G. Fort *et al.* (2014) "Efficiency of the Wang–Landau Algorithm,"
Applied Mathematics Research eXpress, Vol. 2014, No. 2, pp. 275–311
Advance Access publication April 9, 2014
doi:10.1093/amrx/abu003

Efficiency of the Wang–Landau Algorithm: A Simple Test Case

Gersende Fort[1], Benjamin Jourdain[2], Estelle Kuhn[3], Tony Lelièvre[2], and Gabriel Stoltz[2]

[1]LTCI, CNRS & Telecom ParisTech, 46 rue Barrault, 75634 Paris Cedex 13, France, [2]Université Paris-Est, CERMICS (ENPC), INRIA, 6-8 Avenue Blaise Pascal, F-77455 Marne-la-Vallée, France, and [3]INRA Unité MIA, Domaine de Vilvert, 78352 Jouy-en-Josas Cedex, France

Correspondence to be sent to: e-mail: lelievre@cermics.enpc.fr

We analyze the efficiency of the Wang–Landau algorithm to sample a multimodal distribution on a prototypical simple test case. We show that the exit time from a metastable state is much smaller for the Wang–Landau dynamics than for the original standard Metropolis–Hastings algorithm, in some asymptotic regime. Our results are confirmed by numerical experiments on a more realistic test case.

1 Introduction

The Wang–Landau algorithm was originally proposed in the physics literature to efficiently sample the density of states of Ising-type systems [18, 19]. It belongs to the class of *free-energy biasing techniques* [2, 11], which have been introduced in computational statistical physics to efficiently sample thermodynamic ensembles and to compute free-energy differences [13]. From a computational statistical point of view, it can be seen as some adaptive importance sampling strategy combined with a Metropolis algorithm [7, 16]: the target probability distribution is updated at each iteration of the algorithm in order to have a sampling of the configuration space as uniform as possible along a given direction. There are numerous physical and biochemical works using this technique to overcome sampling problems such as the ones encountered in the

Received October 28, 2013; Revised February 5, 2014; Accepted February 17, 2014

computation of macroscopic properties around critical points and phase transitions, or for the sampling of folding mechanisms for proteins. The original paper [19] is cited more than one thousand times, according to Web of Knowledge. The success of the technique motivated its use and study in the statistics literature; see [1, 3, 6, 9, 14, 15] for instance for previous mathematical and numerical studies.

There are in fact several variations of the original Wang–Landau algorithm; see the discussion in [6]. We study here the Wang–Landau algorithm with a deterministic adaption sequence (see Section 2.2 for a precise definition of the algorithm). The aim of this article is to discuss from a mathematical viewpoint the efficiency of the Wang–Landau procedure. The real practical interest of adaptive importance sampling techniques is indeed their improved convergence properties, compared with standard sampling techniques. Although this improvement is obvious to practitioners, it is mathematically more difficult to formalize.

This paper is a companion paper to [6] where a convergence result is proven, without any efficiency analysis. Actually, to our knowledge, the previous mathematical studies on the Wang–Landau algorithm solely focused on the convergence of the algorithm, not on its efficiency. Such insight into improved convergence rates has been obtained for other adaptive importance sampling methods, in particular for Adaptive Biasing Force techniques, see [5, 8, 10, 12]. These analysis have been performed on the nonlinear Fokker–Planck equation obtained in the limit of infinitely many interacting replicas. To the best of our knowledge, there is currently no efficiency analysis of adaptive importance sampling techniques based on a *single* trajectory interacting with its own past. The aim of this work is to gain some insight on the efficiency of the Wang–Landau algorithm, which is an example of such a technique. More precisely, we show here through the analytical study of a toy model and a confirmation by numerical results in a more complicated case, that the Wang–Landau algorithm indeed allows to efficiently escape from metastable states.

The paper is organized as follows. We describe in Section 2 the algorithm that we consider. We next turn to a discussion on the efficiency of the method in Section 3. On a very simple example, we mathematically quantify the improvement on the convergence properties given by the Wang–Landau dynamics, compared with a standard Metropolis–Hastings procedure. Our results are confirmed by numerical experiments on a more realistic 2D test case presented in Section 4. The proofs of our results are gathered in Section 5. Section 6 is devoted to some refinement of the comparison between the standard Metropolis–Hastings procedure and the Wang–Landau algorithm.

2 Description of the Wang–Landau Algorithm

2.1 Notation and preliminaries

Let us consider a normalized target probability density π defined on a Polish space X, endowed with a reference measure λ defined on the Borel σ-algebra $\mathcal{X}$. As for classical Metropolis–Hastings procedure, the practical implementation of the algorithm only requires to specify π up to a multiplicative constant. In statistical physics, the set X is typically composed of all admissible configurations of the system, while π is a Gibbs measure with density $\pi(x) = Z_\beta^{-1} \exp(-\beta U(x))$, U being the potential energy function and β the inverse temperature. In condensed matter physics for instance, actual simulations are performed on systems composed of N particles in Dimension 2 or 3, living in a cubic box with periodic boundary conditions. In this case, $\mathsf{X} = (L\mathbb{T})^{2N}$ or $\mathsf{X} = (L\mathbb{T})^{3N}$, where L is the length of the sides of the box and $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ is the 1D torus.

We now consider a partition $\mathsf{X}_1, \ldots, \mathsf{X}_d$ of X in $d \geqslant 2$ elements, and define, for any $i \in \{1, \ldots, d\}$,

$$\theta_\star(i) \stackrel{\text{def}}{=} \int_{\mathsf{X}_i} \pi(x)\lambda(\mathrm{d}x). \tag{2.1}$$

In the following, X_i will be called the ith *stratum*. Each weight $\theta_\star(i)$ is assumed to be positive and gives the relative likelihood of the stratum $\mathsf{X}_i \subset \mathsf{X}$. In practice, the partitioning could be obtained by considering some smooth function $\xi : \mathsf{X} \to [a, b]$ (called a reaction coordinate in the physics literature) and defining, for $i = 1, \ldots, d-1$,

$$\mathsf{X}_i = \xi^{-1}([\alpha_{i-1}, \alpha_i)), \tag{2.2}$$

and $\mathsf{X}_d = \xi^{-1}([\alpha_{d-1}, \alpha_d])$, with $a = \alpha_0 < \alpha_1 < \cdots < \alpha_d = b$ (possibly, $a = -\infty$ and/or $b = +\infty$).

Let us emphasize here that the choice of an appropriate function ξ is a difficult but central issue. It is mostly based on intuition at the time being: practitioners identify some slowly evolving degrees of freedom responsible for the metastable behavior of the system, and build a function ξ and then a partition using these slow degrees of freedom. Here, metastability refers to the fact that trajectories generated by the reference (nonadaptive) dynamics, which is ergodic with respect to the target probability measure π (for example a Metropolis–Hastings algorithm with target π), remain trapped for a long time in some region of X, and only occasionally hop to another region, where they also remain trapped. There are ways to quantify the relevance of the choice of the reaction coordinate, see for instance the discussion in [4]. There are also ways to adaptively choose the levels $(\alpha_i)_{0 \leqslant i \leqslant d}$; see [3].

The above discussion motivates the fact that the weights $\theta_\star(i)$ typically span several orders of magnitude, some sets X_i having very large weights, and other ones being very unlikely under π. Besides, trajectories bridging two very likely states typically need to go through unlikely regions. To efficiently explore the configuration space, and sample numerous configurations in all the strata X_i, it is therefore a natural idea to resort to importance sampling strategies and to appropriately reweight each subset X_i. A possible way to do so is the following. Let Θ be the subset of (nondegenerate) probability measures on $\{1, \ldots, d\}$ given by

$$\Theta = \left\{ \theta = (\theta(1), \ldots, \theta(d)) \,\middle|\, 0 < \theta(i) < 1 \text{ for all } i \in \{1, \ldots, d\} \text{ and } \sum_{i=1}^{d} \theta(i) = 1 \right\}.$$

For any $\theta \in \Theta$, we denote by π_θ the probability density on $(\mathsf{X}, \mathcal{X})$ (endowed with the reference measure λ) defined as

$$\pi_\theta(x) = \left(\sum_{i=1}^{d} \frac{\theta_\star(i)}{\theta(i)} \right)^{-1} \sum_{i=1}^{d} \frac{\pi(x)}{\theta(i)} \, \mathbb{1}_{\mathsf{X}_i}(x). \tag{2.3}$$

This measure is such that the weight of the set X_i under π_θ is proportional to $\theta_\star(i)/\theta(i)$. In particular, all the strata X_i have the same weight under $\pi_{\theta_\star}$. Unfortunately, the vector $\theta_\star$ is unknown, and sampling under $\pi_{\theta_\star}$ is typically unfeasible.

The Wang–Landau algorithm allows precisely to overcome these difficulties: at each iteration of the algorithm, a weight vector $\theta_n = (\theta_n(1), \ldots, \theta_n(d))$ is updated based on the past behavior of the algorithm and a new point is drawn from a Markov kernel P_{θ_n} with invariant density π_{θ_n}. The update of $\{\theta_n, n \geqslant 0\}$ is chosen in such a way to penalize the already visited strata. The intuition for the convergence of this algorithm is that if $\{\theta_n, n \geqslant 0\}$ converges to θ_∞, then the draws are asymptotically distributed according to the density π_{θ_∞} and it can be checked from the updating rule (see Equation (2.4)) that necessarily $\theta_\infty = \theta_\star$.

2.2 The Wang–Landau algorithm with deterministic adaption

We now describe the algorithm we study in this article. Let $\{\gamma_n, n \geqslant 1\}$ be a $[0, 1)$-valued deterministic sequence. For any $\theta \in \Theta$, denote by P_θ a Markov transition kernel onto $(\mathsf{X}, \mathcal{X})$ with unique stationary distribution $\pi_\theta(x)\lambda(\mathrm{d}x)$; for example, P_θ is one step of a Metropolis–Hastings algorithm [7, 16] with target probability measure $\pi_\theta(x)\lambda(\mathrm{d}x)$.

Consider an initial value $X_0 \in \mathsf{X}$ and an initial set of weights $\theta_0 \in \Theta$ (typically, in absence of any prior information, $\theta_0(i) = 1/d$). Define the process $\{(X_n, \theta_n), n \geqslant 0\}$ as follows: given the current value (X_n, θ_n),

(1) draw X_{n+1} under the conditional distribution $P_{\theta_n}(X_n, \cdot)$;
(2) the weights are then updated as

$$\theta_{n+1}(i) = \theta_n(i) \frac{1 + \gamma_{n+1} \mathbb{1}_{\mathsf{X}_i}(X_{n+1})}{1 + \gamma_{n+1} \theta_n(I(X_{n+1}))} \quad \text{for all } i \in \{1, \ldots, d\}. \tag{2.4}$$

Here, $I : \mathsf{X} \to \{1, \ldots, d\}$ defined by

$$\forall x \in \mathsf{X}, \quad I(x) = i \quad \text{if and only if } x \in \mathsf{X}_i \tag{2.5}$$

associates to a point x the index $I(x)$ of the stratum where x lies.

As explained above, the idea of the updating strategy (2.4) is that the weights of the visited strata are increased, in order to penalize already visited states. Note that the update (2.4) is such that the sum of the weights remains equal to 1.

Let us recall the result of convergence proved in [6]. Three assumptions are required: on the equilibrium measure (see (A1)), on the transition kernels $\{P_\theta, \ \theta \in \Theta\}$ (see (A2)) and on the step-size sequence $\{\gamma_n, n \geqslant 1\}$ (see (A3)). It is assumed that

(A1) The probability density π with respect to the measure λ is such that $0 < \inf_{\mathsf{X}} \pi \leqslant \sup_{\mathsf{X}} \pi < \infty$. In addition, $\inf_{1 \leqslant i \leqslant d} \lambda(\mathsf{X}_i) > 0$.

Note that Assumption (A1) implies that $\inf_{1 \leqslant i \leqslant d} \theta_\star(i) > 0$, where $\theta_\star$ is given by (2.1).

(A2) For any $\theta \in \Theta$, P_θ is a Metropolis–Hastings transition kernel with invariant distribution $\pi_\theta \, d\lambda$, where π_θ is given by (2.3), and with symmetric proposal kernel $q(x, y)\lambda(dy)$ satisfying $\inf_{\mathsf{X}^2} q > 0$.

(A3) The sequence $\{\gamma_n, n \geqslant 1\}$ is a $[0, 1)$-valued deterministic sequence such that

  (a) $\{\gamma_n, n \geqslant 1\}$ is a (ultimately) nonincreasing sequence and $\lim_n \gamma_n = 0$;
  (b) $\sum_n \gamma_n = \infty$;
  (c) $\sum_n \gamma_n^2 < \infty$.

A typical choice for the step-size sequence $\{\gamma_n, \ n \geqslant 1\}$ is $\gamma_n = \gamma_\star n^{-\alpha}$, with $\frac{1}{2} < \alpha \leqslant 1$.

Under assumptions (A1)–(A3), it is shown in [6] that the algorithm converges:

$$\mathbb{P}\left(\lim_{n \to +\infty} \theta_n = \theta_\star \right) = 1.$$

More precisely, the proof is done for a slightly different update than (2.4), namely the following linearized version:

$$\begin{cases} \theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1}\theta_n(i)(1 - \theta_n(i)), \\ \theta_{n+1}(k) = \theta_n(k) - \gamma_{n+1}\theta_n(k)\theta_n(i) \qquad \text{for } k \neq i. \end{cases} \tag{2.6}$$

The update (2.6) is obtained from (2.4) in the limit of small γ_n. We believe that the arguments used in [6] can be adapted to prove the convergence for the nonlinear update (2.4). In contrast, we would like to emphasize here that the distinction between the two updating strategies (2.6) and (2.4) *does matter* when considering the flat histogram criterium for the update of the step sizes, as proved in [9].

However, this convergence result does not help to understand the success of the Wang–Landau algorithm. This algorithm is actually known to be useful in metastable situations, namely when the original Markov chain (with transition kernel P_{θ_0}) remains trapped for very long times in some regions (called the metastable states). Metastability is one of the major bottleneck of standard Markov Chain Monte Carlo techniques, since ergodic averages should be considered over very long times in order to obtain accurate results. The aim of this article is to show that in such a metastable situation, the Wang–Landau algorithm indeed is an efficient sampling procedure. Our analysis will be based on estimates of exit times from metastable states.

3 Analytical Results in a Simple Case

We present in this section results on the improved convergence properties of the Wang–Landau algorithm (when compared with nonadaptive samplers), by theoretically analyzing the first exit times out of a metastable state. Indeed, adaptive biasing techniques such as the Wang–Landau algorithm have been especially designed to be able to switch as fast as possible from a metastable state to another in order to efficiently explore the whole configuration space.

We show in this section that the Wang–Landau algorithm allows to rapidly escape from a metastable state, namely from a large probability stratum surrounded by small probability strata. More precisely, we consider a toy model composed of only three strata: two large probability strata (the metastable states) separated by a low probability stratum (the transition state). We are able to precisely quantify the time the system needs to go from the first metastable state to the second one, for adaptive and nonadaptive dynamics. We show in particular that the exit time is dramatically reduced with the Wang–Landau dynamics compared with the corresponding nonadaptive dynamics.

