i = 1, ..., 7)$. The lines are drawn to guide the eyes. Figure 4 depicts histograms for the $L = 4 − 8$ tunneling times. In both figures a logarithmic scale is used for $\tau$. The worst realizations have dramatically
larger tunneling times than *typical* ones, defined by the median value $\tau_{0.5}$. This leads to large differences between the mean value $\tau$, which determines the needed computer time, and the median value $\tau_{0.5}$. These values are collected in table 3. With increasing lattice size the discrepancy between mean and median increases dramatically (the $L = 12$ data have to be considered unreliable for this purpose). This lack of self–averaging of the spin glass with respect to the multicanonical tunneling time comes somewhat surprising, and remains to be better understood. Also collected in the table are the smallest $\tau_{0.0}$ and largest $\tau_{1.0}$ tunneling time, found on the investigated realizations.

For typical spin glass realizations, *i.e.* the realizations corresponding to the median $\tau_{0.5}$ tunneling times of table 3, I have performed the same analysis as for the 3d IF in the previous subsection. The results are collected in table 4. An interesting and unexpected result is that I find $\tau_1$ systematically smaller than $\tau$, *i.e.* further applications of the recursion relation make the tunneling worse. My tentative interpretation is that the flat distribution is not optimal. Due to statistical fluctuations, one can then imagine that immediately after one of the first few tunneling events the generated multicanonical parameters are positively correlated towards a more optimal choice. A more detailed future analysis may be desirable.

As before, the recursion times $\tau_0^a$ and $\tau_0^b$ are practically identical. However, a second unexpected result is that now the recursion times take the same order of magnitude as the tunneling times, whereas for the 3d IF the recursion times were considerably large than the tunneling times.

It has to be remarked that the $L = 12$ results are not in line with the subsequent estimates from lattices of size $L = 4, 6$ and 8. (a) The $\tau_1$ estimate is considerably higher than expected. The reason is likely that the typical realization picked is not typical. A reliable estimate of $\tau_{0.5}$ is practically impossible due to the small number of only seven $L = 12$ realizations investigated in [17]. (b) The $\tau_0^b$ value, given in brackets, is much smaller than expected. However, the number is given in brackets as it is not an estimate of said quantity. Altogether twelve attempts were made, to determine multicanonical parameters
by means of the recursion. Of those, two did not lead to a single tunneling event within the maximally allowed CPU time corresponding to approximately 11.2E08 updates. These two attempts are (cannot be) not included in the given average values. This behavior illustrates that one should perform several independent starts, when applying the recursion to difficult situations.

Using only the estimates from $L = 4, 6$ and 8, the subsequent my results are obtained from straight line fits to the equations $\tau = c V^\delta$, $\tau_1 = c_1 V^{\delta_1}$ and $\tau_0 = c_0 V^{\delta_0}$:

\[
\ln(c) = -3.04 \pm 0.29, \quad \delta = 3.24 \pm 0.06, \quad (Q = 0.40),
\]

\[
\ln(c_1) = -3.61 \pm 0.24, \quad \delta = 3.28 \pm 0.05, \quad (Q = 0.39),
\]

and

\[
\ln(c_0) = -2.23 \pm 0.24, \quad \delta = 3.09 \pm 0.04, \quad (Q = 0.78),
\]

Here, as well as in the previous section, the routine GFIT from [30] gives results perfectly compatible with the linear fit results. A figure corresponding to (27) and (28) looks similar to figure 2, but is not very instructive as all three fits lines are almost on top of one another. The exponent $\delta$ is smaller than the one reported in [17]. The reason is that it is differently defined. In [17] the tunneling time was averaged over all realization, whereas here I have picked single, typical realizations. There is evidence that for the worst realizations the tunneling time slows down exponentially with $L$. This spoils the power law fit for the average over all realizations.

6 Summary and Conclusions

For the 3d Ising ferromagnet it is clear that the FSS methods employed in [1, 9] provide reliable estimates of the multicanonical parameters more efficiently than the recursion of this paper. On the other hand, the FSS approach breaks down [2] for the important class of disordered systems. Then recursions like the one of this paper become crucial to enable
the method, and the Ising ferromagnet is still a suitable testing ground to set quantitative performance scales. These are now given, for the first time, by tables 2 and 4. Table 4 corresponds to the important case of a typical Edwards–Anderson Ising spin glass. Future investigations will have to cope with these standards. It is my hope that they will bring improvements in the constant factor, and possibly towards a $V^2$ power law behavior, which is optimal for any kind of local random walk behavior.

