Probab. Theory Relat. Fields 111, 215–251 (1998)

Probability Theory and Related Fields

Fluctuations of empirical means at low temperature for finite Markov chains with rare transitions in the general case

Isabelle Gaudron[1,2], **Alain Trouvé**[2,1]

[1] CMLA, Ecole Normale Supérieure de Cachan 61, Av. du Président Wilson, F-94235 Cachan Cedex France
[2] Université Paris 13, LAGA, UMR 7539, Avenue Jean-Baptiste Clément, F-93430 Villetaneuse, France

Received 5 August 1996 / In revised form: 6 August 1997

Summary. The integrated autocovariance and autocorrelation time are essential tools to understand the dynamical behavior of a Markov chain. We study here these two objects for Markov chains with rare transitions with no reversibility assumption. We give upper bounds for the autocovariance and the integrated autocorrelation time, as well as exponential equivalents at low temperature. We also link their slowest modes with the underline energy landscape under mild assumptions. Our proofs will be based on large deviation estimates coming from the theory of Wentzell and Freidlin and others [4, 3, 12], and on coupling arguments (see [6] for a review on the coupling method).

Mathematics Subject Classification (1991): 60F05, 60F10, 60J10, 60M10, 65C05

Keywords: Autocorrelation time – Central limit theorem – Large deviations – Monte Carlo methods

Correspondence to: gaudron@cmla.ens-cachan.fr and trouve@math.univ-paris13.fr

1. Introduction

Consider a family of Markov kernels $(Q_\beta)_{\beta\geq 0}$ on a finite configuration space E. Assume that parameter β plays the role of the inverse of a temperature and that the transitions $Q_\beta(i,j)$ are exponentially vanishing with the inverse of the temperature. More precisely, assume that there exist $\kappa \geq 1$, an irreducible Markov kernel q on E called the communication kernel and $V\colon E \times E \to \mathbb{R}_+ \cup \{+\infty\}$ called the communication cost such that for any $i, j \in E$ we have

$$\tfrac{1}{\kappa} q(i,j)\mathrm{e}^{-V(i,j)\beta} \leq Q_\beta(i,j) \leq \kappa q(i,j)\mathrm{e}^{-V(i,j)\beta} \quad , \tag{1}$$

where we have done the convention that $V(i,j) = +\infty$ iff $q(i,j) = 0$. This framework has been introduced before by Freidlin and Wentzell in their study of small random perturbations of dynamical systems [4]. Such a family $(Q_\beta)_{\beta\geq 0}$ will be called an admissible family. Note that we do not assume any reversibility property of the kernels Q_β so that it extends widely the usual reversible framework of Monte Carlo simulations.

Now, let $h\colon E \to \mathbb{R}$ be any non constant function (real valued observable) on E. If for any $\beta \geq 0$, μ_β denotes the unique equilibrium probability measure of Q_β on E, we consider the problem of the computation of $\mu_\beta(h) = \sum_{i\in E} \mu_\beta(i)h(i)$. Usually, $\mu_\beta(h)$ cannot be computed directly (the explicit expression in terms of $\{i\}$-graphs [4] is too complicated to be used numerically) but should be estimated through the empirical mean on a sample $X_0, \dots, X_{n-1}$ of the Markov chain with transition matrix Q_β and any arbitrary initial probability measure ν

$$S_n(h) = \frac{1}{n}\sum_{k=0}^{n-1} h(X_k) \quad .$$

The rate of convergence of the estimator $S_n(h)$ is given by the central limit Theorem [1]

$$\Phi_n(h) \underset{\text{def}}{=} \sqrt{n}\big(S_n(h) - \mu_\beta(h)\big) \Rightarrow \mathcal{N}(0, 2c_{\text{int},h}) \quad ,$$

where

$$c_{\text{int},h} = \frac{1}{2}\text{Var}(h(X_0)) + \sum_{k=1}^{\infty} \text{cov}(h(X_0), h(X_k))$$

is called the autocovariance of h. Note that this limit does not depend on the initial probability measure ν so that we will assume in the sequel that $\nu = \mu_\beta$. The autocovariance gives us the asymptotical range of the fluctuations of the empirical mean against the length of the sample. Now, if we want to compare these normalized fluctuations with those obtained through an i.i.d sample $h(Y_0), \ldots, h(Y_{n-1})$ of probability law $h \circ \mu_\beta$, we have to introduce the normalized fluctuations given by

$$\Psi_n(h) \underset{\text{def}}{=} \sqrt{n}\left(\frac{S_n(h) - \mu_\beta(h)}{\text{Var}(h(X_0))^{1/2}}\right) ,$$

for which we have $\Psi_n(h) \Rightarrow \mathcal{N}(0, 2\rho_{\text{int},h})$, where $\rho_{\text{int},h} = c_{\text{int},h}/\text{Var}(h(X_0))$ is called the integrated autocorrelation time of h as defined by Sokal in [10]. Roughly speaking, the rate $n/(2\rho_{\text{int},h})$ can be interpreted as the number of "independent" sampling values among the $h(X_k)$'s.

The study of the integrated autocovariances and autocorrelation times is crucial to compare different Markovian dynamics which have the same equilibrium probability measure. We refer in particular to a work of one of the authors which concerns the comparison of the Swendsen-Wang and Metropolis dynamics [5], and which has raised some of the questions we will answer in this paper. The first problem which had to be faced was to find the functions which could give the slowest rates of convergence towards equilibrium, and especially to link these functions with the energy landscapes. The second problem was to compare the behaviors of these dynamics when applied to the same interesting observables h. This led naturally to the comparison of associated empirical distributions for the construction of Kolmogorov-Smirnov tests ([1]). A third problem was to estimate precisely the integrated autocovariance and autocorrelation times. This statistical problem will not be answered here.

We will study in this paper the behaviors of $\rho_{\text{int},h}$ and $c_{\text{int},h}$ at small temperature, i.e. at large β. We will be interested in the values of

$$\overline{I_h} \underset{\text{def}}{=} \limsup_{\beta\to\infty} \tfrac{1}{\beta}\ln(c_{\text{int},h}) \text{ and } \overline{H_h} \underset{\text{def}}{=} \limsup_{\beta\to\infty} \tfrac{1}{\beta}\ln(\rho_{\text{int},h}) ,$$

(see the discussion section 6 about the existence of a true limit for the above quantities) as well as in the slowest modes of Φ and Ψ, i.e. functions h maximizing $\overline{I_h}$ or $\overline{H_h}$.

This problem has been almost completely solved. Let us first introduce the virtual energy $U: E \to \mathbb{R}^+$ defined by $U(i) = \lim_{\beta\to+\infty} -\frac{1}{\beta}\ln(\mu_\beta(i))$ (the existence of this limit follows from a well known result of Wentzell and Freidlin [4]). We give upper-bounds for $\overline{I_h}$ and $\overline{H_h}$, denoted I and H_0, explicitly defined in function of the communication costs $V(i,j)$'s (see Theorem 2 (i) and 3 (i)). Now, if we look more precisely at functions which do not distinguish the different ground states (i.e. configurations $i \in F(E) =_{\text{def}} \{j \in E | \, U(j) = 0\}$), then we show that there exist I^* and H^* such that $\overline{I_h} \leq I^*$ and $\overline{H_h} \leq H^*$. We give in Theorems 2 and 3 sufficient conditions for equality under weak conditions on the energy landscape, (for instance these conditions hold when $F(E)$ is a singleton). We deduce that for the energy function U, $c_{\text{int},U} \propto \exp(I^*\beta)$, but, except in very particular situations, $\overline{H_U} < H^*$. We also give the exponential equivalent of $\rho_{\text{int},U}$ at low temperature in corollary 3: even in the case where the energy U has a unique global minimum, the constant H^* does not govern the normalized fluctuations of $S_n(U)$. However, looking at the energy level functions $U_\lambda = 1_{U \geq \lambda}$, we show that $\rho_{\text{int},U_\lambda} \propto \exp(H^*\beta)$ iff λ belongs to some explicitly given critical set Λ_* (see corollary 2). An important consequence is that this critical constant H^* can not be estimated through the computation of $\rho_{\text{int},U}$, but we have to compute the different $\rho_{\text{int},U_\lambda}$'s!

As a consequence, if we look now for an estimate of the distribution function $F_U(\lambda) =_{\text{def}} \mu_\beta(U_\lambda)$, we get that there exists $C_0 \geq 0$ such that for any $C > C_0$, there exists $0 < \alpha_1 \leq \alpha_2 < 1$ such that

$$\left.\begin{array}{l} \alpha_1 \leq \liminf\limits_{\beta\to+\infty} \liminf\limits_{n\to+\infty} P\left(\sqrt{\exp(-m\beta)} \sup\limits_{\lambda>0} |\Psi_n(U_\lambda)| \geq C\right) \\ \leq \limsup\limits_{\beta\to+\infty} \limsup\limits_{n\to+\infty} P\left(\sqrt{\exp(-m\beta)} \sup\limits_{\lambda>0} |\Psi_n(U_\lambda)| \geq C\right) \leq \alpha_2 \end{array}\right\} \text{iff } m = H^* \ . \tag{2}$$

Hence, the range of the fluctuations of $\sup_{\lambda>0} |\Psi_n(U_\lambda)|$ is given by $\sqrt{\exp(\beta H^*)}$.

Note that this constant H^* is the largest potential barrier which separates a configuration $i \notin F(E)$ from $F(E)$.

