Analytical study of tunneling times in flat histogram Monte Carlo

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Abstract. – We present a model for the dynamics in energy space of multicanonical simulation methods that lends itself to a rather complete analytic characterization. The dynamics is completely determined by the density of states. In the $\pm J$ 2D spin glass the transitions between the ground state level and the first excited one control the long time dynamics. We are able to calculate the distribution of tunneling times and relate it to the equilibration time of a starting probability distribution. In this model, and possibly in any model in which entering and exiting regions with low density of states are the slowest processes in the simulations, tunneling time can be much larger (by a factor of $O(N)$) than the equilibration time of the probability distribution. We find that these features also hold for the energy projection of single spin flip dynamics.

The simulation of models with complicated energy landscapes, such as spin glasses or models of protein folding, has always proved impractical for conventional canonical Monte Carlo methods [1].

In a Monte Carlo simulation of a system of $N$ degrees of freedom, at fixed temperature $T$, energy fluctuations about a mean energy $E(T)$ are of order $k_B T \sqrt{Nc_v}$. As a result, only states in a range of energies $\langle E \rangle - \delta E < E < \langle E \rangle + \delta E$ with $\delta E \sim k_B T \sqrt{Nc_v}$ are accessible in the simulation. In systems with complex energy landscapes, phase space in this narrow energy range breaks up into many regions, connected only by states requiring energy fluctuations $\Delta E \gg \delta E$; tunneling times between these regions become too long to retain any hope of achieving the asymptotic distribution in a reasonable simulation time.

To overcome this problem, one would like to broaden the energy range of the states sampled in a simulation, forsaking the canonical ensemble at a fixed temperature. A variety of methods have been proposed to implement this idea, such as entropic sampling [2], multicanonical Monte Carlo [3, 4], simulated and parallel tempering [5–7], Wang-Landau sampling [8–10], broad histogram and transition matrix methods [11–14]. In some cases, like multicanonical Monte Carlo and Wang-Landau sampling, the aim is to sample all energy levels of the spectrum with equal probability, producing

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flat histograms in energy space. While this allows overcoming large energy barriers in systems with rugged energy landscapes, critical slowing down can remain a problem [14, 15].

Given the practical impossibility of measuring equilibration time of an initial distribution, the performance of these methods is generally assessed by measuring the so called tunneling time [15–17], the time required to cross the entire energy spectrum, from ground states, to states with the energy of maximum density of states, and back, or from ground state to anti-ground states, states of maximum energy.

In this letter we focus on the dynamics of this random walk in energy space. We propose a modification of the directed network of non-zero transition probabilities which underlies the Markov chain of a Monte Carlo simulation, which, while retaining the long time behaviour of the energy projection of conventional simulations, lends itself to a very complete analytic description. Our three most important results concern the $\pm J$ 2D spin glass: (a) the transitions between ground state level and first excited one completely control the long time dynamics of simulations in this model; (b) the equilibration time of a simulation can be considerably shorter than tunneling time; (c) these conclusions also hold for the case of conventional single spin flip (SSF) dynamics.

To calculate thermodynamic averages in any system, we need only specify the set of points of phase space and the corresponding probabilities. To solve this problem using Monte Carlo, we impose on this structure a directed network of non-zero transition rates which defines the Markov chain used to generate the asymptotic distribution. The traditional SSF connects each point of phase space to $N$ first neighbours. The SSF algorithm is, usually, local in energy, i.e., energy differences between connected phase space points being of $O(1)$, independent of system size. It has been claimed that differences in the scaling behaviour of the $\pm J$ 2D spin glass model and a fully frustrated model, both with extensive ground-state entropy, reside in the restrictions imposed by the network defined by SSF dynamics. Still, the scaling laws of relevant time scales with system size found with our dynamics [16] are also similar to those obtained with SSF dynamics [15].

The simplest choice that circumvents the problem of local minima is to construct a Markov chain that connects each point of phase space to all the remaining points that have the same or adjacent energies. In this way, we preserve the locality in energy space of the standard SSF network and avoid the need for long paths to connect states that are adjacent in energy.