Using the notation of the previous section, we have only three strata and three states, and thus $\mathsf{X} = \{1, 2, 3\}$ and $\mathsf{X}_i = \{i\}$ for $i = 1, 2, 3$. Jumps are only allowed between neighboring states, namely from 1 to $\{1, 2\}$, from 2 to $\{1, 2, 3\}$ and from 3 to $\{2, 3\}$. Though being very simple, we believe that this toy model is prototypical of a metastable dynamics. We will check numerically in the next section that our conclusions on this simple test case are indeed also valid for more complicated and more realistic situations.

3.1 Definition of the dynamics

We assume that the first and third strata are visited with high probability, and that the second stratum is visited with low probability. More precisely, we set

$$\theta_\star(2) = \frac{\varepsilon}{2+\varepsilon}, \quad \theta_\star(1) = \theta_\star(3) = \frac{1}{2+\varepsilon}, \tag{3.1}$$

for a small positive parameter $\varepsilon \in (0, 1)$, and consider the limit $\varepsilon \to 0$. The target density π on X is thus defined as: $\pi(\{i\}) = \theta_\star(i)$ for $i = 1, 2, 3$ (the reference measure λ being the uniform measure on $\mathsf{X} = \{1, 2, 3\}$). The parameters $\theta_\star(i)$ depend on ε, even though we do not explicitly indicate this dependence to keep the notation simple. In this specific setting, the biased probability measure (2.3) is

$$\pi_\theta(i) = \left(\sum_{j=1}^{3} \frac{\theta_\star(j)}{\theta(j)} \right)^{-1} \frac{\theta_\star(i)}{\theta(i)} \quad \text{for } i \in \{1, 2, 3\}.$$

Note that $\pi_{\theta_\star} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ is the uniform measure on X.

The basic building block for the reference nonadaptive Markov chain $\{\bar{X}_n, n \geqslant 0\}$ is a symmetric proposal kernel allowing transitions to nearest-neighbor strata only:

$$Q = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{1}{3} & \frac{2}{3} \end{bmatrix}.$$

The corresponding nonadaptive Markov chain is built using a Metropolis–Hastings algorithm [7, 16], with Q as the proposal kernel, and π as the target distribution. To compute the kernel $\bar{P}$ of the Metropolis algorithm, we evaluate its off-diagonal terms, and adjust the diagonal in order for the rows to sum up to 1. For symmetric proposals, the Metropolis procedure consists in proposing a new configuration $\tilde{X}_{n+1}$ from the previous state $\bar{X}_n$ according to the proposal kernel Q, and then to accept this proposal with probability $1 \wedge (\pi(\tilde{X}_{n+1})/\pi(\bar{X}_n))$, in which case $\bar{X}_{n+1} = \tilde{X}_{n+1}$; otherwise, $\bar{X}_{n+1} = \bar{X}_n$.

For instance, the probability to go from 1 to 2 reads

$$\bar{P}_{12} = Q_{12}\left(1 \wedge \frac{\pi(\{2\})}{\pi(\{1\})}\right) = \frac{1}{3}\left(1 \wedge \frac{\theta_\star(2)}{\theta_\star(1)}\right). \tag{3.2}$$

Since $\varepsilon < 1$, the kernel $\bar{P}$ is given by

$$\bar{P} = \begin{bmatrix} 1 - \frac{\varepsilon}{3} & \frac{\varepsilon}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{\varepsilon}{3} & 1 - \frac{\varepsilon}{3} \end{bmatrix}. \tag{3.3}$$

The nonadaptive dynamics $\{\bar{X}_n, n \geqslant 0\}$ is metastable, in the sense that the time to go from the stratum 1 to the stratum 3

$$\bar{T}_{1\to 3} = \min\{n : \bar{X}_n = 3 \text{ starting from } \bar{X}_0 = 1\}$$

is very large, and more precisely of order $6/\varepsilon$ (see Proposition 3.1). This is due to the fact that, in order to go from 1 to 3, the chain has to visit the very low probability transition state 2. This is a prototypical metastable dynamics reminiscent of what happens along molecular dynamics trajectories: due to the very high-dimensional configuration space, only local moves are allowed (otherwise, they would be mostly rejected) and thus, it is difficult to go from a very likely region to another one since they are usually separated by low probability zones.

For the associated adaptive Wang–Landau dynamics $\{(X_n, \theta_n), n \geqslant 0\}$, the transition kernel P_{θ_n} to go from X_n to X_{n+1} is the Metropolis–Hastings kernel corresponding to the proposal kernel Q and the target distribution π_{θ_n}. The expression of P_θ is obtained with computations similar to the ones leading to the expression (3.3) of the transition kernel of the nonadaptive dynamics. In fact, it suffices to replace π by π_θ in equalities such as (3.2). More precisely,

$$P_\theta = \begin{bmatrix} 1 - \frac{1}{3}\left(\varepsilon\frac{\theta(1)}{\theta(2)} \wedge 1\right) & \frac{1}{3}\left(\varepsilon\frac{\theta(1)}{\theta(2)} \wedge 1\right) & 0 \\ \frac{1}{3}\left(\frac{1}{\varepsilon}\frac{\theta(2)}{\theta(1)} \wedge 1\right) & 1 - \frac{1}{3}\left(\frac{1}{\varepsilon}\frac{\theta(2)}{\theta(1)} \wedge 1 + \frac{1}{\varepsilon}\frac{\theta(2)}{\theta(3)} \wedge 1\right) & \frac{1}{3}\left(\frac{1}{\varepsilon}\frac{\theta(2)}{\theta(3)} \wedge 1\right) \\ 0 & \frac{1}{3}\left(\varepsilon\frac{\theta(3)}{\theta(2)} \wedge 1\right) & 1 - \frac{1}{3}\left(\varepsilon\frac{\theta(3)}{\theta(2)} \wedge 1\right) \end{bmatrix}. \tag{3.4}$$

In addition, the step-size sequence in (2.4) is

$$\gamma_n = \gamma_\star n^{-\alpha}, \tag{3.5}$$

for a positive constant $\gamma_\star$, and a parameter $\alpha \in \left[\frac{1}{2}, 1\right]$ (note that we allow here the value $\frac{1}{2}$, see Remark 3.1).

We start from initially equiprobable strata $\theta_0(1) = \theta_0(2) = \theta_0(3) = \frac{1}{3}$, so that $\pi_{\theta_0} = \pi$. Note that the nonadaptive dynamics is simply the Markov chain with transition kernel $P_{(\frac{1}{3},\frac{1}{3},\frac{1}{3})}$. It can be obtained from the adaptive dynamics by setting $\gamma_\star = 0$, in which case $\theta_n = \theta_0 = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ for all $n \geqslant 0$. As above for the nonadaptive dynamics, we define the time to go from the stratum 1 to the stratum 3 for the Wang–Landau dynamics as

$$T_{1\to 3} = \min\{n : X_n = 3 \text{ starting from } X_0 = 1\}.$$

The aim of this section is to show that, in some sense to be made precise, $\bar{T}_{1\to 3}$ is much larger than $T_{1\to 3}$ that is, the Wang–Landau dynamics is much less metastable than the corresponding nonadaptive dynamics. This is related to the fact that, when the stochastic process $\{X_n, n \geqslant 0\}$ remains stuck in the stratum 1, this stratum gets more and more penalized ($\theta_n(1)$ increases, see (2.4)), so that a transition to the stratum 2 becomes more and more favorable. From the stratum 2, a jump to the stratum 3 is then very likely. This is the bottom line of the whole adaptive procedure: penalizing the already visited strata in order to explore very quickly new regions.

3.2 Precise statement on the exit times

We now provide a precise statement on how the exit times $\bar{T}_{1\to 3}$ and $T_{1\to 3}$ scale when ε goes to zero. For the nonadaptive dynamics, it holds (see Section 5.1 for the proof):

Proposition 3.1. The time $\bar{T}_{1\to 3}$ scales like $6/\varepsilon$, in the following sense:

$$\frac{\varepsilon}{6}\mathbb{E}(\bar{T}_{1\to 3}) = 1 + \frac{\varepsilon}{2} \underset{\varepsilon\to 0}{\longrightarrow} 1, \tag{3.6}$$

$$\forall c \geqslant 0, \quad \lim_{\varepsilon\to 0} \mathbb{P}\left(\frac{\varepsilon}{6}\bar{T}_{1\to 3} > c\right) = \mathrm{e}^{-c}. \tag{3.7}$$

□

Equation (3.7) states that when $\varepsilon \to 0$, $\varepsilon \bar{T}_{1\to 3}$ converges in distribution to an exponential random variable with parameter $\frac{1}{6}$.

Let us now consider the Wang–Landau dynamics (5.5). The following result holds (see Section 5.2 for the proof).

Proposition 3.2. Let $\gamma_\star$ and α be the two constants defining the sequence γ_n, as given by (3.5). Let us assume that $\alpha \in \left[\frac{1}{2}, 1\right]$, with $\gamma_\star < 1$ if $\alpha = \frac{1}{2}$.

(1) In the case $\alpha \in [\frac{1}{2}, 1)$, the random variables $(|\ln \varepsilon|^{-1/(1-\alpha)} T_{1\to 3})_{\varepsilon>0}$ converge in probability to $\left(\frac{1-\alpha}{\gamma_\star}\right)^{1/(1-\alpha)}$ when ε goes to 0

(2) In the case $\alpha = 1$, for any function h such that $\lim_{\varepsilon\to 0} h(\varepsilon) = +\infty$,

$$\lim_{\varepsilon\to 0} \mathbb{P}\left(\frac{1}{h(\varepsilon)} < \varepsilon^{1/(1+\gamma_\star)} T_{1\to 3} < h(\varepsilon)\right) = 1. \tag{3.8}$$

□

In the case $\alpha = 1$, one should think of functions h going very slowly to infinity, so that the above result essentially means that

$$\text{as } \varepsilon \to 0, \quad T_{1\to 3} \text{ scales like } \begin{cases} \left(\dfrac{1-\alpha}{\gamma_\star}\right)^{1/(1-\alpha)} |\ln \varepsilon|^{1/(1-\alpha)} & \text{if } \alpha \in [\frac{1}{2}, 1), \\ \varepsilon^{-1/(1+\gamma_\star)} & \text{if } \alpha = 1. \end{cases} \tag{3.9}$$

In any case, the Wang–Landau algorithm is such that $T_{1\to 3}$ is much smaller than $\bar{T}_{1\to 3}$ in the limit $\varepsilon \to 0$ (namely in metastable situations).

Note that at time $T_{1\to 3}$, the Wang–Landau algorithm cannot go back immediately to state 2. It still has to get rid of part of the initial metastability: in particular, $\tilde{\theta}_{T_{1\to 3}}(2) \geqslant \tilde{\theta}_{T_{1\to 3}}(3)$ since state 2 has been visited at least once before $T_{1\to 3}$ and the sequence of step sizes is decreasing. As a consequence, the entry $(3, 2)$ of the matrix $P_{\theta_{T_{1\to 3}}}$ which gives the probability for the algorithm to go back to state 2 at time $T_{1\to 3} + 1$ is smaller than $\frac{\varepsilon}{3}$. Section 6 is dedicated to a formal analysis of the scaling in terms of ε of the successive durations between a visit by the algorithm of one of the extremal states 1 and 3 and the next visit of the other extremal state. Some hint at the total time necessary to get rid of the metastability is also given.

Remark 3.1. Two points should be mentioned about the convergence result from Proposition 3.2:

(1) The convergence in probability in the case $\alpha \in [\frac{1}{2}, 1)$ is equivalent to, for all C_a and C_b such that $0 < C_a < \left(\frac{1-\alpha}{\gamma_\star}\right)^{1/(1-\alpha)} < C_b$,

$$\lim_{\varepsilon\to 0} \mathbb{P}(T_{1\to 3} \in (C_a |\ln \varepsilon|^{1/(1-\alpha)}, C_b |\ln \varepsilon|^{1/(1-\alpha)})) = 1.$$

According to Proposition 5.1, this limiting probability is still one with a lower bound slightly larger than $C_a |\ln \varepsilon|^{1/(1-\alpha)}$.

(2) Note that we obtain results on first exit times also for $\alpha = \frac{1}{2}$, which is an excluded value to obtain the almost sure convergence of the Wang–Landau algorithm (see Assumption (A3)). □

4 Numerical Illustrations

The aim of this section is to show that (most of) the results obtained for the very simple three-state model of Section 3 are still valid for a less simple example inspired by target measures used in computational statistical physics. In these numerical experiments, we also investigate the behavior of the algorithm for values of α in the interval $(0, \frac{1}{2}]$, which are excluded values to prove the theoretical convergence of stochastic approximation procedures in general, and in particular of the Wang–Landau algorithm (see Assumption (A3)). Notice that if $\alpha \in (0, 1/2)$, the Markov process associated to the Wang-Landau algorithm escapes very quickly from metastable states and it is therefore easy to investigate numerically the behavior of the algorithm for such values of α, even for very large values of β.

Our aim is to study the behavior of the exit times out of a metastable state as the temperature in the system goes to zero. The temperature will thus play a role similar to the role of ε in Section 3 (see formula (4.2), where β is the inverse temperature).

4.1 Presentation of the model and of the dynamics

We consider the system based on the 2D potential suggested in [17]. The state space is $\mathsf{X} = [-R, R] \times \mathbb{R}$ (with $R > 0$), and we denote by $x = (x_1, x_2)$ a generic element of X. The reference measure λ is the Lebesgue measure. The density of the target measure reads

$$\pi(x) \propto \mathbb{1}_{[-R,R]}(x_1)\, \mathrm{e}^{-\beta U(x_1,x_2)},$$

for some positive inverse temperature β, with

$$\begin{aligned} U(x_1, x_2) = {} & 3\exp\left(-x_1^2 - \left(x_2 - \frac{1}{3}\right)^2\right) - 3\exp\left(-x_1^2 - \left(x_2 - \tfrac{5}{3}\right)^2\right) \\ & - 5\exp\left(-(x_1 - 1)^2 - x_2^2\right) - 5\exp\left(-(x_1 + 1)^2 - x_2^2\right) + 0.2x_1^4 + 0.2\left(x_2 - \frac{1}{3}\right)^4. \end{aligned} \tag{4.1}$$

We introduce d strata $\mathsf{X}_\ell = (a_\ell, a_{\ell+1}) \times \mathbb{R}$, with $a_\ell = -R + 2(\ell - 1)R/d$ and $\ell = 1, \ldots, d$.

A plot of the level sets of the potential U is presented in Figure 1(Left). The global minima of the potential U are located at the points $x_- = (-1, 0)$ and $x_+ = (1, 0)$. We also provide a plot of the biased potential associated with $\pi_{\theta_\star}$ (for $\beta = 20$, $R = 1.1$ and $d = 22$ strata) in Figure 1(Right).