Let us emphasize the methods employed to tackle the above mentioned problems. In the reversible case, we can express $\rho_{\text{int},h}$ through the eigenvalues of Q_β, and deduce an upper-bound which depends on the spectral gap of Q_β. More precisely, following Sokal in [10], if $\text{Eig}(\beta)$ is the set of all the eigenvalues $\gamma < 1$ of Q_β, there exists a probability measure ν_h (depending on β) on $\text{Eig}(\beta)$ such that we have the spectral representation $\rho_{\text{int},h} = \frac{1}{2}\int(1+\gamma/1-\gamma)\, d\nu_h(\gamma)$. Hence, using convexity and monotonicity of $\gamma \mapsto 1+\gamma/1-\gamma$, we get

$$\frac{1}{2}\left(\frac{1+\gamma_{\text{mean}}}{1-\gamma_{\text{mean}}}\right) \leq \rho_{\text{int},h} \leq \frac{1}{2}\left(\frac{1+\gamma_*}{1-\gamma_*}\right) \ , \tag{3}$$

where γ_* is the greatest eigenvalue in $\text{Eig}(\beta)$ and $\gamma_{\text{mean}} = \int \gamma \, d\nu_h(\gamma)$. Without precise information on the spectral measure ν_h, the inequalities (3) cannot lead to precise estimates of $\rho_{\mathrm{int},h}$, and a precise study of v_h is strongly dependent on the precise structure of the eigenvectors which is not completely understood (for some major steps in this direction see [7]). Note also that this analytical method gives us only poor informations on the values of $c_{\mathrm{int},h}$ and is restricted to the reversible case. In the same spirit, another challenging point of view could be to consider that

$$c_{\mathrm{int},h} = \tfrac{1}{2}\mathscr{E}_{I-Q_\beta^* Q_\beta}(\psi_\beta, \psi_\beta),$$

where $\mathscr{E}_{I-Q_\beta^* Q_\beta}$ is the Dirichlet form associated to the (reversible) generator $I - Q_\beta^* Q_\beta$ in $L^2(\mu_\beta)$, and ψ_β is the unique solution of the Poisson equation

$$\begin{cases} (Q_\beta - I)\psi_\beta = h - \mu_\beta(h) \\ \mu_\beta(\psi_\beta) \qquad = 0. \end{cases} \tag{4}$$

However, one should again deal with the non reversible Markov kernel Q_β in the Poisson equation.

Our approach will be completely different and lies on large deviation estimates on the behavior of the Markov chain $(X_n)_{n\in\mathbb{N}}$ at low temperature initiated by Wentzell and Freidlin in [4], developed for the simulated annealing in the reversible case by Catoni in [3] and extended to general admissible families by one of the authors in [12]. Our starting point will be a usual coupling argument. More precisely, note that $c_{\mathrm{int},h} = \sum_{i,j} h(i)h(j)\widetilde{G}_{ij}$ where

$$\widetilde{G}_{ij} = \frac{1}{2}\mu_\beta(i)\left[(Q_\beta^0(i,j) - \mu_\beta(j)) + 2\sum_{k\geq 1}(Q_\beta^k(i,j) - \mu_\beta(j))\right] .$$

Instead of looking for the $\widetilde{G}_{ij}$'s, it will be more convenient to study $G_{ij} = \widetilde{G}_{ij} + \frac{1}{2}\mu_\beta(i)(Q_\beta^0(i,j) - \mu_\beta(j))$ which verifies

$$G_{ij} = \sum_{k\geq 0}\mu_\beta(i)(Q_\beta^k(i,j) - \mu_\beta(j)) . \tag{5}$$

Now, a straightforward coupling argument shows that $G_{ij} = G_{ij}^1 - G_{ij}^2$ with

$$G_{ij}^l = \mu_\beta(i)\sum_{k\geq 0}\mathrm{P}_{\delta_i\otimes\mu_\beta}\big(X_k^l = j, T_r(\varDelta) > k\big) , \tag{6}$$

where $\mathrm{X} = (X_k^1, X_k^2)_{k\geq 0}$ is the coordinate process on $(E\times E)^{\mathbb{N}}$, $\mathrm{P}_{\delta_i\otimes\mu_\beta}$ is the unique probability measure on $E\times E$ equipped with its natural product σ-algebra for which X is a Markov chain with transition matrix $\mathrm{Q}_\beta = Q_\beta\otimes Q_\beta$ and initial law $\delta_i\otimes\mu_\beta$ and $T_r(\varDelta) = \inf\{k\geq 0 \mid X_k^1 = X_k^2\}$. Since

$$G^1_{ij} = \sum_{a,b} N^{j,b}_{i,a} \text{ and } G^2_{ij} = \sum_{a,b} N^{b,j}_{i,a},$$

where

$$N^{c,d}_{a,b} = \mu_\beta \otimes \mu_\beta(a,b) \sum_{k \geq 0} \mathrm{P}_{\delta_a \otimes \delta_b}(\mathrm{X}_k = (c,d), T_r(\Delta) > k) \ , \tag{7}$$

we compute estimates of the $N^{c,d}_{a,b}$'s through large deviation estimates on the law of the exit time and exit point out of subsets of $E \times E$ for the process X at low temperature.

In section 2, we recall first basic estimates on the behavior of the Markov chain at low temperature associated with an admissible family. In section 3 we state the Theorem 2 which concerns the integrated autocovariance. Section 4 is devoted to the integrated autocorrelation time. Finally, in section 5, we give the proof of these theorems, and in section 5.2 some important lemmas which rely the energy landscape of the coupling X to the initial energy landscape.

Let us mention here the work of L. Miclo on the fluctuations of $\Phi_n(h_i)$ in the simulated annealing framework and for $h_i(j) = 1_{i=j}$. In [8], the process X is assumed to start out of equilibrium and to be driven by a non constant sequence $\beta_n = \ln(1+n)/K$. Moreover, the family Q is assumed to be reversible and the underlying graph of allowed transitions ($q(i,j) > 0$) is assumed to have a tree structure. Since the cooling schedule is logarithmic decreasing, his results are of completely different nature and lie on martingale theory arguments. However, he introduces the potential function $U(i,j) = G_{ij}/\mu_\beta(i)$, and starts with an exponential upper-bound of $\sup_{i \in E} |U(i,j)|$ in β. In our work, we need more precise estimates of G_{ij} for given i and j.

2. Fundamental estimates at low temperature

Since we will work with different processes on different configuration spaces, we consider for the statement of the basic results a generic configuration space $\mathscr{E}$ on which a family $(\mathscr{Q}_\beta)_{\beta \geq 0}$ of Markov kernels is defined, satisfying for any $i, j \in \mathscr{E}$

$$\tfrac{1}{\kappa}\mathfrak{q}(i,j)\mathrm{e}^{-\mathscr{V}(i,j)\beta} \leq \mathscr{Q}_\beta(i,j) \leq \kappa\mathfrak{q}(i,j)\mathrm{e}^{-\mathscr{V}(i,j)\beta} \tag{8}$$

where, as in the introduction, $\mathfrak{q}$ is an irreducible Markov kernel on $\mathscr{E}$ called the communication kernel, $\kappa \geq 1$ and $\mathscr{V} : \mathscr{E} \times \mathscr{E} \to \mathbb{R}_+ \cup \{+\infty\}$ is the communication cost satisfying $\mathscr{V}(i,j) = +\infty$ iff $\mathfrak{q}(i,j) = 0$. We define the virtual energy $\mathscr{U}$ on $\mathscr{E}$ by $\mathscr{U}(i) = -\lim_{\beta \to +\infty} \beta^{-1} \ln(\mu_\beta(i))$ where μ_β is the unique invariant probability measure of $\mathscr{Q}_\beta$ (see [4]) (note that in our definition we have $\min_{i \in \mathscr{E}} \mathscr{U}(i) = 0$).

Definition 1. *Let $\mathfrak{q}_\infty$ be the Markov kernel on $\mathscr{E} \times \mathscr{E}$ defined by*

$$\begin{cases} \mathfrak{q}_\infty(i,j) > 0 & \text{iff } \mathscr{V}(i,j) = 0, \\ \text{and} & \\ \mathfrak{q}_\infty(i,j) = 1/n_i & \text{where } n_i = |\{j \in \mathscr{E} | \mathscr{V}(i,j) = 0\}| \quad . \end{cases}$$

We say that the family $\mathscr{Q} = (\mathscr{Q}_\beta)_{\beta \geq 0}$ is a strongly aperiodic family iff for any irreducible class C of $\mathfrak{q}_\infty$ such that $C \cap F(\mathscr{E}) \neq \emptyset$, the restriction of $\mathfrak{q}_\infty$ to *$C \times C$ is aperiodic.*

Note that if $\mathscr{Q} = (\mathscr{Q}_\beta)_{\beta \geq 0}$ is a strongly aperiodic admissible family, then for any $\beta \geq 0$, $\mathscr{Q}_\beta$ is aperiodic. Moreover, if $F(\mathscr{E})$ is a singleton, then $\mathscr{Q} = (\mathscr{Q}_\beta)_{\beta \geq 0}$ is always strongly aperiodic.

We start with some notations (for an extended presentation see [11, 12]).

Notation 1. Let $B \subset \mathscr{E}$. Let any finite family $g = (g_k)_{0 \leq k \leq n_g}$ of elements of $\mathscr{E}$ such that $g_0 = i$, $g_{n_g} = j$ and $g_k \in B$ for $0 < k < n_g$ be called a path in B from i to j. The integer n_g (depending on g) is called the length of the path g. Let $\mathrm{Pth}_B(i,j)$ denote the set of all paths in B from i to j. A path is said to be empty if its length is equal to 0.

Definition 2.

- *For any non empty path g in $\mathscr{E}$, we define*

$$A_c(g) = \sup_{0 \leq k < n_g} \mathscr{U}(g_k) + \mathscr{V}(g_k, g_{k+1}) \ ,$$

  with the convention that $A_c(g) = \mathscr{U}(g_0)$ if $n_g = 0$ i.e. $g = (g_0)$.
- *We define the communication altitude from i to j by*

$$A_c(i,j) = \inf_{g \in \mathrm{Pth}_{\mathscr{E}}(i,j)} A_c(g) \ .$$

  Moreover, for any $B \subset \mathscr{E}$, we define $A_c(i,B) = \inf_{j \in B} A_c(i,j)$.
- *We say that a non empty subset $\Pi \subset \mathscr{E}$ is a cycle if Π is a singleton or Π satisfies $\sup_{i,j \in \Pi} A_c(i,j) < \inf_{i \in \Pi, j \in \Pi^c} A_c(i,j)$. We note $\mathscr{C}(\mathscr{E})$ the set of all the cycles. Moreover, for any cycle $\Pi \in \mathscr{C}(\mathscr{E})$, we note $A_c(\Pi) = \sup_{i,j \in \Pi} A_c(i,j)$.*
- *For any cycle Π, $H_m(\Pi) = \sup_{i,j \in \Pi}(A_c(i,j) - \mathscr{U}(i))$ will be called the mixing height of Π and $H_e(\Pi) = \sup_{i \in \Pi} \inf_{j \in \Pi^c}(A_c(i,j) - \mathscr{U}(i))$ its exit height.*
- *For any $B \subset \mathscr{E}$, we define*
  $\mathscr{M}(B) = \{\Pi \in \mathscr{C}(\mathscr{E}) | \Pi \subset B$ and maximal for inclusion$\}$
  $\mathscr{M}_*(B) = \{\Pi \in \mathscr{C}(\mathscr{E}) | \Pi \subset B, \Pi \neq B$ and maximal for inclusion$\}$
  $\mathscr{U}(B) = \inf\{\mathscr{U}(i) | i \in B\}$ (potential of B),
  $F(B) = \{i \in B | \mathscr{U}(i) = \mathscr{U}(B)\}$ (bottom of B),

$H_e(B) = \sup\{H_e(\Pi) | \Pi \in \mathscr{C}(\mathscr{E}), \Pi \subset B\}$ (*exit height of B*).