The procedure in best explained in reference to a specific model like the $\pm J$ 2D Ising spin glass. The corresponding energy levels, $E_i$, and degeneracies, $N(E_i)$, can be calculated exactly using the program of Saul and Kardar [18]. Non-zero transition rates connect states with energy $E_i$ to all states with energy $E_i$ or $E_i \pm 1$. The simplest choice of transition rates is to propose the final state uniformly from the set of allowed states, and accept the proposed state with a probability which ensures that the asymptotic probability of each state equals $1/N(E)$. Whereas in a SSF simulation most transition probabilities to states of the same or nearby energy are zero, in our model they are all non zero, with values adjusted to ensure the same equilibrium distribution. This procedure is akin to an averaging of transition rates. While this could lead to significant changes in the dynamics, we nevertheless find that the most relevant features of the long time SSF dynamics in energy space still hold in our model. The advantage of the current model is that the projection of the multicanonical Markov chain in energy space remains a Markov process, allowing us the use of a set of analytic tools to study the dynamics.

We denote by $p_\alpha(t)$ the probability of being in a state $\alpha$; $N_i$ is the degeneracy of energy level $E_i$ and $M_i \equiv N_{i-1} + N_i + N_{i+1} - 1$ is the number of states accessible in a direct transition from any state of energy $E_i$ (the choice of tentative final states excludes the current state). In equilibrium, the flat energy histogram condition requires, for a state $\alpha$ of energy $E_i$,

$$p_\alpha = \frac{1}{N(E_\alpha)} \equiv \frac{1}{N_i}$$

(1)

For reasons of efficiency, we exclude the negative temperature region: for energies greater than $E_m$,......
the energy at the maximum of density of states, we replace \( N(E) \) by \( N(E_m) \) in eq. (1). The transition rate from a state \( \alpha \) to an accessible state \( \beta \), \( \omega_{\beta \alpha} \), satisfies detailed balance, with the equilibrium distribution given in eq. (1) as usual, it is written as a product of a proposal probability, which we take to be uniform among all possible final states, and an acceptance ratio, determined by the detailed balance condition:

\[
\omega_{\beta \alpha} = \frac{1}{M(E_\alpha)} \min \left( 1, \frac{M(E_\alpha)N(E_\alpha)}{M(E_\beta)N(E_\beta)} \right). \tag{2}
\]

In the master equation, the transition probabilities \( \omega_{\beta \alpha} \) do not change if we vary \( \beta \) (or \( \alpha \)) within the same energy level. This makes it possible to write the following master equation for the probability of having energy \( E_i \), \( P_i = \sum_\alpha P_\alpha \delta_{E_\alpha,E_i} \):

\[
P_i(t + 1) = \Gamma_i P_{i+1}(t) + \Gamma_i P_{i-1}(t) + (1 - \Gamma_i - \Gamma_{i-1}) P_i(t) = \sum_j \Omega_{ij} P_j(t) \tag{3}
\]

with

\[
\Gamma_i = \frac{N_i}{M_{i+1}} \min \left( 1, \frac{N_{i+1}M_{i+1}}{M_iN_i} \right). \tag{5}
\]

This equation defines the projection of the original Markov chain onto the energy variable; the random walk in energy space remains a Markov chain with transition probabilities defined by the density of states of the original spin model. This is, of course, an important simplification afforded by our choice of transition rates. With the exception of special models, like the infinite range Ising model [19], the projection of conventional dynamics in energy space is non-markovian and memory effects can have a significant impact on the dynamics [14, 15]. Nevertheless, in the model under study, we find below that important aspects of the long-term SSF dynamics are preserved.