From Laplace's method, the ratio between the weight of the stratum in the transition region around $x_1 = 0$ and the strata located near the global minima of the potential

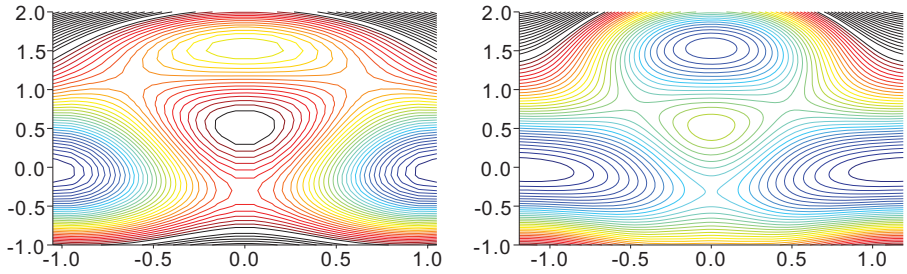

Fig. 1. Left: Level sets of the potential U defined in (4.1). The minima are located at the positions $x_\pm = (\pm 1, 0)$, and there are three saddle points, at the positions $x_\pm^{\mathrm{sd},1} \simeq (\pm 0.6, 1.15)$ and $x^{\mathrm{sd},2} \simeq (0, -0.3)$. The energy differences of these saddle points with respect to the minimal potential energy are, respectively, $\Delta U^1 = 2.2$ and $\Delta U^2 = 2.7$. Right: Level sets of the biased potential $U + \beta^{-1} \log \theta_\star \propto -\beta^{-1} \log \pi_{\theta_\star}$ for $\beta = 20$, $R = 1.1$, and $d = 55$ ($\theta_\star$ being considered as a function with constant values on the strata X_ℓ). The position of the saddle point $x^{\mathrm{sd},2}$ is unaffected, while the saddle points $x_\pm^{\mathrm{sd},1}$ are shifted to $(\pm 0.35, 0.7)$. The energy differences of the saddle points with respect to the minimal energy are now respectively $\Delta U^{1,\mathrm{biased}} \simeq 1.65$ and $\Delta U^{2,\mathrm{biased}} \simeq 1.25$.

U (i.e., around $x_\pm$) scales like $\bar{C} \exp(-\beta \mu_0)$ for some positive values $\bar{C}$ and μ_0, in the limit $\beta \to \infty$. In view of (3.1), we thus expect that the equivalent of the parameter ε of Section 3 in terms of β should be

$$\varepsilon(\beta) = \bar{C} \ \exp(-\beta \mu_0). \tag{4.2}$$

The aim of this section is to check numerically that, assuming this relation between β and ε, the scaling behaviors we obtained in the previous section on exit times for the very simple toy model with three states are indeed also observed for a Markovian dynamics with local moves on the 2D potential U. Let us now make precise the dynamics we consider.

The reference (nonadaptive) Markov chain $\bar{X}_n$ is obtained by a Metropolis algorithm, using an isotropic Gaussian proposal with variance-covariance matrix υ^2 Id, where Id is the 2×2 identity matrix. This dynamics is metastable: for local moves (υ of the order of a fraction of $\|x_+ - x_-\|$, in the following we choose υ in $\{0.025, 0.05, 0.1, 0.2\}$), it takes a lot of time to go from the left to the right, or from the right to the left (note that the potential is symmetric with respect to the y-axis). More precisely, there are two main metastable states: one located around $x_- = (-1, 0)$ and another one around $x_+ = (1, 0)$. These two states are separated by a region of low probability. The metastability of the dynamics increases with β (i.e., as the temperature decreases). The larger β is, the larger is the ratio between the weight under π of the strata located near the main

metastable states and the weight under π of the transition region around $x_1 = 0$, and the more difficult it is to leave the left metastable state to enter the one on the right (and conversely). We compare the reference (nonadaptive) Markov chain with the associated Wang–Landau dynamics X_n. In particular, the proposal kernel used in the Metropolis algorithm is the same for the Wang–Landau dynamics and for the reference dynamics. As in the previous section, the nonlinear update (2.4) is used. The step-size sequence is chosen as in (3.5). The initial weight vector θ_0 is $(1/d, \ldots, 1/d)$. Note that the reference dynamics corresponds to the case when $\gamma_\star = 0$ (no adaption).

4.2 Expected scalings in the small temperature regime

Average exit times are obtained by performing independent realizations of the following procedure: initialize the system in the state $x_- = (-1, 0)$, and run the dynamics until the first time index $\mathcal{N}$ such that $X_{\mathcal{N},1} > 1$ (i.e., the first component of $X_{\mathcal{N}}$ is larger than 1). This average exit time is denoted t_β for the Wang–Landau dynamics, and $\bar{t}_\beta$ for the reference dynamics.

Before giving the numerical results, let us state the expected scaling behaviors for $\bar{t}_\beta$ and t_β in the limit $\beta \to \infty$, in view of Propositions 3.1, 3.2, and (4.2). First, the scaling (3.6) implies that for the reference dynamics, under the relation (4.2) (in the limit $\beta \to \infty$),

$$\bar{t}_\beta \sim \frac{6}{\bar{C}} \exp(\beta \mu_0). \tag{4.3}$$

Secondly, for the Wang–Landau dynamics, (3.9) implies that, under the relation (4.2) (in the limit $\beta \to \infty$): for $\alpha \in [\frac{1}{2}, 1)$ (and we will even consider $\alpha \in (0, 1)$ below),

$$t_\beta \sim \left(\frac{(1-\alpha)\mu_0}{\gamma_\star} \beta \right)^{1/(1-\alpha)}, \tag{4.4}$$

while, for $\alpha = 1$,

$$t_\beta \sim C_{\gamma_\star} \exp\left(\beta \frac{\mu_0}{1+\gamma_\star} \right). \tag{4.5}$$

In practice, the range of values of β required to observe the asymptotic regime $\beta \to \infty$ depends on the values of α and $\gamma_\star$ (see Figure 3).

4.3 Choice of the numerical parameters

For a given value of the inverse temperature β, the computed average exit times t_β and $\bar{t}_\beta$ are obtained by averaging over M independent realizations of the process started at x_-. We use the Mersenne-Twister random number generator as implemented in the GSL

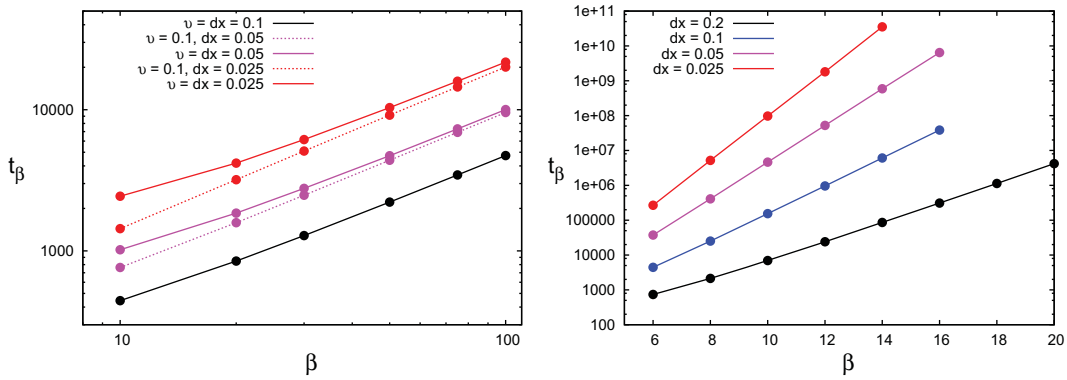

Fig. 2. Left: In the case $\alpha = 0.125$ and $\gamma_\star = 1$ in the step-size sequence (3.5), the scaling of the average exit times is independent of the number of bins, even if υ is of the order of several Δx. Right: In the case $\alpha = 1$ and $\gamma_\star = 8$, the exponential rate a for the scaling $t_\beta \sim C \exp(a\beta)$ depends on Δx (see Table 1).

library. We choose M such that the relative error on t_β or $\bar{t}_\beta$ is less than a few percents in the worst cases. For computational reasons, M is of the order of a few hundreds for the largest exit times, while $M = 10^5$ in the easiest cases.

The choice of the number of bins is a more delicate matter. We consider in the sequel $R = 1.1$ since we want to observe transitions from x_- to x_+, and decompose the interval $[-R, R]$ into d strata of width $2R/d = \Delta x$. In order to sufficiently refine the variations of the potential and to produce a not-too-coarse free-energy profile, we consider bin widths Δx smaller than 0.2. In order to preserve the locality of the moves, the magnitude of the random displacements (which are of order υ) is chosen in order to be comparable with the width Δx of one stratum. Therefore, from one stratum, the neighboring ones are the most likely to be visited. This is reminiscent of the dynamics used on the toy model in the previous section.

Results on the dependence of the average first exit times t_β as a function of Δx are presented in Figure 2. The conclusions which can be drawn from these results are the following:

(i) when $\alpha = 0.125$ and $\gamma_\star = 1$ (as already hinted at in the beginning of Section 4, the interest of this case, which is not covered by the theoretical analysis of Section 3, is that the Wang–Landau algorithm quickly escapes from metastable states and it is easier to investigate numerically very large values of β), the average exit time scales in all cases as $t_\beta \sim C\beta^{1/(1-\alpha)}$, as predicted by (4.4), and only the prefactor depends on the number of bins d. A more

Table 1 Fitted value of a as a function of the bin width $\Delta x = 2R/d$ for the expected scaling relation $t_\beta \sim C \exp(a\beta)$ corresponding to the data presented in Figure 2(Right), when $\alpha = 1$ and $\gamma_\star = 8$

Δx	a
0.025	1.47
0.05	1.21
0.1	0.92
0.2	0.63

precise look at the results shows that the prefactor C is proportional to d. Note also that the average exit time increases when υ decreases, although this increase is moderate;

(ii) when $\alpha = 1$ and $\gamma_\star = 8$, the asymptotic behavior depends more dramatically on the number of bins. For all our choices of Δx, the average exit time scales as $t_\beta \sim C \exp(a\beta)$, as suggested by (4.5), but the value a depends on Δx. More precisely, the rate a decreases as Δx is increased (see the precise results in Table 1).

We expect the same conclusions to hold for other values of α and γ_*, the important distinction being whether $\alpha < 1$ or $\alpha = 1$.

In the sequel (except in Section 6.2), we choose $R = 1.1$ and $d = 22$ in order to have a sufficiently refined free-energy profile. Consistently with the above discussion, we set $\upsilon = 0.1$.

4.4 Numerical results

Let us first check that we indeed recover the correct scaling behavior (4.3) on the average exit times for the reference (nonadaptive) dynamics. In Figure 3.1, we plot, as a function of β, the average exit time $\bar{t}_\beta$ for the nonadaptive dynamics, using a logarithmic scale on the y-axis. The affine fit is very good, and yields an approximate value for the slope: $\mu_0 \simeq 2.32$. This value is of the order of the saddle point energy difference ΔU^1 (see the caption of Figure 1).

We then plot t_β as a function of β in the case $\alpha = 1$ and $\gamma_\star = 2$ in Figure 3.2, still using a logarithmic scale on the y-axis. As expected from (4.5), we indeed observe some exponential asymptotic behavior $t_\beta \sim C_{\gamma_\star} \exp(\beta \mu_{\gamma_\star})$. This is true for other values of $\gamma_\star$. We report the corresponding slopes $\mu_{\gamma_\star}$ for various values of $\gamma_\star$ in Table 2. Although the exponential dependence of t_β on β consistent with (4.5) is reproduced, the exact

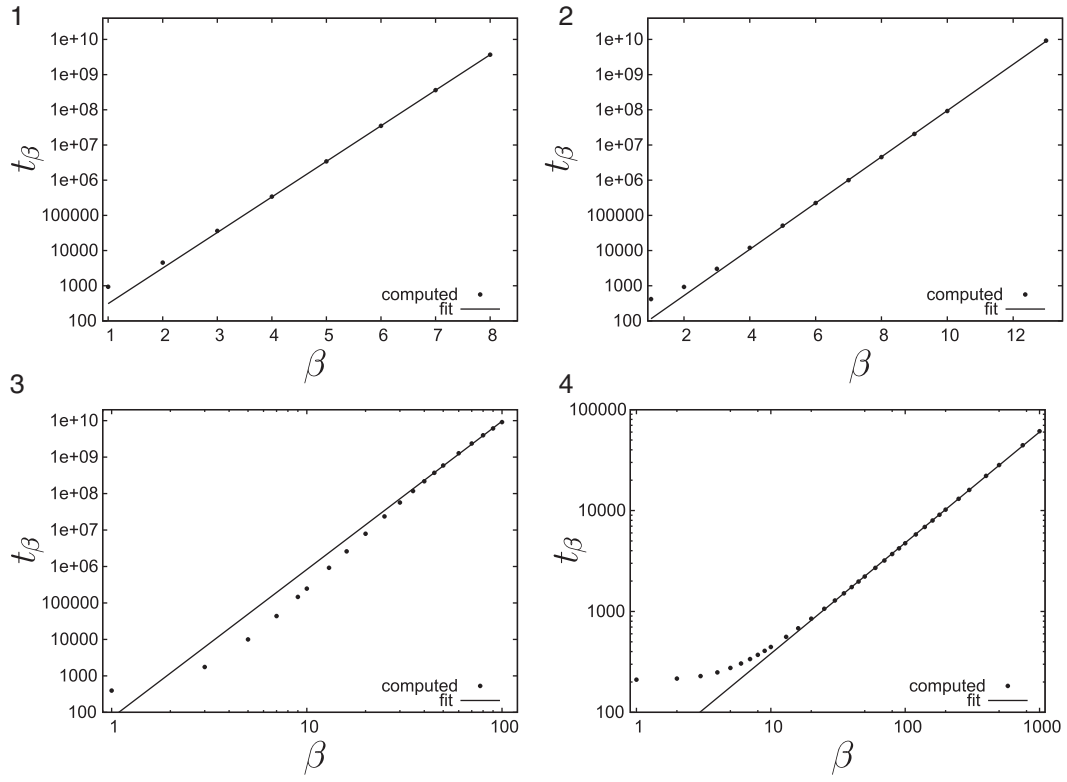

Fig. 3. Average exit time as a function of β for various step-size sequences (3.5). (1) Reference dynamics (logarithmic scale on the y-axis). (2) $\alpha = 1$ and $\gamma_* = 2$ (logarithmic scale on the y-axis). (3) $\alpha = 0.75$ (logarithmic scale on the x and y-axis). (4) $\alpha = 0.125$ (logarithmic scale on the x and y-axis).

dependence on $\gamma_\star$ of the constant in the exponential predicted by the analytical example is not exactly observed here since $\mu_{\gamma_\star} \neq \mu_0/(1+\gamma_\star)$. In fact, $\mu_{\gamma_\star}$ is systematically larger than $\mu_0/(1+\gamma_\star)$. This was expected in view of the results presented in Section 4.3 (since the exponential rate increases as Δx decreases).