Definition 3. *Let* $(\mathscr{X}_n)_{n\in\mathbb{N}}$ *be the coordinate process on* $\mathscr{E}^{\mathbb{N}}$. *For any* $\beta \geq 0$, *we denote P the unique probability measure on* $\mathscr{E}^{\mathbb{N}}$ *with its natural product σ-algebra such that* $(\mathscr{X}_n)_{n\in\mathbb{N}}$ *is a Markov chain satisfying*

- $P(\mathscr{X}_{n+1} = j | \mathscr{X}_n = i) = \mathscr{Q}_\beta(i,j)$,
- $P(\mathscr{X}_0 = i) = \nu_0(i)$ *where* ν_0 *is a fixed initial probability on* $\mathscr{E}$ *whose support is* $\mathscr{E}$.

Definition 4. *Let* $B \subset \mathscr{E}$. *We define for* $i, j \in \mathscr{E}$

$$C_B(i,j) = (\mathscr{U}(i) + \mathscr{V}(i,j) - \inf_{k\in B^c\cup\{j\}} A_c(i,k)) 1_{i\neq j},$$

$$C_B^*(i,j) = \inf\left\{ \sum_{k<n_g} C_B(g_k, g_{k+1}) | \, g \in Pth_B(i,j) \right\}.$$

Moreover, for any $D \subset \mathscr{E}$, *we note* $C_B^*(i,D) = \inf_{j\in D} C_B^*(i,j)$.

Note that, for any $i \in \mathscr{E}$, $C_B(i,i) = C_B^*(i,i) = 0$. For i and j in B, $C_B^*(i,j)$ can be interpreted as the communication cost to go from i to j without escaping from B.

Definition 5. *Let B be a subset of* $\mathscr{E}$. *We define the reaching time of B by* $T_r(B) = \inf\{n \geq 0 | \mathscr{X}_n \in B\}$ *and the exit times of B by* $T_e(B) = \inf\{n \geq 0 | \mathscr{X}_n \notin B\}$ *and* $\tau_e(B) = \inf\{n > 0 | \mathscr{X}_n \notin B\}$.

Theorem 1. *Let* $\beta \geq 0$. *There exist* $a, a' > 0, b \geq 0, c > 0, d > 0, K_1 > 0$ *and* $K_2 > 0$ *depending only on* $\mathscr{E}$, $\mathfrak{q}$ *and* κ *such that*:

(i) *For any non empty* $B \subset \mathscr{E}$, *any* $i \in \mathscr{E}$, $j \in B^c$, $i \neq j$

$$K_1 e^{-C_B^*(i,j)\beta} \leq P(\mathscr{X}_{\tau_e(B)} = j | \mathscr{X}_0 = i) \leq K_2 e^{-C_B^*(i,j)\beta}.$$

(ii) *For any* $B \subset \mathscr{E}$, *any* $n \in \mathbb{N}$ *and any* $i \in B$

$$P(T_e(B) > n | \mathscr{X}_0 = i) \leq (1+b) \exp(-an\, e^{-H_e(B)\beta}).$$

(iii) *For any* $\Pi \in \mathscr{C}(\mathscr{E})$, *any* $n \in \mathbb{N}$ *and any* $i \in \Pi$

$$P(T_e(\Pi) > n | \mathscr{X}_0 = i) \geq c \exp(-a' n e^{-H_e(\Pi)\beta}) 1_{e^{-H_e(\Pi)\beta} \leq d}.$$

Proof. This is an obvious corollary for constant cooling schedules of Theorem 4.1 and 4.7 in [12] or Theorems 1.43 and 1.46 in [11].

Let us precise now a notation we will use in this article.

Notation 2. Let $f: \mathbb{R}_+ \to \mathbb{R}$ and $g: \mathbb{R}_+ \to \mathbb{R}$ be two functions. We will say that $g \propto f$ iff there exist $\beta_0 \geq 0$, $K_1 > 0$ and $K_2 > 0$ such that, for all $\beta \geq \beta_0$, we have the inequalities

$$K_1 g(\beta) \leq f(\beta) \leq K_2 g(\beta).$$

3. Autocovariance at low temperature

This section gives our first main result which concerns the exponential equivalent of the integrated autocovariance at low temperature. We first give the basic definitions which are required to understand this result, and the different hypotheses under which it is valid. The proof will be given later on, in the last part of this paper.

Notation 3. We assume that $Q = (Q_\beta)_{\beta\geq 0}$ is a *strongly aperiodic* admissible family on a finite space E (see definition 1). Then, for any $\beta \geq 0$, we note $\mathbf{Q}_\beta = \mathrm{Q}_\beta \otimes \mathrm{Q}_\beta$, so that $\mathbf{Q} = (\mathbf{Q}_\beta)_{\beta\geq\mathbf{0}}$ becomes an admissible family of Markov kernels on $\mathbf{E} = E \times E$. Now, if U is the virtual energy, $F(E)$ the bottom of E, $A_c(.,.)$ the communication altitude, $V(.,.)$ the communication cost associated with the family Q, we note $\mathbf{F}(\mathbf{E}) = F(E) \times F(E)$ the bottom of $\mathbf{E}$, $\mathbf{U}(a,b) = U(a) + U(b)$ the energy of $(a,b) \in \mathbf{E}$, $\mathrm{A}_c(.,.)$ the communication altitude and $\mathbf{V}((a,b),(a',b')) = V(a,a') + V(b,b')$ the communication cost from (a,b) to (a',b') associated to the family $\mathbf{Q}$. We will also denote $\Delta = \{(i,i) \in \mathrm{E}\}$, and $\mathbf{F} = \Delta \cap \mathbf{F}(\mathbf{E})$.

We now introduce some critical constants appearing in Theorem 2.

Notation 4. Let us note

$I \;= \sup_{a\neq b} A_c(a,b) - 2U(a) - 2U(b)$,
$I^* \;= \sup_{a\notin F(E)} \sup_{b\neq a} A_c(a,b) - 2U(a) - 2U(b)$,
$\mathbf{E}_{I^*} = \{(a,b) \in \mathbf{E} |\, a \neq b, (a,b) \notin \mathbf{F}(\mathbf{E}), A_c(a,b) - 2U(a) - 2U(b) = I^*\}$,
$E_{I^*} = \{a \notin F(E) |\, \exists b \neq a, (a,b) \in \mathbf{E}_{I^*}\}$.

Remark 1. Let us note here that these constants I and I^* are not necessary non-negative.

Notation 5. Let $h : E \to \mathbb{R}$ be a non constant function and denote for all $k \geq 0$

$$c_h(k) = \sum_{i,j\in E} h(i)h(j)\mu_\beta(i)(Q^k_\beta(i,j) - \mu_\beta(j)) \ .$$

We define the integrated autocovariance, denoted $c_{\mathrm{int},h}$, by

$$c_{\mathrm{int},h} = \frac{1}{2}c_h(0) + \sum_{k\geq 1} c_h(k) \ .$$

Moreover, we define the integrated autocorrelation time, denoted $\rho_{\mathrm{int},h}$, by

$$\rho_{\mathrm{int},h} = \frac{c_{\mathrm{int},h}}{c_h(0)} \quad .$$

Theorem 2. *Assume that $Q = (Q_\beta)_{\beta \geq 0}$ is a strongly aperiodic and admissible family. Let f_0 be a fixed point in $F(E)$ and $h : E \to \mathbb{R}$ a non constant function.*

(i) *There exists $K > 0$ such that for all $\beta \geq 0$, $c_{\mathrm{int},h} \leq K \exp(I\beta)$.*
(ii) *Assume now that $h(f) = h(f_0)$, $\forall f \in F(E)$.*

1. *There exists $K > 0$ such that we have for all $\beta \geq 0$, $c_{\mathrm{int},h} \leq K \exp(I^*\beta)$.*
2. *If for any $a \in E_{I^*}$, $h(a) = h(f_0)$, then there exist $I' < I^*$ and $K > 0$ such that, for all $\beta \geq 0$,*
$$c_{\mathrm{int},h} \leq K \exp(I'\beta) \quad .$$
3. *Let us denote $C(E_{I^*})$ the following condition*
$$(C(E_{I^*})) \quad A_c(a, F(E)) > \sup_{f,f' \in F(E)} A_c(f, f'); \quad a \in E_{I^*} \quad .$$

If there exists $i_* \in E_{I^*}$ such that $h(i_*) \neq h(f_0)$, if the condition $C(E_{I^*})$ holds, and if $(h(a) - h(f_0))(h(b) - h(f_0)) \geq 0$ for all $a, b \in E_{I^*}$ verifying $U(a) = U(b)$ and $C^*_{(\{b\} \cup F(E))^c}(a, b) = 0$, then

$$c_{\mathrm{int},h} \propto \exp(I^*\beta) \quad .$$

The proof of Theorem 2 is stated in section 5.3, and is based on one side on both general Lemmas 2 and 3, and on the other side on Lemma 4.