Assume the system starts from an energy level \( r \) at time \( t = 0 \):

\[
P_i(0) = \delta_{i,r}
\]

and let \( Q_i(t) \) now refer to the probability of having energy \( E_i \) at time \( t \), given that the system has never visited energy level \( s \) (\( s > r \)). \( Q_i(t) \) satisfies the master equation in eq. (5) for \( i < s \), with the same initial condition as \( P_i(t) \), namely \( Q_i(0) = \delta_{i,r} \), and an additional condition \( Q_s(t) = 0 \) replacing eq. (3) for \( i = s \). The probability of first passage in \( s \) becomes

\[
H_{sr}(\tau) = \Gamma_{s-1}Q_{s-1}(\tau). \tag{6}
\]

The master equation can be solved using a normal mode expansion, \( Q_i(t) = \sum_\gamma a_\gamma f^\gamma_i \lambda^\gamma_i \). The dimension of the transition matrix in energy space, \( \Omega \), scales linearly with system size, not exponentially as in the case of the transition matrix of the Markov process in phase space. The diagonalization of \( \Omega \), becomes a manageable problem allowing the calculation of the eigenvalues, \( \lambda_\gamma \), the left and right eigenvectors, \( g_\gamma^l \) and \( f_\gamma^r \), and the coefficients \( a_\gamma = g_\gamma^l / \sum_\gamma g_\gamma^l f_\gamma^r \). It is also possible, of course, to diagonalize the transition matrix for the actual probability distribution \( P_i(t) \) using the same formalism, and access the decay time of the various eigenmodes of the master equation. The largest finite one (the equilibrium distribution, \( P_{eq} \), does not decay) is the equilibration time of \( P_i(t), \tau_{eq} \).

The distribution of tunneling time measured in our simulations can be written in the form

\[
H(\tau) = \sum_{\tau'=0}^{\tau} H_{0m}(\tau - \tau') H_{m0}(\tau') \tag{7}
\]
where $E_m$ is the energy level corresponding to the maximum of $N(E)$. In Fig. 1 we superpose a distribution measured in a Monte Carlo simulation with the rates given by eq. 2 with a calculated one for two spin glass samples of linear dimension $L = 6, 12$; the simulation reproduces the calculated distribution very accurately.

The distribution of tunneling time between any two energy levels decays exponentially with a time constant given by $\tau_{\text{max}} = -1 / \log(\lambda_{\text{max}})$, where $\lambda_{\text{max}} < 1$ is the largest eigenvalue of the corresponding $\Omega$ (eq. 5). For a given spin glass sample, we denote by $\tau_u$ and $\tau_d$ the longest decay time for tunneling $E_0 \rightarrow E_m$ and $E_m \rightarrow E_0$, respectively; $H(\tau)$ (eq. 4) will decay exponentially with the largest of $\tau_u$ and $\tau_d$ for the given sample. The power law decay seen in [15] appears only when we aggregate tunneling times from different realizations of the random interactions $\pm J$. If the distribution of the largest decay time, in the ensemble of spin glass samples, has a power law tail, $\rho(\tau_{\text{max}}) \sim \tau^{-\nu_{\text{max}}}$ for $\tau_{\text{max}} \rightarrow \infty$, we obtain, $H(\tau) \sim \int dx \rho(x) e^{-\tau/x} \sim \tau_0^{-\nu}$ as $t \rightarrow \infty$.

This asymptotic behaviour is directly related to features of the density of states of the $\pm J$ spin glass. The inverse transition rate from the ground state level to the first excited level is given by (eq. 5),

$$\tau_0 = \Gamma_0^{-1} = 1 + \frac{N_1 + N_2}{N_0}.$$

It was noted in [15] that $N_1/N_0$ has a Fréchet probability distribution function, in an ensemble of spin glass samples; a similar result occurs for $\tau_0$ (Fig. 2). This fact completely controls the long time dynamics of the Monte Carlo simulations.

In Fig. 3 we plot $\tau_{\text{eq}}$, the equilibration time, and $\tau_u$ and $\tau_d$, the decay time constants for tunneling from $E_0$ to $E_m$ and from $E_m$ to $E_0$, against $\tau_0$. In the samples with larger $\tau_0$, we observe the following relations:

$$\tau_{\text{eq}} \approx \tau_0$$

$$\tau_u \approx \tau_0.$$  \hspace{1cm} (8)  