We now turn to the case $\alpha \in (0,1)$ where we expect $t_\beta \sim C_\alpha \beta^{1/(1-\alpha)}$; see (4.4). Note that we also consider the case $\alpha \in (0, \frac{1}{2})$ which was not covered by the theoretical analysis of Section 3. To confirm the expected behavior, we plot t_β as a function of β in a log–log scale; see Figure 3.3 and 3.4 for the cases $\alpha = 0.75$ and $\alpha = 0.125$, respectively. We observe in all cases a dependence $t_\beta \sim C_\alpha \beta^{\mu_\alpha}$, the value of the exponent μ_α being the slope of the affine fit in the log–log diagram. The estimated exponents are gathered in Table 3 for various values of α when $\gamma_\star = 1$. They compare very well with the value

Table 2 Update with step sizes $\gamma_n = \gamma_\star/n$ ($\alpha = 1$, $d = 22$ or equivalently, $\Delta x = 0.1$). Exponents of the law $t_\beta \sim C_{\gamma_\star} \exp(\mu_{\gamma_\star}\beta)$ for various values of $\gamma_\star$

$\gamma_\star$	$\mu_{\gamma_\star}$	$\mu_0/(1+\gamma_\star)$
0	2.32	2.32
1	1.74	1.16
2	1.51	0.77
4	1.25	0.46
8	0.92	0.26

Table 3 Update with step sizes $\gamma_n = n^{-\alpha}$. Exponents of the scaling law $t_\beta \sim C_\alpha \beta^{\mu_\alpha}$ for $\alpha \in (0,1)$

α	μ_α	$1/(1-\alpha)$
0.125	1.11	1.14
0.25	1.30	1.33
0.375	1.55	1.60
0.5	2.02	2.00
0.625	2.72	2.67
0.75	4.06	4.00

$1/(1-\alpha)$ predicted from (4.4). On the other hand, we were not able to obtain a meaningful dependence of the prefactor C_α on the parameter α. This is related to the dependence of the prefactor on the number of bins (see Section 4.3).

In conclusion, these numerical experiments are in very good agreement with our theoretical findings of Section 3.

5 Proof of the Results Presented in Section 3

In the following, we denote by $\lfloor x \rfloor$ the integer part of $x \in \mathbb{R}$, namely the integer such that $\lfloor x \rfloor \leqslant x < \lfloor x \rfloor + 1$. We will also use the notation $\lceil x \rceil$ for the integer such that $\lceil x \rceil - 1 < x \leqslant \lceil x \rceil$. For $i \neq j \in \{1,2,3\}$, the time to go from i to j for the nonadaptive dynamics is denoted

$$\bar{T}_{i\to j} = \min\{n : \bar{X}_n = j \text{ starting from } \bar{X}_0 = i\}. \tag{5.1}$$

A similar definition holds for the time $T_{i\to j}$ to go from i to j for the Wang–Landau dynamics.

5.1 **Proof of Proposition 3.1**

Using the Markov property and decomposing a trajectory from state 1 to state 3 as successive attempts from 1 to 2 back to 1, and eventually a successful transition from 1 to 2 up to 3, it is easy to check that

$$\bar{T}_{1\to 3} = \sum_{n=1}^{N} \left(\bar{T}^n_{1\to 2} + \bar{T}^n_{2\to\{1,3\}}\right), \tag{5.2}$$

where

$$N \sim \mathcal{G}eo\left(\frac{1}{2}\right), \quad \bar{T}^n_{1\to 2} \sim \mathcal{G}eo\left(\frac{\varepsilon}{3}\right), \quad \bar{T}^n_{2\to\{1,3\}} \sim \mathcal{G}eo\left(\frac{2}{3}\right)$$

are independent geometric random variables. The random variable N is the number of jumps from 1 to 2 before 3 is eventually visited. The random variables $\bar{T}^n_{1\to 2}$ (respectively, $\bar{T}^n_{2\to\{1,3\}}$) are the nth sojourn time in state 1 (respectively, state 2). Notice that we have used here the fact that starting from state 2, the probability to go to state 1 is equal to the probability to go to state 3, which implies that the parameter of the geometric random variable N is $\frac{1}{2}$.

Let us show that (3.6) and (3.7) are easily obtained from (5.2). Indeed, using the fact that for independent geometric random variables $A \sim \mathcal{G}eo(a)$ and $B_k \sim \mathcal{G}eo(b)$ (the random variables B_k being i.i.d.),

$$\sum_{k=1}^{A} B_k \sim \mathcal{G}eo(ab),$$

it is easily seen that $\bar{T}_{1\to 3} \overset{(\mathrm{d})}{=} N_1 + N_2$, where N_1 and N_2 are (nonindependent) geometric random variables

$$N_1 \sim \mathcal{G}eo\left(\frac{\varepsilon}{6}\right), \quad N_2 \sim \mathcal{G}eo\left(\frac{1}{3}\right).$$

Therefore, $\mathbb{E}(\bar{T}_{1\to 3}) = \frac{6}{\varepsilon} + 3$ so that (3.6) holds. Note that, in the limit $\varepsilon \to 0$, we have the following convergences in law:

$$\varepsilon N_1 \to \mathscr{E}(\tfrac{1}{6}), \quad \varepsilon N_2 \to 0,$$

where $\mathscr{E}(\frac{1}{6})$ denotes an exponential random variable with parameter $\frac{1}{6}$. The result (3.7) is then easily obtained by the Slutsky theorem.

5.2 **Proof of Proposition 3.2**

The heuristic of the proof is the following. In the limit of small ε, to go from 1 to 3, a typical path first needs to stay sufficiently long in 1, in order for a transition to 2 to be

more likely (when $\theta_n(1)$ becomes sufficiently large). Then, from 2, the time it takes to go to 3 is small compared with the time spent to leave 1 for the first time. The aim of this proof is to quantify that by: (i) showing that a transition from 1 to 2 in a well-chosen time is very likely and then (ii) showing that once 2 is reached, the time it remains to go to 3 is small compared with the first transition time from 1 to 2. The precise result is the following.

Proposition 5.1. Consider the Wang–Landau dynamics defined in Section 3.1. Let us assume that $\alpha \in [\frac{1}{2}, 1]$ and that, if $\alpha = \frac{1}{2}$, $\gamma_\star < 1$. Then,

$$\lim_{\varepsilon \to 0} \mathbb{P}(T_{1\to 3} \in (a(\varepsilon), b(\varepsilon))) = 1, \tag{5.3}$$

with

(1) for $\alpha \in [\frac{1}{2}, 1)$,

$$a(\varepsilon) = \left(\frac{1-\alpha}{\gamma_\star} [|\ln \varepsilon| - \beta(\varepsilon)] \right)^{1/(1-\alpha)}, \quad b(\varepsilon) = C_b |\ln \varepsilon|^{1/(1-\alpha)},$$

where C_b is any constant such that

$$C_b > \left(\frac{1-\alpha}{\gamma_\star} \right)^{1/(1-\alpha)}$$

and $\beta(\varepsilon)$ is any non-negative function smaller than $|\ln(\varepsilon)|$ and such that

$$\lim_{\varepsilon \to 0} |\ln \varepsilon|^{\alpha/(1-\alpha)} \, \mathrm{e}^{-\beta(\varepsilon)} = 0; \tag{5.4}$$

(2) for $\alpha = 1$,

$$a(\varepsilon) = \varepsilon^{-1/(1+\gamma_\star)} f(\varepsilon), \quad b(\varepsilon) = \varepsilon^{-1/(1+\gamma_\star)} g(\varepsilon),$$

for any positive functions f and g such that

$$\lim_{\varepsilon \to 0} f(\varepsilon) = 0, \quad \lim_{\varepsilon \to 0} g(\varepsilon) = \infty. \qquad \square$$

In the case $\alpha \in [\frac{1}{2}, 1)$, an example of a simple admissible lower bound is $a(\varepsilon) = C_a |\ln \varepsilon|^{1/(1-\alpha)}$ where C_a is any constant such that $C_a < (\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)}$. In this case, one should consider $\beta(\varepsilon) = (1 - \frac{\gamma_\star C_a^{1-\alpha}}{1-\alpha}) |\ln \varepsilon|$, which indeed satisfies (5.4). Therefore, Proposition 5.1 implies Proposition 3.2.

Before proving the proposition, let us first introduce some notation. A convenient rewriting of the Wang–Landau dynamics is: for all $n \geqslant 0$, given $(X_n, \tilde{\theta}_n)$,

$$\begin{cases} X_{n+1} \text{ is sampled according to the kernel } P_{\theta_n}(X_n, \cdot), \\ \tilde{\theta}_{n+1}(i) = \tilde{\theta}_n(i)(1 + \gamma_{n+1} \mathbb{1}_{X_{n+1}=i}), \end{cases} \tag{5.5}$$

where $\tilde{\theta}_0 = (1, 1, 1)$, P_θ is defined by (3.4), and the normalized weights θ_n associated with the unnormalized weights $\tilde{\theta}_n$ are

$$\theta_n(i) = \left(\sum_{j=1}^{3} \tilde{\theta}_n(j) \right)^{-1} \tilde{\theta}_n(i).$$

The updating rule in (5.5) is exactly the standard update (2.4).

A crucial role will be played by the time the dynamics needs to first reach 2:

$$T^0_{1\to 2} = \min\{n : \ X_n = 2 \text{ starting from } X_0 = 1\}. \tag{5.6}$$

The probability to go from state 1 to state 2 in exactly n moves is

$$\mathbb{P}(T^0_{1\to 2} = n) = p^0_{11} \cdots p^{n-2}_{11} p^{n-1}_{12}, \tag{5.7}$$

with

$$p^m_{11} = 1 - \tfrac{1}{3}(\varepsilon \Xi_m \wedge 1), \quad p^m_{12} = 1 - p^m_{11} = \tfrac{1}{3}(\varepsilon \Xi_m \wedge 1),$$

where

$$\Xi_m = \prod_{k=1}^{m} (1 + \gamma_k) \tag{5.8}$$

with the convention $\Xi_0 = 1$. The first $n-1$ factors in (5.7) correspond to staying in state 1 (with the appropriate update of the weights), and the last one corresponds to the transition from state 1 to state 2. An important inequality, which will be used below, is $p^m_{12} \leqslant p^n_{12}$ (and thus $p^m_{11} \geqslant p^n_{11}$) for $m \leqslant n$: when the system is stuck in state 1, as time goes, the probability to go to state 2 increases.

Estimates on the exit time $T_{1\to 3}$ are based on the following equality:

$$T_{1\to 3} = T^0_{1\to 2} + \sum_{i=1}^{N_{2\to 1}} T^i_{1\to 2} + N_2, \tag{5.9}$$

where $N_2 = \sum_{n=0}^{T_{1\to 3}} 1_{\{X_n=2\}}$ is the time the chain spends in 2 before going to 3, $N_{2\to 1}$ is the number of jumps from 2 back to 1 before going to 3, and $T^i_{1\to 2}$ is the time it takes to leave

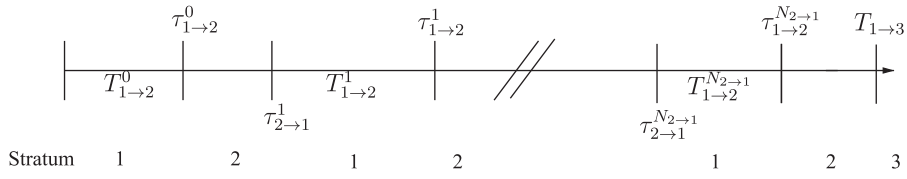

Fig. 4. Schematic representation of the successive passage times and exit times out of 1.

1 at the ith return to the state 1 from 2. Note that

$$N_{2\to1} \leqslant N_2.$$

To make these quantities more precise, let us introduce the successive passage times: for $i \geqslant 1$,

$$\tau^i_{2\to1} = \inf\{n > \tau^{i-1}_{1\to2},\ X_n = 1\}, \tag{5.10}$$

with, by convention $\tau^0_{1\to2} = T^0_{1\to2}$ and,

$$\tau^i_{1\to2} = \inf\{n > \tau^i_{2\to1},\ X_n = 2\}.$$

Note that $T^i_{1\to2} = \tau^i_{1\to2} - \tau^i_{2\to1}$. We refer the reader to Figure 4 for a schematic representation of all these times.

Let us first state a simple result concerning N_2, which is based on the fact that before visiting the state 3, $\tilde\theta_n(3) = 1$ remains unchanged while $\tilde\theta_n(2) \geqslant 1$. This means that for $n \leqslant T_{1\to3}$,

$$P_{\theta_n}(2,3) = \frac{1}{3}\left(\frac{\tilde\theta_n(2)}{\varepsilon\tilde\theta_n(3)} \wedge 1\right) = \frac{1}{3}\left(\frac{\tilde\theta_n(2)}{\varepsilon} \wedge 1\right) = \frac{1}{3},$$

where we have used the inequality $\varepsilon < 1$. At each time the system is in state 2, it stays in state 2 or goes to state 1 at the next time with probability $\frac{2}{3}$. This gives the intuition of the following result, the formal proof of which is postponed to Section 5.3.

Lemma 5.1. The random variable N_2 is geometric with parameter $\frac{1}{3}$: for all $n \geqslant 0$,

$$\mathbb{P}(N_2 \geqslant n) = (\tfrac{2}{3})^n.$$

□

Thus, in (5.9), the last term plays no role in the limit $\varepsilon \to 0$. We show below that this is also true for the second term: the main role is played by $T^0_{1\to2}$. This is why we first need to precisely estimate the time $T^0_{1\to2}$. This can be done for any $\alpha \in (0,1]$ (and not only in $[\frac{1}{2},1]$), and without any restriction on $\gamma_\star$.

Lemma 5.2. Fix $\alpha \in (0,1]$. For $\alpha \in [\frac{1}{2},1]$, let a be the function defined in Proposition 5.1. For $\alpha \in (0,\frac{1}{2})$, let the function a be defined in the same way as for $\alpha \in [\frac{1}{2},1)$. Then,

$$\lim_{\varepsilon\to 0}\mathbb{P}(T^0_{1\to 2}\in(a(\varepsilon),\tilde{b}(\varepsilon)))=1, \tag{5.11}$$

where

(1) if $\alpha\in(0,1)$, $\tilde{b}(\varepsilon)=C_{\tilde{b}}|\ln\varepsilon|^{1/(1-\alpha)}$, where $C_{\tilde{b}}$ is any constant such that $C_{\tilde{b}}>(\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)}$;
(2) if $\alpha=1$, $\tilde{b}(\varepsilon)=\tilde{g}(\varepsilon)\varepsilon^{-1/(1+\gamma_\star)}$ for any positive function $\tilde{g}$ such that $\lim_{\varepsilon\to 0}\tilde{g}(\varepsilon)=\infty$. □

The proof of Lemma 5.2 can be read in Section 5.3.

Remark 5.1. To guess the correct scaling for $T^0_{1\to 2}$, one may consider the typical time $n(\varepsilon)$ for which $\mathbb{P}(T^0_{1\to 2}\leqslant n(\varepsilon))=1-\prod_{k=0}^{n(\varepsilon)-1}(1-\frac{1}{3}(\varepsilon\Xi_k\wedge 1))$ has a positive limit when ε goes to 0. Using an expansion when ε goes to 0, assuming that $\varepsilon\Xi_{n(\varepsilon)}$ goes to zero, we obtain that $n(\varepsilon)$ satisfies $\sum_{k=0}^{n(\varepsilon)-1}\Xi_k\sim\frac{C}{\varepsilon}$ for some constant $C>0$. A guess for the scaling of the time $T^0_{1\to 2}$ is thus $n(\varepsilon)=\arg\min_n\{\sum_{k=0}^{n-1}\Xi_k\geqslant\frac{1}{\varepsilon}\}$ (obtained by choosing $C=1$). Using Lemma 5.4, this yields various asymptotic behaviors for $n(\varepsilon)$ depending on the values of α and $\gamma_\star$ in (3.5):

(1) When $\alpha\in(0,1)$, from (5.14), we obtain that $n(\varepsilon)\sim(\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)}|\ln\varepsilon|^{1/(1-\alpha)}$.
(2) When $\alpha=1$, from (5.13), we obtain $n(\varepsilon)\sim\Gamma(2+\gamma_\star)^{1/(1+\gamma_\star)}\varepsilon^{-1/(1+\gamma_\star)}$.