Note that $C(E_{I^*})$ holds as soon as the energy U has a unique global minimum (which happens for instance in meta-stability problems), and more generally, as soon as U has all its global minimums in a cycle which does not contain points of E_{I^*}. This condition implies that if the states i and j are such that G^1_{ij} is of the largest exponential order as possible, then G^2_{ij} can not be of the same order. Otherwise, since $G_{ij} = G^1_{ij} - G^2_{ij}$, we should have sharp large deviations estimates, and control the different constants in front of the exponentials. In fact this condition, which seems technical at a first glance, has a real physical meaning. If it is not satisfied, different qualitative behaviors, which highly depend on the models, are possible. The simplest example is the Metropolis dynamics applied to the 2D Ising model with no external field. The energy U has in this case two global minimums, a_0 and $-a_0$, separated by a high energy barrier, and which satisfy $I = A_c(a_0, -a_0)$. The constant I^* is very close to I. Let h be a symmetric function on E, which satisfies $h(x) = h(-x)$ for any configuration x. Since all is symmetric in this problem, the exponential order of $c_{\mathrm{int},h}$ will never be equal to $I^*\beta$. The greatest exponential order of $c_{\mathrm{int},h}$ for such a symmetric function will be $I_2\beta$, with $I_2 = \sup_{a\notin F(E)} \inf(A_c(a, a_0) - 2U(a), A_c(a, -a_0) - 2U(a))$.

Corollary 1. *Assume that $Q = (Q_\beta)_{\beta\geq 0}$ is a strongly aperiodic and admissible family. Assume that the condition $(C(E_{I^*}))$ holds. The energy function U satisfies*

$$c_{\mathrm{int},U} \propto \exp(I^*\beta) \ .$$

Then the energy U is a slowest mode for the autocovariance function, among the non constant functions which are constant on $F(E)$.

4. Autocorrelation times at low temperature

This section is organized as the previous one. Note that Theorem 3 relies explicitly the slowest modes of the autocorrelation times to the energy landscape, and that corollary 2 gives examples of functions for which the autocorrelation time is the largest among those which are constant on the bottom of E. It also shows that the largest potential barrier H^* which separates a configuration $i \notin F(E)$ from $F(E)$ naturally appears in the estimation of the integrated autocorrelation times for level functions associated to the energy U.

Notation 6. We denote H_0 and H^* the quantities defined by

$$H_0 = \sup_{i\neq j} A_c(i,j) - U(i) - U(j) \text{ and}$$
$$H^* = \sup_{i\notin F(E)} \sup_{j\neq i} A_c(i,j) - U(i) - U(j) \ .$$

Moreover, we denote

$$\mathbf{E}_{H^*} = \{(i,j) \notin \mathbf{F}(\mathbf{E}) | \, A_c(i,j) - U(i) - U(j) = H^*\} \ ,$$

and

$$E_{H^*} = \{i \notin F(E) | \, \exists j \in E, (i,j) \in \mathbf{E}_{H^*}\}.$$

Theorem 3. *Assume that $Q = (Q_\beta)_{\beta\geq 0}$ is a strongly aperiodic and admissible family. Let f_0 be a fixed point in $F(E)$ and $h\colon E \to \mathbb{R}$ a non constant function.*

(i) *There exists $K > 0$ such that for any $\beta \geq 0$, $\rho_{\mathrm{int},h} \leq K \exp(H_0\beta)$.*
(ii) *Assume that $h(f) = h(f_0)$, $\forall f \in F(E)$, and let us denote $U_h = \inf\{U(i) | \, h(i) \neq h(f_0)\}$.*

1. *There exists* $K > 0$ *such that for any* $\beta \geq 0$, $\rho_{\text{int},h} \leq K \exp(H^* \beta)$.
2. *If for any* $i \in E_{H^*}$, $U(i) \neq U_h$, *then there exist* $K > 0$, *and* $H' < H^*$ *such that* $\rho_{\text{int},h} \leq K \exp(H' \beta)$.
3. *Let us denote now* $(C(E_{H^*}))$ *the following condition*

$$(C(E_{H^*})) \quad A_c(a, F(E)) > \sup_{f, f' \in F(E)} A_c(f, f'); a \in E_{H^*} \ .$$

If there exists $i_* \in E_{H^*}$ *such that* $U_h = U(i_*)$, *if the condition* $(C(E_{H^*}))$ *holds, and if* $(h(i) - h(f_0))(h(j) - h(f_0)) \geq 0$ *for any* $i, j \in E_{H^*}$ *verifying* $U(i) = U(j) = U_h$ *and* $C^*_{(\{j\} \cup F(E))^c}(i, j) = 0$, *then*

$$\rho_{\text{int},h} \propto \exp(H^* \beta) \ .$$

The proof of this theorem, which is based on Lemmas 2, 3 and 5, is stated in section 5.4. Condition $C(E_{H^*})$ is similar to condition $C(E_{I^*})$.

Remark 2. Under the condition $C(E_{H^*})$, we have

$$H^* = H_1 \underset{\text{def}}{=} \sup\{H_e(\Pi) | \, \Pi \in \mathscr{C}(E), \Pi \cap F(E) = \emptyset\} \ .$$

Notation 7. We denote $\Lambda_* = \{U(i) | \, i \in E_{H^*}\}$, and for any $\lambda > 0$, U_λ the function from E to $\mathbb{R}_+$ defined by $U_\lambda(i) = 1_{U(i) \geq \lambda}$.

Corollary 2. *Under condition* $C(E_{H^*})$, $\rho_{\text{int},U_\lambda} \propto \exp(\beta H^*)$ *iff there exists* $\lambda_* \in \Lambda_*$ *such that* $U_\lambda(i) = 1_{U(i) \geq \lambda_*}$.

Corollary 3. *Assume that the conditions of corollary* 1 *hold and let us denote* $U_* = \inf\{U(i) | \, i \notin F(E)\}$. *Then the integrated autocorrelation time of the energy function U satisfies*

$$\rho_{\text{int},U} \propto \exp(\beta(I^* + U_*)) \ .$$

Since $U_* + I^* \leq H^*$ (*and since we usually have* $U_* + I^* < H^*$), *the energy function U is usually not a slowest mode for the integrated autocorrelation time.*

5. Proof of our results

As announced in the introduction, proofs are based on two main tools: the first one is a coupling argument, the second one uses large deviation estimates for Markov chains with rare transitions. These estimates come from the theory of Wentzell and Freidlin and have been developed by O. Catoni [3] to study optimal cooling schedules for simulated annealing, and by one of the authors [12] to study non reversible versions of simulated annealing.

We first give in this part a general result which gives estimates of the cumulated mass in a fixed point before reaching a subset of the bottom of a general set $\mathscr{E}$. It is the first step to study the asymptotic behavior of the $N_{(a,b)}^{(c,d)}$'s (see equation (7)). The second section is devoted to two lemmas which are both used in Theorems 2 and 3. The third section is devoted to Theorem 2, and the fourth one to Theorem 3.

5.1. *Cumulative mass before reaching the bottom of an energy landscape*

Since the result stated in this section will be applied to different processes, we will use here the same notations as in the first part of this paper (Section 2).

Lemma 1. *Let F be a subset of $F(\mathscr{E})$ and let $\beta \geq 0$. For all $i, j \in \mathscr{E}$, we note*

$$M_i^j = \mu_\beta(i) \sum_{k \geq 0} P(\mathscr{X}_k = j, T_r(F) > k | \mathscr{X}_0 = i) \ .$$

(i) *We have $M_i^j = 0$ if $i \in F$ or $j \in F$ and*

$$M_i^j \propto \exp(I_i^j \beta); i, j \notin F$$

where $I_i^j = C^*_{(\{j\} \cup F)^c}(j, F) - C^*_{(\{j\} \cup F)^c}(i, j) - \mathscr{U}(i)$.

(ii) *Let $I_F = \sup_{j \notin F} A_c(j, F) - 2\mathscr{U}(j)$, we have $I_i^j \leq I_F$ for all $i, j \notin F$. Moreover, for all $i, j \notin F$*

$$I_i^j = I_F \text{ iff } \begin{cases} \mathscr{U}(i) = \mathscr{U}(j) \\ C^*_{(\{j\} \cup F)^c}(i, j) = 0 \\ A_c(j, F) - 2\mathscr{U}(j) = A_c(i, F) - 2\mathscr{U}(i) = I_F \ . \end{cases}$$

(iii) *Let $I_F^* = \sup_{j \notin F(\mathscr{E})} A_c(j, F) - 2\mathscr{U}(j)$, we have $I_i^j \leq I_F^*$ for all $i, j \notin F(\mathscr{E})$. Moreover, for all $i, j \notin F(\mathscr{E})$*

$$I_i^j = I_F^* \text{ iff } \begin{cases} \mathscr{U}(i) = \mathscr{U}(j) \\ C^*_{(\{j\} \cup F)^c}(i, j) = 0 \\ A_c(j, F) - 2\mathscr{U}(j) = A_c(i, F) - 2\mathscr{U}(i) = I_F^* \ . \end{cases}$$

Proof. We start here the proof of (i). Let us note for any $i, j \in \mathscr{E}$

$$R_i^j = \sum_{k \geq 0} P(\mathscr{X}_k = j, T_r(F) > k | \mathscr{X}_0 = i) \ .$$

One obviously has that $R_i^j = 0$ as soon as $i \in F$ or $j \in F$. Let us now consider $i, j \notin F$. From the Markov property, we get easily that

$$R_i^j = P(T_r(\{j\}) < T_r(F) | \mathscr{X}_0 = i) R_j^j \ ,$$

and

$$R_j^j = 1 + P(\tau_r(\{j\}) < T_r(F) | \mathscr{X}_0 = j) R_j^j \ ,$$

where $\tau_r(A) = \inf\{n > 0 | \mathscr{X}_n \in A\}$ for all $A \subset \mathscr{E}$. Hence, we deduce that

$$R_i^j = \frac{P(T_r(\{j\}) < T_r(F) | \mathscr{X}_0 = i)}{P(\tau_r(\{j\}) > T_r(F) | \mathscr{X}_0 = j)}; \quad i, j \notin F \ ,$$

so that using Theorem 1 (i), we get that

$$R_i^j \propto \exp\Big(\beta(C^*_{(\{j\}\cup F)^c}(j,F) - C^*_{(\{j\}\cup F)^c}(i,j))\Big)$$

and the proof of (i) is ended.