7 Appendix

In this appendix I describe the actually used computer implementation for the accumulative recursion of the multicanonical parameters. The relevant Fortran subroutine is listed next. It is not claimed that this subroutine is in any sense optimal. It just worked sufficiently well for the described examples.

```fortran
SUBROUTINE UPMUCA(IRPT)
C Update of multicanonical parameters.
C HAMUA(*,1): over-all sum (record keeper only).
C HAMUA(*,2): LRTRT adjusted over-all sum (record keeper only).
C HAMUA(*,3): 1. weighted sum.
C HAMUA(*,4): 2. weighted sum.
C
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT LOGICAL (L)
PARAMETER (ND=3,NL=08,NS=NL**ND,NRPT=100,NSW=NS)
PARAMETER (NNH=(ND*NS)/2,NAMIN=NNH/2,FRTRT=3.D0,EPS=1.D-8)
PARAMETER (HMIN=1.0D0*FLOAT(NS)*FLOAT(NSW))
COMMON /MEAH/ HA(0:NNH),IAMIN,IAMAX,ITMIN,ITMAX
COMMON /MUCA/ B(0:NNH),A(0:NNH),HAMU(0:NNH,4),LRTRT(NRPT)

DO IA=ITMIN,ITMAX
HAMU(IA,1)=HAMU(IA,1)+HA(IA)
HAMU(IA,2)=HAMU(IA,2)+HA(IA)
END DO

C Retreat strategy (below) implies: range up to IAMAX.GE.ITMAX.
IAMAM1=IAMAX-1
DO IA=NAMIN,IAMAM1
IAP1=IA+1
HAMIN=MIN(HA(IA),HA(IAP1))
HAMAX=MAX(HA(IA),HA(IAP1))
IF(HAMIN.GT.0.5D00) THEN
W1=HAMIN/HAMAX
HAMU(IA,3)=HAMU(IA,3)+W1*HA(IA)
END IF
END DO
```

17
HAMU(IA,4)=HAMU(IA,4)+W1*HA(IAP1)*EXP(-4.0D00*B(IAP1))
END IF

C BETA update (after retreat HAMIN.LE.0.5 possible):
HAMUMIN=MIN(HAMU(IA,3),HAMU(IA,4))
IF(HAMUMIN.GT.EPS) THEN
B(IAP1)=-0.25D00*LOG(HAMU(IA,4)/HAMU(IA,3))
ELSE
B(IAP1)=B(IA)
END IF
END DO

C

C Retreat strategy for hung-up situations:
LRTRT(IRPT)=.FALSE.
C Besides retreat, update of MUCA A-array is performed
C (range up to IAMAX.GE.ITMAX is needed for this reason).
DO IA=NAMIN,IAMAM1
IAP1=IA+1
IF(HAMU(IAP1,2).GT.HMIN.AND.HAMU(IAP1,2).GT.FRTRT*HAMU(IA,2)) THEN
C The program may need modifications, if there are
C energy values without states in the .LE.IAMAX range.
IF(HAMU(IA,2).EQ.0) PRINT*,'UPMUCA Warning: IA = ',IA
IF(.NOT.LRTRT(IRPT)) PRINT*,
& 'RETREAT! IRPT,IA,HAMUs:',IRPT,IA,HAMU(IAP1,2),HAMU(IA,2)
LRTRT(IRPT)=.TRUE.
END IF
IF(LRTRT(IRPT)) THEN
HAMU(IAP1,2)=HAMU(IAP1,2)/FRTRT
B(IAP1)=0.0D00
HAMU(IAP1,3)=HAMU(IAP1,3)/FRTRT
HAMU(IAP1,4)=HAMU(IAP1,4)/FRTRT
END IF
A(IAP1)=A(IA)-4.0D00*(B(IAP1)-B(IA))*FLOAT(IA)
END DO
C
IAMAP1=IAMAX+1
DO IA=IAMAP1,NNH
B(IA)=B(IA-1)
A(IA)=A(IA-1)
END DO
C
RETURN
END

Relevant parameters (to be set) are the dimension ND, and lattice size NL. The presented choice is an $8^3$ lattice. NS encodes the lattice size and NNH is needed to dimension a number of arrays.