Note that $\tau_d$ can be two orders of magnitude larger than $\tau_u$; tunneling from $E_m$ to $E_0$ is much slower than from $E_0$ to $E_m$. In fact, as can be seen in the inset of Fig. 3 (b), the following relation holds asymptotically:

$$\tau_d \approx N_b \tau_u.$$  \hspace{1cm} (10)
Figure 2 – Comparison between the histogram of $\tau_0$ from 10000 uniformly generated samples of $\pm J$ 2D spin glass with $L = 10$ and the maximum likelihood fit to a Frechet distribution function obtained from the original data.

where $N_b \sim O(N)$ is the number of energy levels between $E_0$ and $E_m$ (recall that in our simulation the energy histogram is limited to this energy range). These results are quite simple consequences of the existence of a bottleneck in the dynamics due to transitions between $E_0$ and $E_1$ (large $\tau_0$).

The equation for $P_0$ is (for long time we replace $P_i(t + 1) - P_i(t)$ by $dP_i/dt$)

$$\frac{dP_0(t)}{dt} = -\Gamma_0 (P_0(t) - P_1(t)).$$

(11)

We denote the tunneling time scale between $E_1$ and $E_m$ by $\tau_1$; for samples with very large $\tau_0$, we assume $\tau_0 \gg \tau_1$. For $t \gg \tau_1$, we will have for $i \neq 0$

$$P_i(t) \approx \frac{1 - P_0(t)}{N_b - 1} = \frac{N_b}{N_b - 1}P_{eq}(1 - P_0(t))$$

where $P_{eq} = 1/N_b$ is the equilibrium distribution. Replacing in eq. (11) we obtain a time constant for the decay of $P_0(t) - P_{eq}$ given by

$$\tau_{eq} = \left(\frac{\Gamma_0 N_b}{N_b - 1}\right)^{-1} \approx \Gamma_0^{-1}.$$

To calculate the distribution of tunneling time from $E_0$ to $E_m$, $H(\tau)$, we use the initial condition $P_i(t) = \delta_{i,0}$. Defining $P_i(t) = Q_i(t) + R_i(t)$, where $Q_i(t)$ is the probability of having energy $E_i$ at time $t$ given that the system has not reached $E_m$, $Q(t) = \sum_{i=0}^{N_b-1} Q_i(t)$ is the probability that the tunneling time is greater than $t$, $Q(t) = \int_t^{\infty} d\tau H(\tau)$. For $t \gg \tau_1$ we have

$$P_0(t) \approx Q_0(t) \approx R_0(t)$$

$$P_i(t) \approx R_i(t) \quad \text{for } i \neq 0$$

This expresses the fact that the system either has energy $E_0$, and has not tunneled, or has left the ground state and has almost certainly tunneled to $E_m$. Therefore

$$\frac{dQ(t)}{dt} \approx \frac{dQ_0}{dt} \approx \frac{dP_0}{dt}.$$
The decay time of \(Q(t)\) (and \(H(t)\)) is \(\tau_u \approx \tau_0\).

The asymmetry of \(\tau_d\) and \(\tau_u\) should by now be obvious. For tunneling from \(E_m\) to \(E_0\) the initial condition is \(P_i(0) = \delta_{i,m}\) and \(Q(t) = \sum_{i=1}^{N_b} Q_i(t)\). For times much larger than \(\tau_1\) we expect, now,

\[
Q_i(t) \approx \frac{Q(t)}{N_b - 1} \quad \text{for } i \neq 0
\]

Since \(dQ(t)/dt = -\Gamma_0 Q_1(t)\) (\(Q(t)\) only changes due to transitions between \(E_1\) and \(E_0\)), we obtain

\[
\frac{dQ(t)}{dt} = -\frac{\Gamma_0}{N_b - 1} Q_1(t),
\]

i.e.

\[
\tau_d = (N_b - 1) \tau_u \approx N_b \tau_u.
\]

In simple language, these results can be understood as follows. Tunneling from \(E_0\) to \(E_m\) is controlled by the process of exiting the ground state level: the system cannot have tunneled if it is still in a ground state. On the other hand, a system can only enter the ground state level if it is in energy level \(E_1\); therefore the tunneling rate from \(E_m\) to \(E_0\) has an extra factor \(P_{eq} = 1/N_b\) corresponding to the probability of having energy \(E_1\).