At this point, we should make the following remark. Since using Lemma 9 in appendix B, we get that $C^*_{(\{j\}\cup F)^c}(j,F) = A_c(j,F) - \mathscr{U}(j)$ for any $j \in \mathscr{E}$, we deduce that

$$I_i^j \le A_c(j,F) - \mathscr{U}(j) - \mathscr{U}(i) \ .$$

Now, noticing that if $A_c(i,F) < A_c(j,F)$ then $C^*_{(\{j\}\cup F)^c}(i,j) \ge A_c(j,F) - A_c(i,F)$ (this relation is proved in Lemma 11 in appendix B), we get finally that

$$I_i^j \le A_c(j,F) \wedge A_c(i,F) - \mathscr{U}(j) - \mathscr{U}(i) \ . \tag{9}$$

We turn now to the proof of (ii). Let $i, j \notin F$ and let $a \in \{i, j\}$ such that $\mathscr{U}(a) = \mathscr{U}(i) \wedge \mathscr{U}(j)$. Then using (9) we deduce immediately that

$$I_i^j \le A_c(a,F) - 2\mathscr{U}(a) \le I_F \ .$$

Since the first inequality is strict as soon as $\mathscr{U}(i) \ne \mathscr{U}(j)$, we get that for all $i, j \notin F$, if $I_i^j = I_F$, then

$$\mathscr{U}(i) = \mathscr{U}(j) \text{ and } A_c(i,F) - 2\mathscr{U}(i) = A_c(j,F) - 2\mathscr{U}(j) = I_F \ . \tag{10}$$

However, if (10) is satisfied, then $I_i^j = A_c(j,F) - 2\mathscr{U}(j) - C^*_{(\{j\}\cup F)^c}(i,j)$ so that for all $i, j \notin F$, if $I_i^j = I_F$ we have in fact

$$\begin{gathered} \mathscr{U}(i) = \mathscr{U}(j), A_c(i,F) - 2\mathscr{U}(i) = A_c(j,F) - 2\mathscr{U}(j) = I_F \\ \text{and} \\ C^*_{(\{j\}\cup F)^c}(i,j) = 0 \ . \end{gathered} \tag{11}$$

Since we verify easily that for any $i, j \notin F$, if (11) is satisfied, then $I_i^j = I_F$, the proof of (ii) is ended.

The proof of (iii) is completely similar to the proof of (ii) and is let to the reader.

5.2. Relations between the coupling $\mathbf{X}$ *and the single chain* X

This section is devoted to two lemmas which are both used in Theorems 2 and 3. The first one gives a very important relation between the localized communication costs of the Markov chain $\mathbf{X}$ and those of the single chain X. The second gives, for some states i and j, a lower bound for the G^1_{ij}'s. Note that these lemmas will be applied to points of E_{I^*} and E_{H^*} in the proofs of Theorems 2 and 3. The fact that conditions $C(E_{I^*})$ and $C(E_{H^*})$ are satisfied is crucial.

Lemma 2. *Let* $Q = (Q_\beta)_{\beta \geq 0}$ *be an admissible and strongly aperiodic family on* E, *let* $i \in E$ *and assume that* $A_c(i, F(E)) > \sup\{A_c(f, f') |\, f, f' \in F(E)\}$. *Let* Π *be the smallest cycle for the inclusion such that* $i \in \Pi$ *and* $\Pi \cap F(E) \neq \emptyset$.

(i) *There exists* $\Pi_0 \in \mathscr{M}_*(\Pi)$ *such that* $F(E) \subset \Pi_0$ *and* $i \notin \Pi_0$.
(ii) *For any* $j \in \Pi \setminus \Pi_0$ *and* $b, b' \in F(E)$, *then*

$$\text{if } \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0 \text{ then } C^*_{(\{j\}\cup F(E))^c}(i,j) = 0 \enspace .$$

(iii) *For any* $j \in \Pi \setminus \Pi_0$ *and any* $b, b' \in F(E)$ *we have*

$$\mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) > 0 \enspace .$$

Proof. From the above definition of Π, we get that $A_c(\Pi) = A_c(i, F(E))$. However, since for any $f, f' \in F(E)$, we have $A_c(f, f') < A_c(i, F(E))$, there exists Π' such that $A_c(\Pi') < A_c(\Pi)$ and $F(E) \subset \Pi'$. Since $\Pi' \cap \Pi \neq \emptyset$, we deduce that Π' is strictly included in Π. Hence, there exists $\Pi_0 \in \mathscr{M}_*(\Pi)$ such that $F(E) \subset \Pi_0 \subset \Pi$. From the definition of Π, we get obviously that $i \notin \Pi_0$ so that part (i) is proved.

We turn now to the proof of part (ii). Let $j \in \Pi \setminus \Pi_0$ and let $b, b' \in F(E)$. Assume that $C^*_{(\{j\}\cup F(E))^c}(i,j) > 0$. We will show that $\mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) > 0$. From Theorem 1 (i), we get that there exists a constant $K > 0$ such that

$$\mathbf{P}_{(i,b)}(T_r(\mathbf{F}) > T_r(\{(j,b')\})) \geq K \exp\Big(-\beta \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b'))\Big) \enspace .$$

Hence, if we prove that

$$\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}(T_r(\mathbf{F}) < T_r(\{(j,b')\})) = 1 \enspace , \tag{12}$$

we will deduce immediately that $\mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) > 0$. To prove equality (12), let us show that

$$\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \Pi_0 \times F(E)\big) = 1 \enspace , \tag{13}$$

and

$$\lim_{\beta\to\infty} \mathbf{P}_{(c,f)}(T_r(\mathbf{F}) < T_e(\Pi_0 \times \Pi_0)) = 1, \forall (c,f) \in \Pi_0 \times F(E) \ , \quad (14)$$

where the set D is equal to $(\Pi \setminus (\Pi_0 \cup \{j\})) \times \Pi_0$.

Let us prove first the relation (13). We denote $D^1 = \Pi \setminus (\Pi_0 \cup \{j\})$. Considering the two events $(T_e^2(\Pi_0) \le T_e^1(D^1))$ and $(T_e^1(D^1) < T_e^2(\Pi_0))$, we deduce the upper bound

$$\begin{aligned}\mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \notin \Pi_0 \times F(E)\big) \le \mathbf{P}_{(i,b)}\big(T_e^2(\Pi_0) \le T_e^1(D^1)\big) \\ + \sum_{k\ge 0} \mathbf{P}_{(i,b)}\big(T_e^1(D^1) = k, X_k^2 \notin F(E)\big) \\ + \mathbf{P}_{(i,b)}\Big(X^1_{T_e(D^1)} \in \{j\} \cup \Pi^c\Big) \ . \quad (15)\end{aligned}$$

Since $H_e(\Pi_0) > H_e(D^1)$, we get that $\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}(T_e^2(\Pi_0) \le T_e^1(D^1)) = 0$. Let us note now that if $\mathcal{Q}$ is an irreducible Markov kernel, v its unique invariant probability measure, v_0 an initial probability measure and $v_n = v_0 \mathcal{Q}^n$ for any $n \ge 0$, then, denoting $g_n(p) = v_n(p)/v(p)$, we have $\sup g_{n+1} \le \sup g_n$ so that

$$v_n(p) \le v(p) \sup g_0 \ . \quad (16)$$

Hence, we deduce that $\sum_{k\ge 0} \mathbf{P}_{(i,b)}\big(T_e^1(D^1) = k, X_k^2 \notin F(E)\big)) \le \mu_\beta(F(E)^c)/\mu_\beta(b)$, which tends to 0 as β tends to infinity (b belongs to $F(E)$). Concerning the last term of the right hand side of (15), the event depends only on the first coordinate, so that applying Theorem 1, we deduce that there exists $K > 0$ such that

$$\mathbf{P}_{(i,b)}\Big(X^1_{T_e^1(D^1)} \in \{j\} \cup \Pi^c\Big) \le K \exp\big(-\beta C^*_{D^1}(i, \{j\} \cup \Pi^c)\big).$$

Since $D^1 \subset (\{j\} \cup F(E))^c$, we get that $C^*_{D^1}(i,j) \ge C^*_{(\{j\}\cup F(E))^c}(i,j) > 0$. Moreover, $D^1 \subset \Pi \setminus F(E)$ so that $C^*_{D^1}(i, \Pi^c) \ge C^*_{\Pi\setminus F(E)}(i, \Pi^c) > 0$. Hence we deduce that $C^*_{D^1}(i, \{j\} \cup \Pi^c) > 0$ and equality (13) is proved.

Let us prove now the equality (14). Let (c,f) be a state in $\Pi_0 \times F(E)$, and denote $\Pi_{(c,f)} = \{(a',b'); \mathbf{A}_c((c,f),(a',b')) < H_e(\Pi_0)\}$. Let us first notice that $\Pi_{(c,f)}$ is a cycle contained in $\Pi_0 \times \Pi_0$. Indeed, let (a',b') be any state of $\Pi_{(c,f)}$. Since $H_e(\Pi_0) > \mathbf{A}_c((c,f),(a',b')) \ge A_c(c,a') \vee A_c(f,b')$, we have $A_c(c,a') < H_e(\Pi_0)$ and $A_c(f,b') < H_e(\Pi_0)$. Since $c \in \Pi_0$, and $f \in \Pi_0$, then $a' \in \Pi_0$ and $b' \in \Pi_0$. Moreover, since the family $Q = (Q_\beta)_{\beta\ge 0}$ is strongly aperiodic, we have $\mathbf{A}_c((a,f),(f,f)) = A_c(a,f) \le H_m(\Pi_0) < H_e(\Pi_0)$ so that (f,f) belongs to $\Pi_{(c,f)}$.

We deduce now from the property of $\Pi_{(c,f)}$ that

$$\mathbf{P}_{(c,f)}(T_e(\Pi_0 \times \Pi_0) < T_r(\mathbf{F})) \le \mathbf{P}_{(c,f)}\big(T_e(\Pi_{(c,f)}) < T_r(\{(f,f)\})\big)$$

and

$$\lim_{\beta\to\infty} \mathbf{P}_{(c,f)}(T_e(\Pi_{(c,f)}) < T_r(\{(f,f)\})) = 0$$

so that (14) is proved and the proof of part (ii) is complete.