This motivates the scaling for $T^0_{1\to 2}$. □

We are now in position to prove Proposition 5.1.

Proof of Proposition 5.1. Let a and b satisfy the assumptions of Proposition 5.1. Since $T_{1\to 3}\geqslant T^0_{1\to 2}+1$, the lower bound in Proposition 5.1 (i.e., the fact that $\lim_{\varepsilon\to 0}\mathbb{P}(T_{1\to 3}\leqslant a(\varepsilon))=0$) immediately follows from Lemma 5.2. The upper bound requires some more work. We choose $\tilde{b}(\varepsilon)$ satisfying the assumptions of Lemma 5.2 with $(\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)}<C_{\tilde{b}}<C_b$ if $\alpha\in[\frac{1}{2},1)$ and $\tilde{g}<g$ if $\alpha=1$. In particular, $\tilde{b}<b$. Let us also introduce a positive function

$\Delta(\varepsilon)$ going to infinity as $\varepsilon \to 0$, that will be specified later on. Then, using (5.9),

$$\begin{aligned}\mathbb{P}(T_{1\to 3} \geqslant b(\varepsilon)) &\leqslant \mathbb{P}(T^0_{1\to 2} \notin (a(\varepsilon), \tilde{b}(\varepsilon))) + \mathbb{P}(N_2 \geqslant \Delta(\varepsilon)) \\ &\quad + \mathbb{P}(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ T_{1\to 3} \geqslant b(\varepsilon)) \\ &\leqslant \mathbb{P}(T^0_{1\to 2} \notin (a(\varepsilon), \tilde{b}(\varepsilon))) + \mathbb{P}(N_2 \geqslant \Delta(\varepsilon)) \\ &\quad + \mathbb{P}\left(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to 1}} T^i_{1\to 2} \geqslant b(\varepsilon) - \Delta(\varepsilon) - \tilde{b}(\varepsilon)\right).\end{aligned} \tag{5.12}$$

The first term in the right-hand side goes to zero as $\varepsilon \to 0$ by Lemma 5.2. Since $\Delta(\varepsilon)$ tends to ∞ when ε goes to zero, the second term goes to zero by Lemma 5.1. Concerning the third term, the idea is the following: we would like to choose $\tilde{b}$ and Δ such that, on the event $T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon))$ and $N_2 \leqslant \Delta(\varepsilon)$, the times $T^i_{1\to 2}$ can be simply controlled using the fact that state 1 has already been visited for a long time (namely $T^0_{1\to 2} > a(\varepsilon)$ and therefore $\tilde{\theta}_{T^0_{1\to 2}}(1)$ is large) and state 2 is not visited many times (this corresponds to $N_2 \leqslant \Delta(\varepsilon)$ so that $\tilde{\theta}_n(2)$ remains small). This idea will be quantified in Lemma 5.5 in Section 5.3 from which we will deduce.

Lemma 5.3. Assume that $\Delta(\varepsilon) = \mathrm{O}(a^\alpha(\varepsilon))$ as $\varepsilon \to 0$. Then, there exist constants $C, C', \bar{\varepsilon} > 0$ such that for $\varepsilon \in (0, \bar{\varepsilon})$,

$$\begin{aligned}&\mathbb{P}\left(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to 1}} T^i_{1\to 2} \geqslant b(\varepsilon) - \Delta(\varepsilon) - \tilde{b}(\varepsilon)\right) \\ &\leqslant \begin{cases} \Delta(\varepsilon) \exp\left(-C \dfrac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{2-\gamma_\star^2} \exp(-\beta(\varepsilon))\right) & \text{if } \alpha = \dfrac{1}{2}, \\ \Delta(\varepsilon) \exp\left(-C \dfrac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{1/(1-\alpha)} \exp(-\beta(\varepsilon))\right) & \text{if } \alpha \in \left(\dfrac{1}{2}, 1\right), \\ C' \Delta(\varepsilon) \exp\left(-C \dfrac{g(\varepsilon) - \tilde{g}(\varepsilon)}{\Delta(\varepsilon)} f(\varepsilon)^{\gamma_\star}\right) & \text{if } \alpha = 1. \end{cases}\end{aligned}$$

□

Let us first conclude in the case $\alpha \in [\frac{1}{2}, 1)$. We may choose Δ satisfying $\Delta(\varepsilon) = \mathrm{O}(a^\alpha(\varepsilon))$ and going to infinity as slowly as needed. Then, for the upper bound of the third term of the right-hand side of (5.12) given by Lemma 5.3 to vanish as $\varepsilon \to 0$, it is enough that

$$\begin{aligned}\lim_{\varepsilon \to 0} |\ln \varepsilon|^{1/(1-\alpha)} \exp(-\beta(\varepsilon)) &= +\infty \text{ if } \alpha \in \left(\frac{1}{2}, 1\right), \\ \lim_{\varepsilon \to 0} |\ln \varepsilon|^{2-\gamma_\star^2} \exp(-\beta(\varepsilon)) &= +\infty \text{ if } \alpha = \frac{1}{2}.\end{aligned}$$

For this limit to hold, it is always possible to decrease β as long as (5.4) holds, that is,

$$\lim_{\varepsilon \to 0} |\ln \varepsilon|^{\alpha/(1-\alpha)} \, \mathrm{e}^{-\beta(\varepsilon)} = 0$$

since the smaller β, the larger a, and stronger the conclusion (5.3) of Proposition 5.1. This is possible without restriction when $\alpha \in (\frac{1}{2}, 1)$ and if and only if $2 - \gamma_\star^2 > 1$ when $\alpha = \frac{1}{2}$.

Let us now suppose that $\alpha = 1$. Up to increasing f, which makes the conclusion of Proposition 5.1 stronger, while preserving $\lim_{\varepsilon \to 0} f(\varepsilon) = 0$, one may assume that $g(\varepsilon) f(\varepsilon)^{\gamma_\star}$ goes to infinity as ε goes to zero. In addition, it is always possible to choose $\tilde{g} \leqslant g$ such that $(g(\varepsilon) - \tilde{g}(\varepsilon)) f(\varepsilon)^{\gamma_\star}$ goes to infinity as ε goes to zero. Then one can choose Δ, which grows sufficiently slowly at infinity so that $\Delta(\varepsilon) \exp(-C \frac{g(\varepsilon) - \tilde{g}(\varepsilon)}{\Delta(\varepsilon)} f(\varepsilon)^{\gamma_\star})$ tends to 0. ■

5.3 Proofs of the technical lemmas

Proof of Lemma 5.1. Let $(\mathcal{F}_n)_{n \geqslant 0}$ denote the filtration generated by the Markov chain $\{(X_n, \tilde{\theta}_n), n \geqslant 0\}$. Let us also introduce the successive visit times of state 2. For $i \geqslant 1$ let $\eta_i = \inf\{n > \eta_{i-1} : X_n = 2\}$ with convention $\eta_0 = 0$. For $n \in \mathbb{N}^*$, one has $\{N_2 \geqslant n+1\} = \bigcap_{k=1}^{n} \{X_{\eta_k + 1} \in \{1, 2\}\}$. Therefore,

$$\begin{aligned}
\mathbb{P}(N_2 \geqslant n+1) &= \mathbb{E}\left(\mathbb{E}\left(\prod_{k=1}^{n} 1_{\{X_{\eta_k+1} \in \{1,2\}\}} | \mathcal{F}_{\eta_n}\right)\right) = \mathbb{E}\left(\prod_{k=1}^{n-1} 1_{\{X_{\eta_k+1} \in \{1,2\}\}} \mathbb{P}(X_{\eta_n+1} \in \{1,2\} | \mathcal{F}_{\eta_n})\right) \\
&= \mathbb{E}\left(\prod_{k=1}^{n-1} 1_{\{X_{\eta_k+1} \in \{1,2\}\}} (1 - P_{\theta_{\eta_n}}(2,3))\right),
\end{aligned}$$

where we used that the event $\bigcap_{k=1}^{n-1} \{X_{\eta_k+1} \in \{1,2\}\}$ is $\mathcal{F}_{\eta_n}$-measurable for the second equality and the strong Markov property for the chain $\{(X_l, \tilde{\theta}_l), l \geqslant 0\}$ for the last equality. On $\bigcap_{k=1}^{n-1} \{X_{\eta_k+1} \in \{1,2\}\}$, the sequence $\{X_l, l \geqslant 0\}$ has not visited state 3 before the stopping time η_n, which implies $P_{\theta_{\eta_n}}(2,3) = \frac{1}{3}$. Hence,

$$\mathbb{P}(N_2 \geqslant n+1) = \frac{2}{3} \mathbb{E}\left(\prod_{k=1}^{n-1} 1_{\{X_{\eta_k+1} \in \{1,2\}\}}\right) = \frac{2}{3} \mathbb{P}(N_2 \geqslant n)$$

and one concludes by induction on n. ■

To prove Lemmas 5.2 and 5.3, we need the following estimations on Ξ_n.

Lemma 5.4. For $\alpha = 1$,

$$\Xi_n \sim \frac{n^{\gamma_\star}}{\Gamma(1+\gamma_\star)} \quad \text{as } n \to \infty. \tag{5.13}$$

For $\alpha \in (0,1)$,

$$\ln(\Xi_n) \sim \frac{\gamma_\star}{1-\alpha} n^{1-\alpha} \quad \text{as } n \to \infty, \tag{5.14}$$

$$\forall n,\ \Xi_n \leqslant \exp\left(\frac{\gamma_\star}{1-\alpha} n^{1-\alpha}\right), \tag{5.15}$$

and there exists a constant $C > 0$ independent of n such that

$$\forall n,\ \Xi_n \geqslant \begin{cases} C \exp\left(2\gamma_\star \sqrt{n} - \dfrac{\gamma_\star^2}{2} \ln n\right) & \text{for } \alpha = \dfrac{1}{2}, \\ C \exp\left(\dfrac{\gamma_\star}{1-\alpha} n^{1-\alpha}\right) & \text{for } \alpha \in \left(\dfrac{1}{2}, 1\right). \end{cases} \tag{5.16}$$

□

Proof of Lemma 5.4. In the case $\alpha = 1$, using the Stirling formula, we have

$$\Xi_n = \prod_{k=1}^{n} (1+\gamma_k) = \prod_{k=1}^{n} \left(1 + \frac{\gamma_\star}{k}\right) = \frac{\Gamma(n+1+\gamma_\star)}{\Gamma(1+\gamma_\star)\Gamma(n+1)} \sim \frac{n^{\gamma_\star}}{\Gamma(1+\gamma_\star)},$$

which is (5.13). Now, for $\alpha \in (0,1)$, as $n \to \infty$,

$$\ln(\Xi_n) = \ln\left(\prod_{k=1}^{n} (1+\gamma_k)\right) \sim \gamma_\star \sum_{k=1}^{n} k^{-\alpha} \sim \frac{\gamma_\star}{1-\alpha} n^{1-\alpha}.$$

Moreover,

$$\ln(\Xi_n) \leqslant \gamma_\star \sum_{k=1}^{n} k^{-\alpha} \leqslant \gamma_\star \sum_{k=1}^{n} \int_{k-1}^{k} x^{-\alpha}\, \mathrm{d}x = \frac{\gamma_\star}{1-\alpha} n^{1-\alpha}.$$

To prove (5.16), we start from the lower bound

$$\ln(\Xi_n) \geqslant \sum_{k=1}^{n} \gamma_k - \frac{1}{2} \sum_{k=1}^{n} \gamma_k^2.$$

For $\alpha \in (0,1)$,

$$\sum_{k=1}^{n} \gamma_k \geqslant \gamma_\star \sum_{k=1}^{n} \int_{k}^{k+1} x^{-\alpha}\, \mathrm{d}x = \frac{\gamma_\star}{1-\alpha}((n+1)^{1-\alpha} - 1) \geqslant \frac{\gamma_\star}{1-\alpha}(n^{1-\alpha} - 1),$$

so that

$$\ln(\Xi_n) \geqslant \frac{\gamma_\star}{1-\alpha}(n^{1-\alpha} - 1) - \frac{1}{2} \sum_{k=1}^{n} \gamma_k^2.$$

We now distinguish between two cases. For $\alpha \in (\frac{1}{2}, 1)$,

$$\sum_{k=1}^{n} \gamma_k^2 = \gamma_\star^2 \sum_{k=1}^{n} k^{-2\alpha} \leqslant \gamma_\star^2 + \gamma_\star^2 \sum_{k=2}^{n} \int_{k-1}^{k} x^{-2\alpha}\, \mathrm{d}x = \gamma_\star^2 + \frac{\gamma_\star^2}{2\alpha - 1}(1 - n^{1-2\alpha}) \leqslant \frac{2\gamma_\star^2 \alpha}{2\alpha - 1}.$$

Therefore, for $n \geqslant 1$,

$$\ln(\Xi_n) \geqslant \frac{\gamma_\star}{1-\alpha}(n^{1-\alpha} - 1) - \frac{\gamma_\star^2 \alpha}{2\alpha - 1},$$

which gives the expected result. For $\alpha = \frac{1}{2}$,

$$\sum_{k=1}^{n} \gamma_k^2 \leqslant \gamma_\star^2 + \gamma_\star^2 \sum_{k=2}^{n} \int_{k-1}^{k} x^{-1}\, \mathrm{d}x = \gamma_\star^2 (1 + \ln n),$$

so that, for $n \geqslant 1$,

$$\ln(\Xi_n) \geqslant 2\gamma_\star(\sqrt{n} - 1) - \frac{\gamma_\star^2}{2}(1 + \ln n),$$

which also gives the claimed result. ∎

Proof of Lemma 5.2. Let us first deal with $\alpha \in (0, 1)$. We start by the lower bound on $T^0_{1\to 2}$. Let a be of the form $a(\varepsilon) = (\frac{1-\alpha}{\gamma_\star}(|\ln \varepsilon| - \beta(\varepsilon)))^{1/(1-\alpha)}$ for any non-negative function $\beta(\varepsilon)$ smaller than $|\ln(\varepsilon)|$ and satisfying (5.4). By (5.7),

$$\begin{aligned}\ln(\mathbb{P}\{T^0_{1\to 2} > a(\varepsilon)\}) &= \ln\left(\prod_{k=0}^{\lfloor a(\varepsilon)\rfloor} p_{11}^k\right) = \sum_{k=0}^{\lfloor a(\varepsilon)\rfloor} \ln\left(1 - \frac{1}{3}(\varepsilon \Xi_k \wedge 1)\right) \geqslant -\frac{C_0}{3} \sum_{k=0}^{\lfloor a(\varepsilon)\rfloor} (\varepsilon \Xi_k \wedge 1) \\ &\geqslant -\frac{C_0 \varepsilon}{3} \sum_{k=0}^{\lfloor a(\varepsilon)\rfloor} \Xi_k,\end{aligned}$$

where we have used that, by concavity of the function ln, $\ln(1 - x) \geqslant -C_0 x$ for $x \in (0, \frac{1}{3})$ with $C_0 = -3\ln(2/3) > 0$. Now, by (5.15),

$$\begin{aligned}\sum_{k=0}^{n} \Xi_k &\leqslant \sum_{k=0}^{n} \exp\left(\frac{\gamma_\star}{1-\alpha} k^{1-\alpha}\right) \leqslant \sum_{k=0}^{n} \int_{k}^{k+1} \exp\left(\frac{\gamma_\star}{1-\alpha} x^{1-\alpha}\right) \mathrm{d}x \\ &= \int_0^{n+1} \exp\left(\frac{\gamma_\star}{1-\alpha} x^{1-\alpha}\right) \mathrm{d}x \leqslant \frac{(n+1)^\alpha}{\gamma_\star} \int_0^{n+1} \gamma_\star x^{-\alpha} \exp\left(\frac{\gamma_\star}{1-\alpha} x^{1-\alpha}\right) \mathrm{d}x \\ &\leqslant \frac{1}{\gamma_\star}(n+1)^\alpha \exp\left(\frac{\gamma_\star}{1-\alpha}(n+1)^{1-\alpha}\right).\end{aligned}$$