These results provide a very clear explanation of the correlation between tunneling time and \(N_1/N_0\) found in [15]. The controlling time scale \(\tau_0 = 1 + (N_1 + N_2)/N_0\) is clearly related to the ratio \(N_1/N_0\). This difference in time scales \(\tau_u\) and \(\tau_d\) should be present in other models; namely,
those in which the slowest processes in the simulations involve getting across steep entropy changes. The $2D \pm J$ spin glass is an extreme case of this behavior, the dynamics being controlled by the transition between the two lowest energy levels. One could ask if this result is an artifact of our simplified dynamics. In fact, we verified the same behavior with SSF dynamics. Fig. 4 shows the same type of plot as in Fig. 3 with averaged tunneling time (averages taken within a sample) in SSF dynamics: for long times the relation of eq. (10) is still verified. Notice that the equilibration time scale of a probability distribution, $\tau_{eq}$, may be much smaller than tunneling time scale, which, as usually measured, is dominated by $\tau_d$. This can lead to a very pessimistic estimate of the time required to reach equilibrium.

In summary, modelling the dynamics of a multicanonical simulation in a sort of mean-field way, by averaging transition rates to states of the same or nearby energies, we were able to define a Markov process in the energy variable, reducing the dimension of the Markov matrix to a manageable size. Nevertheless, this procedure preserves the main features of the long time dynamics of a conventional simulation. A very complete and physically transparent description of the more salient features of the dynamics of multicanonical simulations becomes possible. In particular, we clarified the relation between equilibration and tunneling time, and the difference between tunneling and $\tau_d$. This can lead to a very pessimistic estimate of the time required to reach equilibrium.

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References

[1] Newman M. E. J. and Barkema G. T., *Monte Carlo Methods in Statistical Physics* (Oxford University Press) 1999.
[2] Lee J. Y., *Phys. Rev. Lett.*, 71 (1993) 2353.
[3] Berg B. A. and Neuhaus T., *Phys. Rev. Lett.*, 68 (1992) 9.
[4] Berg B. A. and Neuhaus T., *Phys. Lett. B*, 267 (1991) 249.
[5] Marinari E. and Parisi G., *Europhys. Lett.*, 19 (1992) 451.
[6] Hukushima K. and Nemoto K., *J. Phys. Soc. Jpn.*, 65 (1996) 1604.
[7] Lyubartsev A. P., Martsinovski A. A., Shevchenko S. V. and Vorontsov-Velyaminov P. N., *J. Chem. Phys.*, 96 (1992) 1776.
[8] Wang F. G. and Landau D. P., *Phys. Rev. E*, 64 (2001) 056101.
[9] Wang F. G. and Landau D. P., *Phys. Rev. Lett.*, 86 (2001) 2050.
[10] Troyer M., Wessel S. and Alet F., *Phys. Rev. Lett.*, 90 (2003) 120201.
[11] Oliveira P. M. C., Penna T. J. P. and Herrmann H. J., *Braz. J. Phys.*, 26 (1996) 677.
[12] Wang J. S. and Swendsen R. H., *J. Stat. Phys.*, 106 (2002) 245.
[13] Wang J. S., Tay T. K. and Swendsen R. H., *Phys. Rev. Lett.*, 82 (1999) 476.
[14] Trebst S., Huse D. A. and Troyer M., *Phys. Rev. E*, 70 (2004) 046701.
[15] Dayal P., Trebst S., Wessel S., Wurtz D., Troyer M., Sabhapandit S. and Coppersmith S. N., *Phys. Rev. Lett.*, 92 (2004) 097201.
[16] Lopes J. V., Costa M. D. and Lopes dos Santos J. M. B., *in preparation*.
[17] Berg B. A. and Celik T., *Int. J. Mod. Phys. C*, 3 (1992) 1521.
[18] Saul L. and Kardar M., *Nucl. Phys.*, 432 (1994) 641.
[19] Wu Y., Koerner M., Colonna-Romano L., Trebst S., Gould H., Machta J. and Troyer M., *condmat/0412076*, (2004).