The argument IRPT keeps track of the number of repeated calls to UPMUCA. In an outside DO–loop IRPT runs from 1 to NRPT. Inside our subroutine NRPT is only needed to dimension
the **LOGICAL** array **LRTRT**, which keeps track of the number of “retreats”, to be discussed later. A parameter not needed at all in our subroutine is **NSW**. It denotes the number of update sweeps performed in between the calls to **UPMUCA**. In the presented code it is set equal to the lattice size, corresponding the recursion time \( \tau_b^0 \) of section 5.

**NAMIN** sets the lower bound on the IA range \((I_A \text{ of section } 5)\) to which the recursion is applied: \( B(I_A) = 0 \) for \( I_A \leq \text{NMIN} \) implements \( \beta(I_A) = 0 \) for \( I_A \leq N_{\text{min}} \). The other parameters will be discussed later on.

Most arguments are passed through **COMMON** blocks. On entry the array **HA** contains the newly assembled statistics, *i.e.* the histogram of the number of times a certain IA value (corresponding to an energy via (23)) has been visited during the last **NSW** sweeps. (The information is collected after each single spin update. The array **HA** has to be set to **HA** \( \equiv 0 \) after each call to **UPMUCA**.) Further arguments passed by the **COMMON** block **MEAH** (measurements) are: **IAMIN**, the smallest IA value encountered so far (not used in **UPMUCA**); **IAMAX**, the largest IA value encountered so far; **ITMIN**, the smallest IA value encountered during the last **NSW** sweeps, and **ITMAX**, the largest IA value encountered during the last **NSW** sweeps.

The meaning of the array(s) **HAMU** is explained by the comments at the beginning of the subroutine. Central for the code are the lines

\[
W_1 = \frac{\text{HMIN}}{\text{HAMAX}} \\
\text{HAMU}(I_A, 3) = \text{HAMU}(I_A, 3) + W_1 \times \text{HA}(I_A) \\
\text{HAMU}(I_A, 4) = \text{HAMU}(I_A, 4) + W_1 \times \text{HA}(I_A) \times \exp(-4.0D00 \times B(I_A))
\]

which implement our equations (19) and (20) recursively. Next, the arrays **A** and **B** correspond to the multicanonical functions \( \beta \) and \( \alpha \) the lines

\[
B(I_A) = -0.25D00 \times \log(\text{HAMU}(I_A, 4)/\text{HAMU}(I_A, 3))
\]

and

\[
A(I_A) = A(I_A) - 4.0D00 \times (B(I_A) - B(I_A)) \times \text{FLOAT}(I_A)
\]

implement equations (21) and (11). Of course, \( A(\text{NMIN}) = 0 \). The parameter **EPS** prevents that the \( \beta \)-recursion takes place without sufficient statistics, and otherwise equation
(22) is chosen.

Some complications arise, mainly because a “retreat” strategy has been implemented to get out of certain “hung-up” situations. To discuss them is beyond the scope of this paper, as the relevant (spin glass) configurations require more detailed investigations first. In short, an extreme difference between $\text{HAMU}(\text{IA}+1,2)$ and $\text{HAMU}(\text{IA},2)$ can turn out to be artificial, such that its statistics is better not trusted. “Extreme” is defined by the parameter $\text{FRTRT}$, put to 3 in the presented code. When the thus defined limit is exceeded the assembled statistics is reduced in weight by the factor $1/\text{FRTRT}$ and $\beta(I_A)$ is put in the corresponding energy region to $\beta(I_A) = 0$ for the next recursion. The program may thus escape certain traps successfully. However, I like to remark that one has to chose $\text{FRTRT}$ to be very large (around 200), if one likes to calculate multicanonical parameters for an $24^3$ IF in the range described in section 5.1. The reason is the peculiar IF density of states anomaly from $I_A = (3N/2) - 7$ to $I_A = (3N/2) - 6$ (see table 1). The choice $\beta \equiv 0$ re-creates an $\text{FRTRT}$ factor of order $N$.