Hence, using the inequality $(x + y)^\delta \leqslant x^\delta + y^\delta$ for any $(x, y) \in \mathbb{R}_+^2$ and $\delta \in (0, 1)$,

$$\begin{aligned}\ln(\mathbb{P}\{T^0_{1\to 2} > a(\varepsilon)\}) &\geqslant -\frac{C_0 \varepsilon}{3\gamma_\star}(a(\varepsilon) + 1)^\alpha \exp\left(\frac{\gamma_\star}{1-\alpha}(a(\varepsilon) + 1)^{1-\alpha}\right) \\ &\geqslant -C_1 \varepsilon a(\varepsilon)^\alpha \exp\left(\frac{\gamma_\star}{1-\alpha} a(\varepsilon)^{1-\alpha}\right),\end{aligned}$$

where C_1 is a constant independent of ε. Therefore,

$$\ln(\mathbb{P}\{T^0_{1\to 2} > a(\varepsilon)\}) \geqslant -C_1\varepsilon\left(\frac{1-\alpha}{\gamma_\star}(|\ln\varepsilon| - \beta(\varepsilon))\right)^{\alpha/(1-\alpha)} \exp(|\ln\varepsilon| - \beta(\varepsilon))$$
$$= -C_2(|\ln\varepsilon| - \beta(\varepsilon))^{\alpha/(1-\alpha)}\exp(-\beta(\varepsilon)), \tag{5.17}$$

where $C_2 = C_1(\frac{1-\alpha}{\gamma_\star})^{\alpha/(1-\alpha)}$ is a constant independent of ε. Thus, under the assumption (5.4), we indeed obtain that $\lim_{\varepsilon\to 0}\mathbb{P}(T^0_{1\to 2} \leq a(\varepsilon)) = 0$.

We now turn to an estimate of an upper bound for $T^0_{1\to 2}$. Let us introduce a function $\tilde{b}(\varepsilon) = C_{\tilde{b}}|\ln\varepsilon|^{1/(1-\alpha)}$ where $C_{\tilde{b}}$ is any constant such that $C_{\tilde{b}} > (\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)}$. We also define an intermediate time $\tilde{n}(\varepsilon) \leqslant \tilde{b}(\varepsilon)$ such that $p_{12}^{\tilde{n}(\varepsilon)} = \frac{1}{3}$, which equivalently writes

$$\tfrac{1}{3}(\varepsilon\Xi_{\tilde{n}(\varepsilon)} \wedge 1) = \tfrac{1}{3} \quad \text{that is } \varepsilon\Xi_{\tilde{n}(\varepsilon)} \geqslant 1.$$

We choose

$$\tilde{n}(\varepsilon) = \lceil \tilde{C}|\ln\varepsilon|^{1/(1-\alpha)}\rceil, \quad \left(\frac{1-\alpha}{\gamma_\star}\right)^{1/(1-\alpha)} < \tilde{C} < C_{\tilde{b}}.$$

In view of (5.14), and since $\tilde{C}^{\alpha-1} < \frac{\gamma_\star}{1-\alpha}$, it holds $\Xi_n \geqslant \exp(\tilde{C}^{\alpha-1}n^{1-\alpha})$ for n large enough. Thus, for ε small enough, we obtain

$$\Xi_{\tilde{n}(\varepsilon)} \geqslant \exp(\tilde{C}^{\alpha-1}\lceil\tilde{C}|\ln\varepsilon|^{1/(1-\alpha)}\rceil^{1-\alpha}) \geqslant \frac{1}{\varepsilon},$$

so that $p_{12}^{\tilde{n}(\varepsilon)} = \frac{1}{3}$. An upper bound on $T^0_{1\to 2}$ is then obtained as (note that for ε small enough, $\lceil\tilde{b}(\varepsilon)\rceil - 2 \geqslant \tilde{n}(\varepsilon)$):

$$\mathbb{P}(T^0_{1\to 2} \geqslant \tilde{b}(\varepsilon)) = \prod_{k=0}^{\lfloor\tilde{b}(\varepsilon)\rfloor-2} p_{11}^k \leqslant \prod_{k=\tilde{n}(\varepsilon)}^{\lfloor\tilde{b}(\varepsilon)\rfloor-2} p_{11}^k \leqslant \left(\frac{2}{3}\right)^{\lfloor\tilde{b}(\varepsilon)\rfloor-2-\tilde{n}(\varepsilon)}$$
$$\leqslant \frac{81}{16}\exp\left[\left(\ln\frac{3}{2}\right)(\tilde{C} - C_{\tilde{b}})|\ln\varepsilon|^{1/(1-\alpha)}\right].$$

The right-hand side goes to zero when ε goes to 0, which yields the result for the asymptotic upper bound $\tilde{b}(\varepsilon)$. This ends the proof of Lemma 5.2 in the case $\alpha \in (0,1)$.

In the case $\alpha = 1$, for the lower bound, we choose $a(\varepsilon) = f(\varepsilon)\varepsilon^{-1/(1+\gamma_\star)}$ for any function f such that $\lim_{\varepsilon\to 0} f(\varepsilon) = 0$. We have, using (5.13) for the fourth inequality and

denoting by C a positive constant which may change from line to line

$$\begin{aligned}
\mathbb{P}(T^0_{1\to 2}\leqslant a(\varepsilon)) &= 1-\mathbb{P}(T_{1\to 2}>\lfloor a(\varepsilon)\rfloor) = 1-\prod_{k=0}^{\lfloor a(\varepsilon)\rfloor-1} p_{11}^k \\
&\leqslant 1-(p_{11}^{\lfloor a(\varepsilon)\rfloor})^{\lfloor a(\varepsilon)\rfloor} = 1-\exp(\lfloor a(\varepsilon)\rfloor \ln(p_{11}^{\lfloor a(\varepsilon)\rfloor})) \leqslant -\lfloor a(\varepsilon)\rfloor \ln(p_{11}^{\lfloor a(\varepsilon)\rfloor}) \\
&= -\lfloor a(\varepsilon)\rfloor \ln\left(1-\frac{1}{3}(\varepsilon \Xi_{\lfloor a(\varepsilon)\rfloor}\wedge 1)\right) \leqslant -\lfloor a(\varepsilon)\rfloor \ln\left(1-\frac{1}{3}\varepsilon\Xi_{\lfloor a(\varepsilon)\rfloor}\right) \\
&\leqslant -\lfloor a(\varepsilon)\rfloor \ln(1-C\varepsilon a(\varepsilon)^{\gamma_\star}) \leqslant -\lfloor a(\varepsilon)\rfloor \ln(1-C\varepsilon^{1/(1+\gamma_\star)} f(\varepsilon)^{\gamma_\star}) \\
&\leqslant C\lfloor a(\varepsilon)\rfloor \varepsilon^{1/(1+\gamma_\star)} f(\varepsilon)^{\gamma_\star} \leqslant C f(\varepsilon)^{1+\gamma_\star},
\end{aligned}$$

which converges to 0 as ε goes to 0.

We now consider the upper bound. We set $b(\varepsilon)=g(\varepsilon)\varepsilon^{-1/(1+\gamma_\star)}$ with $\lim_{\varepsilon\to 0} g(\varepsilon)=\infty$. In the following, we assume that g grows sufficiently slowly so that $\lim_{\varepsilon\to 0}\varepsilon(b(\varepsilon))^{\gamma_\star}=0$. This is not a restrictive assumption since the probability $\mathbb{P}(T^0_{1\to 2}\geqslant b(\varepsilon))$ is even lower when the function g goes faster to infinity. Moreover, upon replacing $g(\varepsilon)$ by $\varepsilon^{1/(1+\gamma_\star)}\lfloor \varepsilon^{-1/(1+\gamma_\star)} g(\varepsilon)\rfloor$, we may assume that $b:(0,1)\to\mathbb{N}$. One has

$$\mathbb{P}(T^0_{1\to 2}\geqslant b(\varepsilon)) = \prod_{k=0}^{b(\varepsilon)-2} p_{11}^k = \prod_{k=0}^{b(\varepsilon)-2}\left(1-\frac{1}{3}(\varepsilon\Xi_k\wedge 1)\right).$$

For $k\leqslant b(\varepsilon)$, it holds $\varepsilon\Xi_k\leqslant \varepsilon\Xi_{\lfloor b(\varepsilon)\rfloor}$ with the right-hand side smaller than $C\varepsilon b(\varepsilon)^{\gamma_\star}$ by (5.13). This upper bound goes to zero as ε goes to zero by assumption. Thus, for ε sufficiently small,

$$\mathbb{P}(T^0_{1\to 2}\geqslant b(\varepsilon)) = \prod_{k=0}^{b(\varepsilon)-2}\left(1-\frac{1}{3}\varepsilon\Xi_k\right) \leqslant \prod_{k=0}^{b(\varepsilon)-2}(1-C\varepsilon k^{\gamma_\star}), \tag{5.18}$$

where C is a constant independent of ε. Then, using the fact that $\varepsilon b(\varepsilon)^{\gamma_\star}$ is smaller than $1/C$ for ε sufficiently small, we have in this limit

$$\begin{aligned}
\ln\left(\prod_{k=0}^{b(\varepsilon)-2}(1-C\varepsilon k^{\gamma_\star})\right) &= \sum_{k=0}^{b(\varepsilon)-2}\ln(1-C\varepsilon k^{\gamma_\star}) \leqslant -C\varepsilon\sum_{k=1}^{b(\varepsilon)-2} k^{\gamma_\star} \\
&\leqslant -C\varepsilon\sum_{k=1}^{b(\varepsilon)-2}\int_{k-1}^{k} x^{\gamma_\star}\,\mathrm{d}x = -C\varepsilon\int_0^{b(\varepsilon)-2} x^{\gamma_\star}\,\mathrm{d}x \\
&= -\frac{C}{\gamma_\star+1}\varepsilon(b(\varepsilon)-2)^{\gamma_\star+1} \leqslant -\frac{C}{\gamma_\star+1}\left(1-\frac{2}{b(\varepsilon)}\right)^{\gamma_\star+1} g(\varepsilon)^{\gamma_\star+1}.
\end{aligned}$$

Using this estimate in (5.18) leads to the existence of a modified positive constant C such that for ε small enough, $\mathbb{P}(T^0_{1\to 2}\geqslant b(\varepsilon))\leqslant \exp(-Cg(\varepsilon)^{\gamma_\star+1})$, the right-hand side going to 0 as $\varepsilon\to 0$. This therefore concludes the proof of Lemma 5.2 in the case $\alpha=1$. ■

Remark 5.2. Considering the Equation (5.17), one could think of replacing the assumption (5.4) on β by the seemingly weaker one:

$$\lim_{\varepsilon\to 0}(|\ln\varepsilon| - \beta(\varepsilon))^{\alpha/(1-\alpha)}\exp(-\beta(\varepsilon)) = 0.$$

But both conditions are equivalent since

$$\begin{aligned}|\ln\varepsilon|^{\alpha/(1-\alpha)}\exp(-\beta(\varepsilon)) \leqslant\ & 1_{\{\beta(\varepsilon)\leqslant|\ln\varepsilon|/2\}}2^{\alpha/(1-\alpha)}(|\ln\varepsilon| - \beta(\varepsilon))^{\alpha/(1-\alpha)}\exp(-\beta(\varepsilon))\\ &+ 1_{\{\beta(\varepsilon)>|\ln\varepsilon|/2\}}(|\ln\varepsilon|)^{\alpha/(1-\alpha)}\exp(-|\ln\varepsilon|/2).\end{aligned}$$

□

In order to prove Lemma 5.3, we need, as explained in the proof of Proposition 5.1, to ensure that $\tilde{\theta}_n(2)$ remains small when $T^0_{1\to 2} > a(\varepsilon)$ and $N_2 \leqslant \Delta(\varepsilon)$.

Lemma 5.5. Let us assume that $\alpha \in (0,1]$. Let us consider a non-negative constant Δ and a constant $a \geqslant 1$. Let $\nu_2(n)$ denote the number of visits of state 2 up to time n included. Then, on the event $\{T^0_{1\to 2} > a\}$, for any n such that $\nu_2(n) \leqslant \Delta$,

$$\tilde{\theta}_n(2) \leqslant \begin{cases}\exp\left(\dfrac{\gamma_\star}{1-\alpha}\lfloor a\rfloor^{1-\alpha}\left(\left(\dfrac{\lceil a+\Delta\rceil+1}{\lfloor a\rfloor}\right)^{1-\alpha} - 1\right)\right) & \text{if } \alpha\in(0,1),\\ \left(\dfrac{\lceil a+\Delta\rceil+1}{\lfloor a\rfloor}\right)^{\gamma_\star} & \text{if } \alpha = 1.\end{cases} \tag{5.19}$$

□

Proof of Lemma 5.5. On the event $\{T^0_{1\to 2} > a\}$, for n such that $\nu_2(n) \leqslant \Delta$, it holds

$$\tilde{\theta}_n(2) \leq \prod_{k=\lfloor a\rfloor+1}^{\lceil a+\Delta\rceil+1}\left(1+\frac{\gamma_\star}{k^\alpha}\right).$$

Now,

$$\begin{aligned}\ln\left(\prod_{k=\lfloor a\rfloor+1}^{\lceil a+\Delta\rceil+1}\left(1+\frac{\gamma_\star}{k^\alpha}\right)\right) &= \sum_{k=\lfloor a\rfloor+1}^{\lceil a+\Delta\rceil+1}\ln\left(1+\frac{\gamma_\star}{k^\alpha}\right) \leqslant \sum_{k=\lfloor a\rfloor+1}^{\lceil a+\Delta\rceil+1}\frac{\gamma_\star}{k^\alpha}\\ &\leqslant \sum_{k=\lfloor a\rfloor+1}^{\lceil a+\Delta\rceil+1}\int_{k-1}^{k}\frac{\gamma_\star}{x^\alpha}\,\mathrm{d}x = \int_{\lfloor a\rfloor}^{\lceil a+\Delta\rceil+1}\frac{\gamma_\star}{x^\alpha}\,\mathrm{d}x.\end{aligned}$$