We turn now to the proof of part (iii). Using Theorem 1 (i), we deduce that it is sufficient to prove that $\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}(T_r(\mathbf{F}) < T_e^2(\Pi_0)) = 1$. Let us denote $B^1 = \Pi \setminus \Pi_0$ and $B = B^1 \times \Pi_0$. We will prove in fact that

$$\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(B)} \in \Pi_0 \times F(E)\big) = 1 \ , \tag{17}$$

and

$$\lim_{\beta\to\infty} \mathbf{P}_{(c,f)}(T_r(\mathbf{F}) < T_e(\Pi_0 \times \Pi_0)) = 1 \ \ \forall\, (c,f) \in \Pi_0 \times F(E) \ .$$

This last inequality has been proved before in the proof of part (ii). As regards (17), we have for $\mathbf{P}_{(i,b)}(\mathbf{X}_{T_e(B)} \notin \Pi_0 \times F(E))$ the upper bound

$$\mathbf{P}_{(i,b)}\big(T_e^2(\Pi_0) \leq \ T_e^1(B^1)\big) + \sum_{k\geq 0} \mathbf{P}_{(i,b)}(T_e^1(B^1) = k, X_k^2 \notin F(E)) + \mathbf{P}_{(i,b)}\Big(X_{T_e^1(B^1)} \in \Pi^c\Big) \ .$$

Since $H_e(B^1) < H_e(\Pi_0)$, the first term vanishes when β tends to infinity. Moreover, using the same argument than in part (ii), we get that the second term in the right hand side vanishes also. Now, since $\mathbf{P}_{(i,b)}\big(X_{T_e^1(B^1)} \in \Pi^c\big)$ is bounded by $\mathbf{P}_{(i,b)}\big(X_{T_e^1(\Pi\setminus F(E))} \in \Pi^c\big)$ which tends to 0 when β tends to infinity, the proof of (17) is complete.

Lemma 3. *Let $Q = (Q_\beta)_{\beta\geq 0}$ be an admissible and strongly aperiodic family on E, let $i \in E$ and assume that $A_c(i, F(E)) > \sup\{\, A_c(f,f') | \, f, f' \in F(E) \,\}$. Let Π and Π_0 as defined in Lemma* 2. *Let $j \in \Pi \setminus \Pi_0$ such that $C^*_{(\{j\}\cup F(E))^c}(i,j) = 0$. Then we have*

$$G_{ij}^1 \geq K \exp\big(\beta(H_j - U(i))\big) \ ,$$

where $H_j =_{\mathrm{def}} \sup\{H_e(\Pi') | \, \Pi' \in \mathscr{C}(E), \ j \in F(\Pi')\}$.

Proof. Let $b \in F(E)$. Since $G_{ij}^1 = \mu_\beta(i) \sum_{k\geq 0} \mathbf{P}_{\delta_i \otimes \mu_\beta}\big(X_k^1 = j, T_r(\Delta) > k\big)$, we deduce that

$$\begin{aligned} G_{ij}^1 &\geq \mu_\beta(i)\mu_\beta(b) \sum_{k\geq 0} \mathbf{P}_{(i,b)}\big(X_k^1 = j, T_r(\Delta) > k\big) \\ &\geq \mu_\beta(i)\mu_\beta(b) \mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \{j\} \times \Pi_0\big) \\ &\quad \times \inf_{c\in\Pi_0} \sum_{k\geq 0} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k, T_e^2(\Pi_0) > k\big) \ , \end{aligned}$$

where $D = (\Pi \setminus (\Pi_0 \cup \{j\})) \times \Pi_0$ and Π_j is the greatest cycle among all the cycles Π' such that $j \in F(\Pi')$. Note, from the definitions of Π and Π_0, that we have $\Pi_j \subset \Pi \setminus \Pi_0$. For all integer $M > 0$ and all $c \in \Pi_0$, we have

$$\begin{aligned}\sum_{k\geq 0} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k, T_e^2(\Pi_0) > k\big) \\ \geq \sum_{k=0}^{M} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k, T_e^2(\Pi_0) > k\big) \\ \geq \sum_{k=0}^{M} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k\big)\mathbf{P}_{(j,c)}\big(T_e^2(\Pi_0) > k\big) \ .\end{aligned}$$

Since $\mathbf{P}_{(j,c)}\big(T_e^2(\Pi_0) > k\big)$ is decreasing in k, we deduce that

$$\begin{aligned}\sum_{k\geq 0} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k, T_e^2(\Pi_0) > k\big) \\ \geq \mathbf{P}_{(j,c)}\big(T_e^2(\Pi_0) > M\big) \sum_{k=0}^{M} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k\big) \ . \qquad (18)\end{aligned}$$

Then, applying the Lemma 7 proved in appendix, we obtain that there exist $R_0 > 0$, $\beta_0 \geq 0$, and $C > 0$, such that for any $\beta \geq \beta_0$,

$$\sum_{k=0}^{[R_0 \exp(H_j\beta)]} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k\big) \geq C \exp\big(H_j\beta\big) \ . \qquad (19)$$

Moreover, applying Theorem 1 (iii), there exist $\beta_1 \geq 0$, $C > 0$, and $a > 0$ such that for all $\beta \geq \beta_1$,

$$\mathbf{P}_{(j,c)}\big(T_e^2(\Pi_0) > [R_0 e^{H_j\beta}]\big) \geq C \exp\Big(-aR_0 e^{\beta(H_j - H_e(\Pi_0))}\Big) \ . \qquad (20)$$

Hence, since $H_j < H_e(\Pi_0)$, we deduce from equations (18), (19) and (20) that there exists a constant $C > 0$, such that for all $\beta \geq \sup(\beta_0, \beta_1)$

$$\sum_{k\geq 0} \mathbf{P}_{(j,c)}\big(X_k^1 = j, T_e^1(\Pi_j) > k, T_e^2(\Pi_0) > k\big) \geq C \exp\big(\beta H_j\big) \ .$$

Since $b \in F(E)$, $\mu_\beta(b)$ is bounded from below uniformly in β by a strictly positive constant, and there exists a constant $K > 0$ such that, for all $\beta \geq \sup(\beta_0, \beta_1)$

$$G_{ij}^1 \geq K\mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \{j\} \times \Pi_0\big) \exp\big(\beta(H_j - U(i))\big) \ . \qquad (21)$$

If $i = j$, the announced result is clear. Let now i be different from j. Since

$$\mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \{j\} \times \Pi_0\big) = \mathbf{P}_{(i,b)}\Big(X^1_{T^1_e(D^1)} = j,\ T^1_e(D^1) < T^2_e(\Pi_0)\Big)\ ,$$

where $D^1 = \Pi \backslash (\Pi_0 \cup \{j\})$, we get the inequality

$$\mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \{j\} \times \Pi_0\big) \geq P_i(X^1_{T^1_e(D^1)} = j) - \mathbf{P}_{(i,b)}\big(T^2_e(\Pi_0) \leq T^1_e(D^1)\big).$$

Since $H_e(\Pi_0) > H_e(D^1)$, we get finally $\lim_{\beta\to\infty} \mathbf{P}_{(i,b)}\big(T^2_e(\Pi_0) \leq T^1_e(D^1)\big) = 0$. Moreover, there exists a constant $C > 0$, such that, for all $\beta \geq 0$,

$$P_i(X^1_{T^1_e(D^1)} = j) \geq C\exp\big(-\beta C^*_{D^1}(i,j)\big).$$

We just need to prove now that $C^*_{D^1}(i,j)$ is equal to 0.

Let Π' be any cycle and B a subset of E. Assume that $a \in \Pi'$, $b' \notin \Pi'$, and $B^c \cap \Pi' \neq \emptyset$. Then, $A_c(a, B^c) \leq A_c(a, B^c \cap \Pi') \leq A_c(\Pi')$. But since $b' \notin \Pi'$, we have $U(a) + V(a,b') > A_c(\Pi')$. So that $C_B(a,b') = U(a) + V(a,b') - A_c(a,B^c) \geq U(a) + V(a,b') - A_c(\Pi') > 0$.

As a consequence, since $F(E) \subset \Pi_0 \subset \Pi$, we deduce that for $(p,q) \in \Pi_0 \times \Pi_0^c$ and $(p',q') \in \Pi \times \Pi^c$, we have $C_{(F(E)\cup\{j\})^c}(p,q) > 0$ and $C_{(F(E)\cup\{j\})^c}(p',q') > 0$. Hence, if $g \in \mathrm{Pth}_{(F(E)\cup\{j\})^c}(i,j)$ is such that $C_{(F(E)\cup\{j\})^c}(g) = 0$ (such a path exists because $C^*_{(F(E)\cup\{j\})^c}(i,j) = 0$), we get that $g \in \mathrm{Pth}_{D^1}(i,j)$. Now, since we verify easily that for any $p \in D^1$, we have $A_c(p, F(E) \cup \{j\}) = A_c(p, (D^1)^c)$, we deduce that $C_{D^1}(g) = C_{(F(E)\cup\{j\})^c}(g) = 0$, so that $C^*_{D^1}(i,j) = 0$.

Hence, we deduce that there exist $C > 0$ and $\beta_2 > 0$, such that for all $\beta \geq \beta_2$, $\mathbf{P}_{(i,b)}\big(\mathbf{X}_{T_e(D)} \in \{j\} \times \Pi_0\big) \geq C$. From this result and the equation (21), we have that there exist $K > 0$ and $\beta_* > 0$ ($\beta_* = \sup(\beta_0, \beta_1, \beta_2)$), such that for all $\beta \geq \beta_*$

$$G^1_{ij} \geq K\exp\big(\beta(H_j - U(i))\big)\ . \tag{22}$$

so that the proof of the lemma is complete.

5.1. *Integrated autocovariance*

This section gives the proof of Theorem 2. It is organized as follows. A first lemma gives upper bounds for the constants $I^{(c,d)}_{(a,b)}$ defined in Lemma 1 applied to the coupling $\mathbf{X}$ and to the subset $\mathbf{F}$ of $\mathbf{F}(\mathbf{E})$ as well as necessary and sufficient conditions to reach these upper bounds. The proof of Theorem 2 follows.