**Acknowledgements:** I would like to thank Wolfhard Janke and Claus Vohwinkel for useful discussions. The manuscript was partly written at the Institut für Physik, Johannes Gutenberg Universität, Mainz. The author likes to thank Kurt Binder and his group for their hospitality.

**References**

[1] B. Berg and T. Neuhaus, Phys. Lett. B 267, 249 (1991); Phys. Rev. Lett. 68, 9 (1992).

[2] B. Berg and T. Celik, Phys. Rev. Lett. 69, 2292 (1992); Int. J. Mod. Phys. C 3, 1251 (1992).

[3] A.P. Lyubartsev, A.A. Martsinowski, S.V. Shevkunov, and P.N. Vorontsov–Velyaminow, J. Chem. Phys. 96, 1176 (1992).
[4] E. Marinari and G. Parisi, Europhys. Lett. 19, 451 (1992).

[5] B. Berg, Int. J. Mod. Phys. C 3, 311 (1992).

[6] A. Hüller, Z. Phys. B 88, 79 (1992).

[7] B. Hesselbo and R. Stinchcombe, Phys. Rev. Lett. 74, 2151 (1995).

[8] C. Borgs and S. Kappler, Phys. Lett. A 171, 2011 (1992).

[9] B. Berg, U. Hansmann, and T. Neuhaus, Z. Phys. B 90, 229 (1993).

[10] B. Grossmann and M.L. Laursen, Nucl. Phys. B 408, 637 (1993).

[11] K. Rummukainen, Nucl. Phys. B 390, 621 (1993).

[12] A. Billoire, T. Neuhaus, and B. Berg, Nucl. Phys. B 396, 779 (1993); 413, 795 (1994).

[13] J. Lee, Phys. Rev. Lett. 71, 211 (1993); Erratum 71, 2353 (1993).

[14] B. Berg, (unpublished); B. Berg, U. Hansmann, and Y. Okamoto, J. Phys. Chem. 99 (1995) 2236-2237.

[15] U. Hansmann and Y. Okamoto, J. Comput. Chem. 14, 1333 (1993).

[16] M.-H. Hao and H.A. Scheraga, J. Phys. Chem. 98, 4940 (1994).

[17] B. Berg, U. Hansmann, and T. Celik, Phys. Rev. B 50, 16444 (1994).

[18] W. Kerler and P. Rehberg, Phys Rev. E 50, 4220 (1994).

[19] W. Janke and S. Kappler, Phys. Rev. Lett. 74, 212 (1995).

[20] W. Janke, Recent Developments ins Monte–Carlo Simulations of First-Order Phase Transitions, in Computer Simulations Studies in Condensed Matter Physics VII, D.P. Landau, K.K Mon and H.-B. Schüttler (Eds), Proceedings in Physics 78, Springer, 1994, pp. 29–44.
[21] B. Berg, Nature **361**, 708 (1993).

[22] G.M. Torrie and J.P. Valleau, J. Comp. Phys. **23**, 187 (1977).

[23] Note that the recursions given in [2] and [13] are algebraically identical [14] in their central parts. Details, like the energy range to which the recursion is applied, and the prescription given for values outside this range, may vary. They are discussed in section 3 of this paper.

[24] H.T. Diep, P. Lallemand, and O. Nagai, J. Phys. C **18**, 1067 (1985).

[25] Kerson Huang, *Statistical Mechanics*, John Wiley & Sons, 1987, p.134.

[26] M. Mézard, G. Parisi, and M.A. Virasoro, *Spin Glasses and Beyond*, World Scientific, 1987.

[27] B. Baumann, Nucl. Phys. B **285**, 391 (1987).

[28] It is straightforward, but tedious, to modify the subroutine `UPMUCA` of the appendix, such that it can cope with \( n(I_A) = 0 \) for (isolated) \( I_A \) values.

[29] B. Berg and S. Weaver, work in progress.

[30] W.H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling, *Numerical Recipes*, (Cambridge University Press, 1988).