When $\alpha = 1$, the right-hand side is equal to $\gamma_\star\ln\left(\frac{\lceil a+\Delta\rceil+1}{\lfloor a\rfloor}\right)$, which gives the claimed result. When $\alpha \in (0,1)$, the right-hand side is equal to

$$\frac{\gamma_\star}{1-\alpha}\lfloor a\rfloor^{1-\alpha}\left(\left(\frac{\lceil a+\Delta\rceil+1}{\lfloor a\rfloor}\right)^{1-\alpha} - 1\right),$$

which concludes the proof. ■

Proof of Lemma 5.3. Let $c(\varepsilon) = \lceil \frac{b(\varepsilon)-\tilde{b}(\varepsilon)}{\Delta(\varepsilon)} \rceil - 1$. Using the fact that $N_{2\to 1} \leqslant N_2$, and recalling that $(\mathcal{F}_n)_{n\geqslant 0}$ denotes the filtration generated by $((X_n, \theta_n))_{n\geqslant 0}$, it holds

$$\begin{aligned}
&\mathbb{P}\left(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to 1}} T^i_{1\to 2} \geqslant b(\varepsilon) - \Delta(\varepsilon) - \tilde{b}(\varepsilon) \right) \\
&\quad \leqslant \mathbb{P}\left(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \exists i \in \{1, \dots, N_{2\to 1}\},\ T^i_{1\to 2} \geqslant \frac{b(\varepsilon) - \tilde{b}(\varepsilon)}{\Delta(\varepsilon)} - 1 \right) \\
&\quad \leqslant \sum_{l=1}^{\Delta(\varepsilon)} \mathbb{P}(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ N_{2\to 1} = l,\ \exists i \in \{1, \dots, l\},\ T^i_{1\to 2} \geqslant c(\varepsilon)) \\
&\quad \leqslant \sum_{l=1}^{\Delta(\varepsilon)} \sum_{i=1}^{l} \mathbb{P}(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ N_{2\to 1} = l,\ T^i_{1\to 2} \geqslant c(\varepsilon)) \\
&\quad = \sum_{i=1}^{\Delta(\varepsilon)} \mathbb{P}(T^0_{1\to 2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ N_{2\to 1} \geqslant i,\ T^i_{1\to 2} \geqslant c(\varepsilon)) \\
&\quad \leqslant \sum_{i=1}^{\Delta(\varepsilon)} \mathbb{E}(1_{\{T^0_{1\to 2} > a(\varepsilon), N_{2\to 1} \geqslant i\}} \mathbb{P}(N_2 \leqslant \Delta(\varepsilon), T^i_{1\to 2} \geqslant c(\varepsilon) | \mathcal{F}_{\tau^i_{2\to 1}})),
\end{aligned} \tag{5.20}$$

where $\tau^i_{2\to 1}$ is defined by (5.10). We recall that $\nu_2(n)$ denotes the number of visits of state 2 up to time n included. On $N_{2\to 1} \geqslant i$, $N_2 \geqslant \nu_2(\tau^i_{2\to 1} + T^i_{1\to 2})$ and therefore, by using the strong Markov property of the chain $((X_n, \theta_n))_{n\geqslant 0}$, we obtain that, on the event $\{N_{2\to 1} \geqslant i\}$,

$$\begin{aligned}
&\mathbb{P}(N_2 \leqslant \Delta(\varepsilon), T^i_{1\to 2} \geqslant c(\varepsilon) | \mathcal{F}_{\tau^i_{2\to 1}}) \\
&\quad \leqslant \mathbb{E}(1_{\{\nu_2(\tau^i_{2\to 1}+c(\varepsilon)-2) \leqslant \Delta(\varepsilon), X_{\tau^i_{2\to 1}}=1, \dots, X_{\tau^i_{2\to 1}+c(\varepsilon)-2}=1\}} \mathbb{P}(X_{\tau^i_{2\to 1}+c(\varepsilon)-1} = 1 | \mathcal{F}_{\tau^i_{2\to 1}+c(\varepsilon)-2}) | \mathcal{F}_{\tau^i_{2\to 1}}) \\
&\quad = \mathbb{E}(1_{\{\nu_2(\tau^i_{2\to 1}+c(\varepsilon)-2) \leqslant \Delta(\varepsilon), X_{\tau^i_{2\to 1}}=1, \dots, X_{\tau^i_{2\to 1}+c(\varepsilon)-2}=1\}} (1 - P_{\theta_{\tau^i_{2\to 1}+c(\varepsilon)-2}}(1,2)) | \mathcal{F}_{\tau^i_{2\to 1}}).
\end{aligned} \tag{5.21}$$

We recall that

$$P_{\theta_n}(1,2) = \frac{1}{3}\left(\varepsilon \frac{\tilde{\theta}_n(1)}{\tilde{\theta}_n(2)} \wedge 1 \right).$$

On the event $\{T^0_{1\to 2} > a(\varepsilon)\}$, we have, for $n \geqslant a(\varepsilon)$, $\tilde{\theta}_n(1) \geqslant \Xi_{a(\varepsilon)}$, so that $P_{\theta_n}(1,2) \geqslant \frac{\varepsilon \Xi_{a(\varepsilon)}}{3\tilde{\theta}_n(2)} \wedge \frac{1}{3}$. Since $\Delta(\varepsilon) = \mathrm{O}(a(\varepsilon)^\alpha)$, by Lemma 5.5, there exist constants $M \in (0, +\infty)$ and $\bar{\varepsilon} \in (0,1)$ such that for

$$\forall \varepsilon \in (0, \bar{\varepsilon}),\ \text{on the event } \{T^0_{1\to 2} > a(\varepsilon)\},\ \forall n \text{ s.t. } \nu_2(n) \leqslant \Delta(\varepsilon),\ \tilde{\theta}_n(2) \leqslant M. \tag{5.22}$$

As a consequence, for $\varepsilon \in (0, \bar{\varepsilon})$, on the event $\{T^0_{1\to 2} > a(\varepsilon)\} \cap \{N_{2\to 1} \geqslant i\} \cap \{\nu_2(\tau^i_{2\to 1} + c(\varepsilon) - 2) \leqslant \Delta(\varepsilon)\}$, $\tilde{\theta}_{\tau^i_{2\to 1}+c(\varepsilon)-2}(2) \leqslant M$ and therefore $P_{\theta_{\tau^i_{2\to 1}+c(\varepsilon)-2}}(1,2) \geqslant \frac{\varepsilon \Xi_{a(\varepsilon)}}{3M} \wedge \frac{1}{3}$. Since, from (5.15),

$\varepsilon \Xi_{a(\varepsilon)} \leqslant \exp(-\beta(\varepsilon))$ which goes to zero as ε goes to 0, we deduce that, up to diminishing $\bar{\varepsilon}$, for any $\varepsilon \in (0, \bar{\varepsilon})$,

$$P_{\theta_{\tau^i_{2\to1}+c(\varepsilon)-2}}(1,2) \geqslant \frac{\varepsilon \Xi_{a(\varepsilon)}}{3\tilde{M}} \text{ on the event } \{T^0_{1\to2} > a(\varepsilon)\} \cap \{N_{2\to1} \geqslant i\} \cap \{\nu_2(\tau^i_{2\to1} + c(\varepsilon) - 2) \leqslant \Delta(\varepsilon)\}.$$

With (5.21), we deduce that on $\{T^0_{1\to2} > a(\varepsilon)\} \cap \{N_{2\to1} \geqslant i\}$,

$$\mathbb{P}(N_2 \leqslant \Delta(\varepsilon),\ T^i_{1\to2} \geqslant c(\varepsilon) | \mathcal{F}_{\tau^i_{2\to1}}) \leqslant \mathbb{E}\left(1_{\{\nu_2(\tau^i_{2\to1}+c(\varepsilon)-3)\leqslant\Delta(\varepsilon), X_{\tau^i_{2\to1}}=1,\dots,X_{\tau^i_{2\to1}+c(\varepsilon)-3}=1\}} \left(1 - \frac{\varepsilon \Xi_{a(\varepsilon)}}{3M}\right)(1 - P_{\theta_{\tau^i_{2\to1}+c(\varepsilon)-3}}(1,2)) \middle| \mathcal{F}_{\tau^i_{2\to1}} \right).$$

Iterating the reasoning, we obtain that, on $\{T^0_{1\to2} > a(\varepsilon)\} \cap \{N_{2\to1} \geqslant i\}$,

$$\mathbb{P}(N_2 \leqslant \Delta(\varepsilon),\ T^i_{1\to2} \geqslant c(\varepsilon) | \mathcal{F}_{\tau^i_{2\to1}}) \leqslant \left(1 - \frac{\varepsilon \Xi_{a(\varepsilon)}}{3M}\right)^{c(\varepsilon)-1}.$$

With (5.20) and the definition of $c(\varepsilon)$, we deduce that

$$\mathbb{P}\left(T^0_{1\to2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to1}} T^i_{1\to2} \geqslant b(\varepsilon) - \Delta(\varepsilon) - \tilde{b}(\varepsilon) \right) \leqslant \Delta(\varepsilon) \exp\left(\left(\left\lceil \frac{b(\varepsilon) - \tilde{b}(\varepsilon)}{\Delta(\varepsilon)} \right\rceil - 2 \right) \ln\left(1 - \frac{\varepsilon \Xi_{a(\varepsilon)}}{3M}\right) \right) \tag{5.23}$$

For $\alpha \in [\frac{1}{2}, 1)$, we deduce that

$$\mathbb{P}\left(T^0_{1\to2} \in (a(\varepsilon), \tilde{b}(\varepsilon)),\ N_2 \leqslant \Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to1}} T^i_{1\to2} \geqslant b(\varepsilon) - \Delta(\varepsilon) - \tilde{b}(\varepsilon) \right) \leqslant \Delta(\varepsilon) \exp\left(-K \frac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{1/(1-\alpha)} \varepsilon \Xi_{a(\varepsilon)} \right)$$

for some positive constant $K > 0$. We conclude by (5.16), which ensures

$$\frac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{1/(1-\alpha)} \varepsilon \Xi_{a(\varepsilon)} \geqslant C \frac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{1/(1-\alpha)} \varepsilon \exp\left(\frac{\gamma_\star}{1-\alpha} a(\varepsilon)^{1-\alpha} \right) = C \frac{1}{\Delta(\varepsilon)} |\ln \varepsilon|^{1/(1-\alpha)} \exp(-\beta(\varepsilon)),$$

for $\alpha \in (\frac{1}{2}, 1)$ and

$$\begin{aligned}\frac{1}{\Delta(\varepsilon)}|\ln\varepsilon|^{1/(1-\alpha)}\varepsilon\Xi_{a(\varepsilon)} &\geqslant C\frac{1}{\Delta(\varepsilon)}|\ln\varepsilon|^2\varepsilon\exp\left(2\gamma_\star\sqrt{a(\varepsilon)}-\frac{\gamma_\star^2}{2}\ln(a(\varepsilon))\right)\\ &= C\frac{1}{\Delta(\varepsilon)}|\ln\varepsilon|^2\exp(-\beta(\varepsilon))(|\ln\varepsilon|-\beta(\varepsilon))^{-\gamma_\star^2}\\ &\geqslant C\frac{1}{\Delta(\varepsilon)}|\ln\varepsilon|^{2-\gamma_\star^2}\exp(-\beta(\varepsilon)),\end{aligned}$$

for $\alpha = \frac{1}{2}$.

When $\alpha = 1$, (5.23) implies

$$\begin{aligned}&\mathbb{P}\left(T^0_{1\to 2}\in(a(\varepsilon),\tilde{b}(\varepsilon)),\ N_2\leqslant\Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to 1}}T^i_{1\to 2}\geqslant b(\varepsilon)-\Delta(\varepsilon)-\tilde{b}(\varepsilon)\right)\\ &\leqslant\Delta(\varepsilon)\exp\left(\left(\frac{g(\varepsilon)-\tilde{g}(\varepsilon)}{\Delta(\varepsilon)}\varepsilon^{-1/(1+\gamma_\star)}-2\right)\ln\left(1-\frac{\varepsilon\Xi_{a(\varepsilon)}}{3M}\right)\right).\end{aligned}$$

Using the fact that, by (5.13), there exists a constant C independent of ε such that

$$\varepsilon\Xi_{a(\varepsilon)}\leqslant C f(\varepsilon)^{\gamma_\star}\varepsilon^{1/(1+\gamma_\star)},$$

so that the left-hand side goes to zero when ε goes to zero, we obtain (the constants C, C' are independent from ε small enough, and their values may change from one occurrence to another)

$$\begin{aligned}&\mathbb{P}\left(T^0_{1\to 2}\in(a(\varepsilon),\tilde{b}(\varepsilon)),\ N_2\leqslant\Delta(\varepsilon),\ \sum_{i=1}^{N_{2\to 1}}T^i_{1\to 2}\geqslant b(\varepsilon)-\Delta(\varepsilon)-\tilde{b}(\varepsilon)\right)\\ &\leqslant C'\Delta(\varepsilon)\exp\left(-C\frac{g(\varepsilon)-\tilde{g}(\varepsilon)}{\Delta(\varepsilon)}\varepsilon^{-1/(1+\gamma_\star)}\varepsilon\Xi_{a(\varepsilon)}\right)\\ &\leqslant C'\Delta(\varepsilon)\exp\left(-C\frac{g(\varepsilon)-\tilde{g}(\varepsilon)}{\Delta(\varepsilon)}f(\varepsilon)^{\gamma_\star}\right).\end{aligned}$$

■

6 Discussion of the Successive Exit Times of the Metastable States

In this section, we consider the scaling of the successive transition times back and forth between states 1 and 3, and not only of the first transition time from 1 to 3. For the sake of conciseness, we do not provide complete proofs of the results, but only indicate how to adapt the previous reasoning to the successive exit times.

For the nonadaptive dynamics $\{\bar{X}_n,\ n\geq 0\}$, the analysis is very easy. Let $\bar{T}_{3\to 1}$ denote the time between $\bar{T}_{1\to 3}$ and the first subsequent return to state 1 : $\bar{T}_{3\to 1} = \min\{n > \bar{T}_{1\to 3} : \bar{X}_n = 1\} - \bar{T}_{1\to 3}$. Of course by symmetry, the asymptotic behavior of $\varepsilon\bar{T}_{3\to 1}$ as $\varepsilon\to 0$

is the same as the one of $\varepsilon \bar{T}_{1\to 3}$ given by Proposition 3.1: $\varepsilon \bar{T}_{3\to 1}$ scales like $6/\varepsilon$ and converges in distribution to an exponential random variable with parameter $1/6$. And more generally, all the successive durations needed by the Metropolis–Hastings algorithm to go from one of the extremal states 1 and 3 to the other scale like $6/\varepsilon$.

Let us now discuss the successive exit times of the Wang–Landau algorithm. We first consider the easier case $\alpha \in [\frac{1}{2}, 1)$ in Section 6.1, which is illustrated by numerical experiments in Section 6.2. We finally discuss the case $\alpha = 1$ in Section 6.3.