Remark 3. Let us denote

$$\begin{cases} N^{(a',b')}_{(a,b)} & = \mu_\beta(a)\mu_\beta(b)\sum_{k\geq 0}\mathbf{P}_{(a,b)}(\mathbf{X}_k = (a',b'), T_r(\Delta) > k) \\ \text{and} & \\ M^{(a',b')}_{(a,b)} & = \mu_\beta(a)\mu_\beta(b)\sum_{k\geq 0}\mathbf{P}_{(a,b)}(\mathbf{X}_k = (a',b'), T_r(\mathbf{F}) > k)\ . \end{cases}$$

Since we have obviously

$$N_{(a,b)}^{(a',b')} \le M_{(a,b)}^{(a',b')} \text{ and } \begin{cases} G_{ij}^1 & = \sum_{b,b' \in E} N_{(i,b)}^{(j,b')}, \\ G_{ij}^2 & = \sum_{b,b' \in E} N_{(i,b)}^{(b',j)} \end{cases},$$

we can obtain exponential upper bounds of the G_{ij}'s through upper bounds on the $I_{(a,b)}^{(c,d)}$'s.

Lemma 4. *Let* i, j, b and $b' \in E$ *and assume that* $(i,b) \notin \mathbf{F}$ *and* $(j,b') \notin \mathbf{F}$.

(i) *We have* $I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} \le I$.
(ii) *Assume that* $i, j \notin F(E)$. *Then we have* $I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} \le I^*$.
(iii) *Assume that* $i, j \notin F(E)$. *Then*

$$I_{(i,b)}^{(j,b')} = I^* \text{ iff } \begin{cases} (i,b),(j,b') \in \mathbf{E}_{I^*} \\ U(i) = U(j) \\ \mathbf{C}^*_{(\{(j,b')\}\cup \mathbf{F})^c}((i,b),(j,b')) = 0 \end{cases}$$

and

$$I_{(i,b)}^{(b',j)} = I^* \text{ iff } \begin{cases} (i,b),(b',j) \in \mathbf{E}_{I^*} \\ U(i) = U(j) \\ \mathbf{C}^*_{(\{(b',j)\}\cup \mathbf{F})^c}((i,b),(b',j)) = 0 \end{cases} .$$

Moreover, if the condition $(C(E_{I^*}))$ *holds*

$$(C(E_{I^*})) \quad A_c(a, F(E)) > \sup_{f,f' \in F(E)} A_c(f,f'); a \in E_{I^*},$$

then $I_{(i,b)}^{(b',j)} < I^*$.

Proof. Before starting the proof, let us make several remarks. First of all, if $(i,b) \in \mathbf{E}_{I^*}$ with $i \notin F(E)$, then $b \in F(E)$.

Remark 4. For any $(a,b) \in \mathbf{E}$, we have

$$\mathbf{A}_c((a,b),\mathbf{F}) \ge A_c(a,b) \ . \tag{23}$$

Indeed, for any $f \in F(E)$, we have $\mathbf{A}_c((a,b),(f,f)) \ge A_c(a,f) \vee A_c(f,b) \ge A_c(a,b)$, where the last inequality comes from the ultrametricity property of the communication altitude.

Now, if a or b belongs to $F(E)$, then

$$\mathbf{A}_c((a,b),\mathbf{F}) \le A_c(a,b) \ . \tag{24}$$

Indeed, assume that $b \in F(E)$, then $\mathbf{A}_c((a,b),\mathbf{F}) = \inf_{f \in F(E)} \mathbf{A}_c((a,b),(f,f))$. However, let $\Pi = \{c \in E | A_c(b,c) = 0\}$. The set Π is a cycle and $U(c) = 0$ for any $c \in \Pi$. From the strong aperiodicity of Q, we get that for any $c, c' \in \Pi$, there exists a path $\mathbf{g} = (\mathbf{g}_0, \ldots, \mathbf{g}_n)$ such that $\mathbf{g}_0 = (c, c')$, $\mathbf{g}_n = (c, c)$ and $\mathbf{A}_c(\mathbf{g}) = 0$. Moreover, there exists a path $\mathbf{p} = (\mathbf{p}_0, \ldots, \mathbf{p}_r)$ such that if $p^1 = (p^1_0, \ldots, p^1_r)$ and $p^2 = (p^2_0, \ldots, p^2_r)$ (where $\mathbf{p}_k = (p^1_k, p^2_k)$), then

$$\begin{cases} A_c(p^1) = A_c(a, b) \\ \mathbf{p}_0 = (a, b), \ \mathbf{p}_r = (b, c) \in \Pi \times \Pi, \\ A_c(p^2) = 0 \ , \end{cases}$$

so that $\mathbf{A}_c(\mathbf{p}) = A_c(a, b)$. Now, concatenating $\mathbf{p}$ with a path $\mathbf{g}$ of the first type with starting point (b, c), we deduce the inequality (24).

Remark 5. We have in fact

$$I = \sup_{f \in F(E)} \sup_{b \neq f} A_c(f, b) - 2U(b) \ , \tag{25}$$

and

$$I^* = \sup_{f \in F(E)} \sup_{b \notin F(E)} A_c(f, b) - 2U(b) \ . \tag{26}$$

Indeed, for any $a, b \notin F(E)$ and $f \in F(E)$, we have

$$A_c(a, b) \leq A_c(a, f) \vee A_c(b, f),$$

so that if $c \in \{a, b\}$ is chosen such that $A_c(c, f) = A_c(a, f) \vee A_c(b, f)$, then

$$A_c(a, b) - 2U(a) - 2U(b) < A_c(c, f) - 2U(c) \leq I^* \leq I.$$

We start now the proof of (i). We deduce from Lemma 1 (ii) that

$$\sup\{I^{(j,b')}_{(i,b)} \,|\, (i, b) \notin \mathbf{F}, \ (j, b') \notin \mathbf{F}\} = \sup\{ I^{(j,b')}_{(i,b)} \,|\, (i, b, j, b') \in A\},$$

where $A = \{(i, b, j, b') \in E^4 | \, \mathbf{U}(i, b) = \mathbf{U}(j, b'), \ (i, b) \notin \mathbf{F}, \ (j, b') \notin \mathbf{F}\}$. Moreover, for any $i, b, j, b' \in E$, we have $I^{(j,b')}_{(i,b)} \leq L^{(j,b')}_{(i,b)}$ where

$$L^{(j,b')}_{(i,b)} = \mathbf{A}_c((i, b), \mathbf{F}) \wedge \mathbf{A}_c((j, b'), \mathbf{F}) - \mathbf{U}(i, b) - \mathbf{U}(j, b').$$

We will prove that $L^{(j,b')}_{(i,b)} \leq I$ for any $(i, b, j, b') \in A$. Let $(i, b, j, b') \in A$. Note first that

$$\mathbf{A}_c((i, b), \mathbf{F}) \leq (U(i) + A_c(b, F(E))) \vee (\sup_{f \in F(E)} A_c(i, f)) \ . \tag{27}$$

This inequality is clear when $b \in F(E)$, the left hand term being then less than $A_c(i, b)$. Let now $b \notin F(E)$ and $f_b \in F(E)$ such that $A_c(b, f_b) = A_c(b, F(E))$. There exists a path $g^2 \in \mathrm{Pth}(b, f_b)$, such that $A_c(g^2) = A_c(b, F(E))$. Now, there exists $i_1 \in E$ and $g^1 \in \mathrm{Pth}(i, i_1)$ with the same length than g^2 such that $A_c(g^1) \leq U(i)$ (it is sufficient to follow edges (c,d) such that $V(c,d) = 0$). Hence $\mathbf{g} = (g^1, g^2)$ is a path from (i,b) to (i_1, f_b) such that

$$\mathbf{A}_c(\mathbf{g}) \leq A_c(g^1) + A_c(g^2) \leq U(i) + A_c(b, F(E)) \ .$$

Since $A_c(i_1, f_b) \leq A_c(i_1, i) \vee A_c(i, f_b)$, and $A_c(i, i_1) \leq U(i) \leq A_c(i, f_b)$, we deduce that $A_c(i_1, f_b) \leq A_c(i, f_b)$. Hence, there exists a path $p^1 \in \mathrm{Pth}(i_1, f_b)$ such that $A_c(p^1) \leq A_c(i, f_b)$. Moreover we easily construct a path $p^2 \in \mathrm{Pth}(f_b, f_b')$ with the same length than p^1 such that $A_c(p^2) = U(f_b) = 0$ $(f_b' \in F(E))$. Thus, considering $\mathbf{p} = (p^1, p^2)$, we have

$$\mathbf{A}_c(\mathbf{p}) \leq A_c(p^1) + A_c(p^2) \leq A_c(i, f_b) \ .$$

Finally, let $\Pi = \{a \in E | A_c(a, f_b) = 0\}$. The set Π is a cycle containing f_b and f_b', and Π is an irreducible class for q_∞ defined in (2). Hence, since Q is strongly aperiodic, we deduce that $q_\infty \otimes q_\infty$ restricted to $\Pi \times \Pi$ is irreducible so that there exists a path $\mathbf{q} \in \mathrm{Pth}((f_b, f_b'), (f_b, f_b))$ such that $q_\infty(q_k^1, q_{k+1}^1) > 0$ and $q_\infty(q_k^2, q_{k+1}^2) > 0$ for any $0 \leq k < n_{\mathbf{q}}$. Thus $\mathbf{A}_c(\mathbf{q}) \leq A_c(q^1) + A_c(q^2) = 0$. Following successively $\mathbf{g}$, $\mathbf{p}$, and $\mathbf{q}$, we get a path $\mathbf{m} \in \mathrm{Pth}((i,b), (f_b, f_b))$ satisfying

$$\mathbf{A}_c(\mathbf{m}) \leq (U(i) + A_c(b, F(E))) \vee A_c(i, f_b) \ ,$$

so that the inequality (27) is proved. We deduce from this result that

$$\begin{aligned} L_{(i,b)}^{(j,b')} &\leq (A_c(b, F(E)) - 2U(b) - U(i)) \\ &\quad \vee (\sup_{f \in F(E)} A_c(i,f) - 2U(i) - 2U(b)) \\ &\leq (I - U(i)) \vee (I - 2U(b)) \ , \end{aligned} \tag{28}$$

and part (i) is proved.