**Tables**
\[
E = I_A - 3N - 3N/2 - 3N + 4 (3N/2) - 1 - 3N + 8 (3N/2) - 2 - 3N + 12 (3N/2) - 3 - 3N + 16 (3N/2) - 4 - 3N + 20 (3N/2) - 5 - 3N + 24 (3N/2) - 6 - 3N + 28 (3N/2) - 7 - 3N + 32 (3N/2) - 8 - 3N + 36 (3N/2) - 9
\]

Table 1: Finite lattice low temperature expansion for the 3d IF \((N = L^3)\).

| \(L\) | \(n_\tau\) | \(\tau\) | \(\tau_{a0}\) | \(\tau_{b0}\) | \(\tau_{a0}^0\) | \(\tau_{b0}^0\) | \(n_{\tau_1}\) | \(\tau_1\) |
|------|-------------|-----------|-------------|-------------|-------------|-------------|-------------|-------------|
| 4    | 548         | 719 (19)  | E01         | 126         | 661 (41) E02| 126         | 557 (46)  E02| 111         | 731 (58)  E01|
| 6    | 354         | 126 (05)  | E03         | 252         | 195 (20) E04| 126         | 219 (23)  E04| 145         | 129 (10)  E03|
| 8    | 559         | 881 (23)  | E03         | 126         | 311 (55) E05| 126         | 253 (50)  E05| 125         | 839 (69)  E03|
| 12   | 322         | 118 (06)  | E05         | 140         | 95 (32) E07 | 164         | 90 (15)   E07 | 141         | 127 (11)  E04|
| 16   | 577         | 760 (30)  | E05         | 180         | 2       | 14 (big)   | E09         | 180         | 746 (54)  E05|

Table 2: Tunneling and recursion times for the 3d IF.

| \(L\) | \(\tau\) | \(\tau_{0.0}\) | \(\tau_{0.5}\) | \(\tau_{1.0}\) |
|------|--------|---------------|---------------|---------------|
| 4    | 398 (15) | 144 E02       | 304 E02       | 411 E03       |
| 6    | 336 (30) | 436 E03       | 131 E04       | 670 E05       |
| 8    | 171 (46) | 505 E04       | 282 E05       | 213 E08       |
| 12   | 139 (77) | 408 E06       | 481 E07       | 544 E08       |

Table 3: Mean \(\tau\) and some q-tiles \(\tau_q\) for the 3d EAI tunneling time.

| \(L\) | \(n_\tau\) | \(\tau\) | \(\tau_{a0}\) | \(\tau_{b0}\) | \(\tau_{a0}^0\) | \(\tau_{b0}^0\) | \(n_{\tau_1}\) | \(\tau_1\) |
|------|-------------|-----------|-------------|-------------|-------------|-------------|-------------|-------------|
| 4    | 185         | 332 (25)  | E02         | 126         | 523 (19) E02| 126         | 409 (22)  E02| 270         | 228 (14)  E02|
| 6    | 256         | 181 (12)  | E04         | 126         | 150 (10) E04| 126         | 172 (11)  E04| 357         | 131 (08)  E04|
| 8    | 134         | 272 (26)  | E05         | 252         | 245 (13) E05| 252         | 253 (16)  E05| 207         | 203 (16)  E05|
| 12   | 10          | 19 (4) E06 | 13          | 92 (31) E08 |             |             |             |             |

Table 4: Tunneling and recursion times for typical 3d EAI spin glass realizations.
Figure 1: Histograms for the 3d IF recursion time $\tau_0^b$ on lattices of size $L^3$. 
This figure "fig1-1.png" is available in "png" format from:

http://arxiv.org/ps/hep-lat/9503019v2
Figure 2: Estimates for recursion time $\overline{\tau}_0$ and tunneling time $\overline{\tau}$ for the 3d IF.
This figure "fig1-2.png" is available in "png" format from:

http://arxiv.org/ps/hep-lat/9503019v2
Figure 3: Sorted 3d EAI tunneling times for various lattices of size $L^3$. 
This figure "fig1-3.png" is available in "png" format from:

http://arxiv.org/ps/hep-lat/9503019v2
Tunneling Time Estimates: Histograms over Realizations.

Figure 4: Histograms over realizations for 3d EAI tunneling time estimates $\tau$ on lattices of size $L^3$. 
This figure "fig1-4.png" is available in "png" format from:

http://arxiv.org/ps/hep-lat/9503019v2