6.1 Successive exit times of the Wang–Landau algorithm for $\alpha \in [\frac{1}{2}, 1)$

Setting $n(\varepsilon) = (\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)} |\ln \varepsilon|^{1/(1-\alpha)}$, one has $T_{1\to 3} \sim n(\varepsilon)$ according to Proposition 3.2. Let $T_{3\to 1}$ denote the time between $T_{1\to 3}$ and the first subsequent return to state 1 : $T_{3\to 1} = \min\{n > T_{1\to 3} : X_n = 1\} - T_{1\to 3}$. To analyze the asymptotic behavior of $T_{3\to 1}$ as $\varepsilon \to 0$, one needs the vector $\tilde{\theta}_{T_{1\to 3}}$ of unnormalized weights at time $T_{1\to 3}$. One has $\tilde{\theta}_{T_{1\to 3}}(3) = 1 + \gamma_\star T_{1\to 3}^{-\alpha} = 1 + o(1)$. By the proof of Proposition 3.2 (see in particular Lemma 5.2 and (5.22)), there is a finite constant M such that $\lim_{\varepsilon\to 0} \mathbb{P}(\tilde{\theta}_{T_{1\to 3}}(2) \leqslant M) = 1$. Last, since before time $T_{1\to 3}$, the algorithm stays in state 1 at least during the time interval $[0, T_{1\to 2} - 1]$ and at most during the time interval $[0, T_{1\to 3} - 2]$,

$$\Xi_{T^0_{1\to 2}-1} \leqslant \tilde{\theta}_{T^0_{1\to 2}}(1) \leqslant \tilde{\theta}_{T_{1\to 3}}(1) \leqslant \Xi_{T_{1\to 3}-2}. \tag{6.1}$$

For $c \in (1, +\infty)$, choosing $C_a = (\frac{1-\alpha}{c\gamma_\star})^{1/(1-\alpha)}$ and $C_b = (\frac{c(1-\alpha)}{\gamma_\star})^{1/(1-\alpha)}$, one deduces by Lemma 5.2, Proposition 3.2, and (5.14), that

$$\lim_{\varepsilon\to 0} \mathbb{P}\left(\frac{1}{c}|\ln \varepsilon| \leqslant \ln(\tilde{\theta}_{T_{1\to 3}}(1)) \leqslant c|\ln \varepsilon|\right) = 1.$$

This means that $\tilde{\theta}_{T_{1\to 3}}(1)$ is approximately of order $\frac{1}{\varepsilon}$. We will perform the analysis of $T_{3\to 1}$, under the simplifying assumption that $\tilde{\theta}_{T_{1\to 3}}(1) \leqslant \frac{C}{\varepsilon}$ so that, as long as state 1 has not been reached again after $T_{1\to 3}$, the transition probability from state 2 to state 1 remains of order 1. Then the only difference with the analysis of $T_{1\to 3}$ is that the step sizes of the Wang–Landau algorithm have been shifted into $(\frac{\gamma_\star}{(T_{1\to 3}+n)^\alpha})_{n\geqslant 1}$. Repeating the analysis performed in the proof of Lemma 5.2, we see that the time $T^0_{3\to 2}$ needed by the algorithm to reach again state 2 will be of order $n_2(\varepsilon)$ such that

$$\sum_{k=n(\varepsilon)}^{n_2(\varepsilon)} \exp\left(\sum_{j=n(\varepsilon)}^{k} \frac{\gamma_\star}{j^\alpha}\right) = O\left(\frac{1}{\varepsilon}\right).$$

This condition gives $n_2(\varepsilon) \sim (\frac{2(1-\alpha)}{\gamma_\star})^{1/(1-\alpha)} |\ln \varepsilon|^{1/(1-\alpha)}$. So, repeating the arguments given in the proof of Proposition 3.2, one expects that $T_{3\to 1}$ is of order $(\frac{2(1-\alpha)}{\gamma_\star})^{1/(1-\alpha)} |\ln \varepsilon|^{1/(1-\alpha)}$

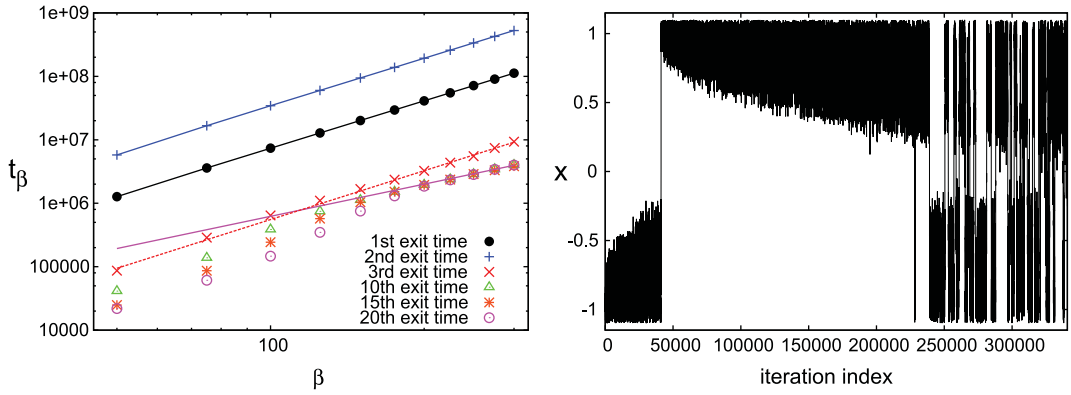

Fig. 5. Left: Scaling of successive exit times as a function of the inverse temperature (in log–log scale) in the case $\alpha = 0.6$ and $\gamma_\star = 1$. The first three exit times are of the same order of magnitude. All the subsequent exit times have similar orders of magnitudes. The exit times starting from the third one are much smaller than the first two. Right: Typical trajectory for $\beta = 15$ when $\alpha = 0.6$ and $\gamma_\star = 1$. Note how the system first explores the two metastability basins before more freely switching from one basin to the other.

and that $\tilde{\theta}_{T_{1\to 3}+T_{3\to 1}}(2)$ remains bounded. Moreover, one also expects that $\tilde{\theta}_{T_{1\to 3}+T_{3\to 1}}(3)$ is approximately of order $\frac{1}{\varepsilon}$.

At time $T_{1\to 3} + T_{3\to 1}$, one has $\tilde{\theta}_{T_{1\to 3}+T_{3\to 1}}(2)$ bounded uniformly in ε whereas $\tilde{\theta}_{T_{1\to 3}+T_{3\to 1}}(1)$ and $\tilde{\theta}_{T_{1\to 3}+T_{3\to 1}}(3)$ are both approximately of order $\frac{1}{\varepsilon}$ so that every entry in the transition matrix $P_{\theta_{T_{1\to 3}+T_{3\to 1}}}$ but the ones with indices $(1,3)$ and $(3,1)$ are approximately of order 1. So one expects, that after time $T_{1\to 3} + T_{3\to 1}$ which is of order $(1 + 2^{1/(1-\alpha)})(\frac{1-\alpha}{\gamma_\star})^{1/(1-\alpha)} |\ln \varepsilon|^{1/(1-\alpha)}$, the Wang–Landau algorithm has got rid of the initial metastability and moves freely from any of the extremal states 1 and 3 to the other one with the only constraint of going through state 2.

6.2 Numerical results

The above theoretical results on the scaling of the exit times for a simple three-state model can be numerically checked for the model presented in Section 4. We present in Figure 5 the average successive exit times as a function of the inverse temperature in the case $\alpha = 0.6$ and $\gamma_\star = 1$, as well as a typical trajectory in order to visualize more clearly the qualitative behavior of the system. We denote by t_β^k the average kth exit time, obtained by averaging exit times obtained for $M = 10^5$ independent realizations for the smallest values of β, and a few thousands for the largest values of β (the other

parameters being the same as in Section 4.4, namely $R = 1.1$, $d = 22$, $\upsilon = 0.1$). The time t_β^1 is the first transition time t_β introduced in Section 4, t_β^2 is the average of the first transition time from the value $x_1 = 1$ back to $x_1 = -1$, t_β^3 is the average of the second transition time from the value $x_1 = -1$ to $x_1 = 1$, and so forth. Our numerical results show that

$$t_\beta^k \sim C_k \beta^a$$

with $a = 2.5$ for $k = 1, 2, 3$, while $a \simeq 1.7$ for $k \geqslant 4$. Several conclusions can be drawn. First, the first two exit times indeed have the same scaling, as expected from the analysis in the previous section. Moreover, the subsequent exit times (except for the third one) also have the same scalings, but are much shorter in average than the first two exit times. They are however still growing with β. This is due to the fact that, in this case which is more complex than the simple three-state model, some metastability remains, as illustrated by Figure 1(Right): there are still energy (or free energy) barriers to cross, even for the biased potential.

6.3 Successive exit times of the Wang–Landau algorithm for $\alpha = 1$

In the case $\alpha = 1$, by Proposition 3.2, $T_{1\to 3}$ is approximately of order $n(\varepsilon) = \varepsilon^{-1/(1+\gamma_\star)}$. One still has $\tilde\theta_{T_{1\to 3}}(3) = 1 + \gamma_\star T_{1\to 3}^{-1} = 1 + \mathrm{o}(1)$ and $\tilde\theta_{T_{1\to 3}}(2)$ bounded uniformly in ε small enough. Moreover, (6.1), Proposition 3.2, Lemma 5.2, and (5.13), imply that for any function h such that $\lim_{\varepsilon\to 0} h(\varepsilon) = +\infty$,

$$\lim_{\varepsilon\to 0} \mathbb{P}(h(\varepsilon)^{-\gamma_\star}\varepsilon^{-\gamma_\star/(1+\gamma_\star)} \leqslant \tilde\theta_{T_{1\to 3}}(1) \leqslant h(\varepsilon)^{\gamma_\star}\varepsilon^{-\gamma_\star/(1+\gamma_\star)}) = 1.$$

In particular, $\tilde\theta_{T_{1\to 3}}(1) \leqslant \frac{C}{\varepsilon}$. Now, the time $T_{3\to 2}^0$ needed by the algorithm to reach again state 2 will be of order $n_2(\varepsilon)$ such that $\sum_{k=n(\varepsilon)}^{n_2(\varepsilon)} \prod_{j=n(\varepsilon)}^{k}(1 + \frac{\gamma_\star}{j}) = \mathrm{O}(\frac{1}{\varepsilon})$. With this condition, we deduce that $T_{3\to 2}^0$ and $T_{3\to 1}$ will be approximately of order $\epsilon^{-\frac{1+2\gamma_\star}{(1+\gamma_\star)^2}}$. As a consequence $T_{1\to 3} = \mathrm{o}(T_{3\to 1})$, which we could guess from the explosion as $\alpha \to 1$ of the factor $2^{1/(1-\alpha)}$ appearing in the analysis for $\alpha \in [\frac{1}{2}, 1)$. Now, while $\tilde\theta_{T_{1\to 3}+T_{3\to 1}}(2)$ remains bounded, $\tilde\theta_{T_{1\to 3}+T_{3\to 1}}(1)$ is approximately of order $\varepsilon^{-\gamma_\star/(1+\gamma_\star)}$ while $\tilde\theta_{T_{1\to 3}+T_{3\to 1}}(3)$ is approximately of order $\prod_{j=n(\varepsilon)}^{n_2(\varepsilon)}(1 + \frac{\gamma_\star}{j})$, that is, of order $\varepsilon^{-(\frac{\gamma_\star}{1+\gamma_\star})^2}$. So there remains some metastability preventing the algorithm to move quickly from any of the extremal states to the other one. For instance, the time it will need after $T_{1\to 3} + T_{3\to 1}$ to go back to state 3 will be approximately of order $\varepsilon^{-(1+2\gamma_\star+2\gamma_\star^2)/(1+\gamma_\star)^3}$, which is intermediate between the orders of $T_{1\to 3}$ and $T_{3\to 1}$. Next, it will take a time of approximate order $\varepsilon^{-(1+2\gamma_\star)/(1+\gamma_\star)^2}$ to go back to state 1 and the next transition times should be smaller since the orders of $\tilde\theta(1)$ and $\tilde\theta(3)$ have increased but the shift in the sequence of step sizes is only multiplied by a constant.

Acknowledgement

We thank Eric Moulines for stimulating discussions.

Funding

This work was supported by the French National Research Agency under the grants ANR-09-BLAN-0216-01 (MEGAS) and ANR-08-BLAN-0218 (BigMC).

References

[1] Atchade, Y. F. and J. S. Liu. "The Wang–Landau algorithm for Monte Carlo computation in general state spaces." *Statistica Sinica* 20, no. 1 (2010): 209–33.

[2] Babin, V., C. Roland, and C. Sagui. "Adaptively biased molecular dynamics for free energy calculations." *Journal of Chemical Physics* 128, no. 13 (2008): 134101.

[3] Bornn, L., P. Jacob, P. Del Moral, and A. Doucet. "An adaptive interacting Wang–Landau algorithm for automatic density exploration." *Journal of Computational and Graphical Statistics* 22, no. 3 (2013): 749–73.

[4] Chopin, N., T. Lelièvre, and G. Stoltz. "Free energy methods for efficient exploration of mixture posterior densities." *Statistics and Computing* 22, no. 4 (2012): 897–916.

[5] Darve, E. and A. Pohorille. "Calculating free energies using average force." *Journal of Chemical Physics* 115, no. 20 (2001): 9169–83.

[6] Fort, G., B. Jourdain, E. Kuhn, T. Lelièvre, and G. Stoltz. "Convergence of the Wang–Landau algorithm." *Mathematics of Computation*, (2014).

[7] Hastings, W. K. "Monte Carlo sampling methods using Markov chains and their applications." *Biometrika* 57, no. 1 (1970): 97–109.

[8] Hénin, J. and C. Chipot. "Overcoming free energy barriers using unconstrained molecular dynamics simulations." *Journal of Chemical Physics* 121, no. 7 (2004): 2904–14.

[9] Jacob, P. E. and R. J. Ryder. "The Wang–Landau algorithm reaches the Flat Histogram criterion in finite time." *The Annals of Applied Probability* 24, no. 1 (2014): 34–53.

[10] Lelièvre, T. and K. Minoukadeh. "Longtime convergence of an adaptive biasing force method: The bi-channel case." *Archive for Rational Mechanics and Analysis* 202, no. 1 (2011): 1–34.

[11] Lelièvre, T., M. Rousset, and G. Stoltz. "Computation of free energy profiles with adaptive parallel dynamics." *Journal of Chemical Physics* 126, no. 13 (2007): 134111.

[12] Lelièvre, T., M. Rousset, and G. Stoltz. "Long-time convergence of an adaptive biasing force method." *Nonlinearity* 21, no. 6 (2008): 1155–81.

[13] Lelièvre, T., M. Rousset, and G. Stoltz. *Free-Energy Computations: A Mathematical Perspective*. London: Imperial College Press, 2010.

[14] Liang, F. "A generalized Wang–Landau algorithm for Monte Carlo computation." *Journal of the American Statistical Association* 100, no. 472 (2005): 1311–27.

[15] Liang, F., C. Liu, and R. J. Carroll. "Stochastic Approximation in Monte Carlo Computation." *Journal of the American Statistical Association* 102, no. 477 (2007): 305–20.

[16] Metropolis, N., A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller. "Equations of state calculations by fast computing machines." *Journal of Chemical Physics* 21, no. 6 (1953): 1087–91.

[17] Park, S., M. K. Sener, D. Lu, and K. Schulten. "Reaction paths based on mean first-passage times." *Journal of Chemical Physics* 119, no. 3 (2003): 1313–9.

[18] Wang, F. and D. P. Landau. "Determining the density of states for classical statistical models: A random walk algorithm to produce a flat histogram." *Physical Review E* 64, no. 5 (2001): 056101.

[19] Wang, F. G. and D. P. Landau. "Efficient, multiple-range random walk algorithm to calculate the density of states." *Physical Review Letters* 86, no. 10 (2001): 2050–3.