From now, we assume that $i, j \notin F(E)$. Let $b, b' \in E$ and assume first that $\mathbf{U}(i,b) = \mathbf{U}(j,b')$. We will show that $L_{(i,b)}^{(j,b')} \leq I^*$. Consider the right hand side of the first inequality of (28). We have

$$A_c(b, F(E)) - 2U(b) - U(i) \leq \begin{cases} -U(i) \leq I^* & \text{if } b \in F(E) \\ I^* - U(i) & \text{if } b \notin F(E) \end{cases} \ , \tag{29}$$

and

$$\sup_{f \in F(E)} A_c(i,f) - 2U(i) - 2U(b) \leq I^* - 2U(b) \ , \tag{30}$$

so that $L_{(i,b)}^{(j,b')} \leq I^*$. Since $L_{(i,b)}^{(j,b')} = L_{(i,b)}^{(b',j)}$ we get $L_{(i,b)}^{(b',j)} \leq I^*$ and using Lemma 1 (iii) we deduce part (ii) and $I_{\mathbf{F}}^* \leq I^*$.

Let now $a \in E_{I^*}$, and $f \in F(E)$ such that $(a,f) \in \mathbf{E}_{I^*}$. We have that $I^{(a,f)}_{(a,f)} = I^*$. Indeed $I^{(a,f)}_{(a,f)} = \mathbf{A}_c((a,f),\mathbf{F}) - 2U(a)$. Using remark 4, $\mathbf{A}_c((a,f),\mathbf{F}) - 2U(a) = A_c(a,f) - 2U(a) = I^*$. Hence $I^*_{\mathbf{F}} \geq I^*$, and $I^*_{\mathbf{F}} = I^*$.

Moreover, we get from (29) and (30) that if $L^{(j,b')}_{(i,b)} = I^*$ then $U(b) = 0$. Now, since $L^{(j,b')}_{(i,b)} = L^{(i,b)}_{(j,b')}$ we get also $U(b') = 0$ so that we have in fact $b, b' \in F(E)$.

Hence, using Lemma 1 (iii), we deduce that

$$I^{(j,b')}_{(i,b)} = I^* \text{ iff } \begin{cases} (i,b),(j,b') \in \mathbf{E}_{I^*}, \\ U(i) = U(j), \\ \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0 \end{cases} ,$$

and

$$I^{(b',j)}_{(i,b)} = I^* \text{ iff } \begin{cases} (i,b),(b',j) \in \mathbf{E}_{I^*}, \\ U(i) = U(j), \\ \mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) = 0 \end{cases} .$$

To end the proof, we have to show now that if $(i,b),(b',j) \in \mathbf{E}_{I^*}$ and $U(i) = U(j)$, then, under $(C(E_{I^*}))$,

$$\mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) > 0 \ .$$

However, since in this case $b, b' \in F(E)$, and since $(C(E_{I^*}))$ holds, we deduce that if Π and Π_0 are defined as in Lemma 2, then $j \in \Pi \backslash \Pi_0$ and using part (iii) of Lemma 2, we get $\mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) > 0$. Hence the proof is complete.

Here follows the statement of Theorem 2.

Proof. Let us start with some notations. Note that, if we call $m_h = \sum_{k\geq 0} c_h(k)$,

$$m_h = \sum_{i,j} h(i)h(j)G_{ij} \ . \tag{31}$$

Moreover, since $\sum_i G_{ij} = \sum_j G_{ij} = 0$, denoting $\tilde{h}(i) = h(i) - h(f_0)$ for any $i \in E$, we have $m_h = m_{\tilde{h}}$. Now, denoting $E_h = \{i \in E | \tilde{h}(i) \neq 0\}$, we get

$$m_{\tilde{h}} = \sum_{i,j \in E_h} \tilde{h}(i)\tilde{h}(j)G_{ij} \ . \tag{32}$$

Now, let us note that $c_h(0) = c_{\tilde{h}}(0) \geq 0$. Hence we deduce that $0 \leq c_{\text{int},h} \leq m_{\tilde{h}}$. Now, applying Lemma 4 (i), Lemma 1 and remark 3, we deduce that there exists $K > 0$ such that, for all $\beta \geq 0$, $m_{\tilde{h}} \leq K\exp(I\beta)$, and that

$$c_{\text{int},h} \leq K\exp(I\beta) \ .$$

Part (i) is proved.

Assume now that $h(f) = h(f_0), \ \forall f \in F(E)$. Then, using Lemma 4 (ii), we deduce that there exists $K > 0$ such that for any $\beta \geq 0$ we have

$$c_{\text{int},h} \leq K \exp(I^* \beta),$$

and part (ii)(1) is proved.

We turn now to the proof of part (ii)(2). We assume then that for any $i \in E_{I^*}$ we have $\tilde{h}(i) = 0$. Then, using Lemma 4 (iii), we deduce that there exists $I' < I^*$ and $K > 0$ such that for any $\beta \geq 0$ and any $i, j \notin E_{I^*} \cup F(E)$, we have

$$|G_{ij}| \leq K \exp(I' \beta) \ .$$

Hence, there exists $I' < I^*$ and $K > 0$ such that for any $\beta \geq 0$,

$$c_{\text{int},h} \leq m_{\tilde{h}} \leq K \exp(I' \beta) \ .$$

Let us prove now part (ii)(3) and assume that $C(E_{I^*})$ holds and that there exists $i_* \in E_{I^*}$ such that $\tilde{h}(i_*) \neq 0$. Let $i, j \notin F(E)$ and note $U_{ij} =_{\text{def}} U(i) \wedge U(i)$. Using Lemma 4 (iii), we deduce that there exists $I' < I^*$ such that for any $b, b' \in E$, we have $I_{(i,b)}^{(b',j)} \leq I'$. Hence there exists $K > 0$ such that for any $\beta \geq 0$

$$G_{ij}^2 \leq K \exp(I' \beta) \ .$$

Let us study now the behavior of the G_{ij}^1's. Let us note

$$A = \{(i,j) \in E_{I^*} \times E_{I^*} \,|\, U(i) = U(j), \ C^*_{(\{j\} \cup F(E))^c}(i,j) = 0\}.$$

Since we assume that for any $(i,j) \in A$, we have $\tilde{h}(i)\tilde{h}(j) \geq 0$, we deduce that

$$\sum_{(i,j) \in A} \tilde{h}(i)\tilde{h}(j) G_{ij}^1 \geq \tilde{h}(i_*)\tilde{h}(i_*) G_{i_* i_*}^1 \ .$$

Now, since we assume that $(C(E_{I^*}))$ holds, we deduce from Lemma 3 that there exists $\beta_0 \geq 0$ and $K > 0$ such that

$$G_{i_* i_*}^1 \geq K \exp(I^* \beta) \ .$$

Hence, to end the proof, it will be sufficient to prove that for any $(i,j) \notin A$, with $U_{ij} \geq U_h =_{\text{def}} \inf\{U(l) \,|\, h(l) \neq h(f_0)\}$, there exists $K > 0$ and $I' < I^*$ such that for any $\beta \geq 0$ we have

$$G_{ij}^1 \leq K \exp(I' \beta) \ . \tag{33}$$

Moreover, to get (33) it is sufficient to prove that for any $b, b' \in E$, we have $I_{(i,b)}^{(j,b')} < I^*$. However, using Lemma 4, we get that if $I_{(i,b)}^{(j,b')} = I^*$ then $U(i) = U(j), \ i, j \in E_{I^*}$ and $\mathbf{C}^*_{(\{(j,b')\} \cup \mathbf{F})^c}((i,b),(j,b')) = 0$. Hence we deduce easily from Lemma 2 (ii) that $C^*_{(\{j\} \cup F(E))^c}(i,j) = 0$. This is in contradiction with the fact that $(i,j) \notin A$ so that (33) is proved. Since

$c_{\mathrm{int},h} = m_{\tilde{h}} - \frac{1}{2}c_{\tilde{h}}(0)$, and $c_{\tilde{h}}(0) = \sum_{i\in E_h}\mu_\beta(i)\tilde{h}^2(i) - \left(\sum_{i\in E_h}\mu_\beta(i)\tilde{h}(i)\right)^2$, we also have

$$c_{\tilde{h}}(0) \propto \exp(-\beta U_h) \ . \tag{34}$$

Denote now $U_* =_{\mathrm{def}} \inf\{U(l) | \, l \notin F(E)\}$. Hence, if $I^* + U_* > 0$ or if $U_h > U_*$ (let us note here that we always have $I^* + U_* \geq 0$), the proof of (ii)(3) is complete.

Let us assume now that $I^* + U_* = 0$ and that $U_h = U_*$. Let us note, for all $i,j \in E$ and $l \in \{1,2\}$,

$$G'^{l}_{ij} = \mu_\beta(i)\sum_{k\geq 1}\mathbf{P}_{\delta_i\otimes\mu_\beta}\left(X^l_k = j, T_r(\Delta) > k\right) \ .$$

We can write

$$c_{\mathrm{int},h} = \frac{1}{2}c_{\tilde{h}}(0) + \sum_{i,j}\tilde{h}(i)\tilde{h}(j)(G'^{1}_{ij} - G'^{2}_{ij}) \ .$$

It is clear that $0 \leq G'^{l}_{ij} \leq G^l_{ij}$, for all $i,j \in E$ and $l \in \{1,2\}$. Hence there exists $I' < I^*$ such that for all $\beta \geq 0$, $\left|\sum_{i,j}\tilde{h}(i)\tilde{h}(j)G'^{2}_{ij}\right| \leq K\exp(\beta I')$, and $\left|\sum_{(i,j)\notin A}\tilde{h}(i)\tilde{h}(j)G'^{1}_{ij}\right| \leq K\exp(\beta I')$. Now, since $\sum_{(i,j)\in A}\tilde{h}(i)\tilde{h}(j)G'^{1}_{ij} \geq 0$, and since $c_{\tilde{h}}(0) \propto \exp(-\beta U_*)$, the proof of (ii)(3) is complete.

Remark 6. We recall here that the condition $(C(E_{I^*}))$ holds as soon as U has a unique global minimum. In this case, the energy U is a slowest mode for the autocovariance function.

5.2. Autocorrelation times

This section is organized as the preceding one. A first lemma relies the constants associated to the Markov chain $\mathbf{X}$ to the energy landscape of the initial chain X, and is followed by the proof of Theorem 3.

Lemma 5. Let i, j, b and $b' \in E$, and $U_{ij} = U_i \wedge U_j$.

(i) *We have* $I^{(j,b')}_{(i,b)} \vee I^{(b',j)}_{(i,b)} \leq H_0 - U_{ij}$.

(ii) *Assume that* $i,j \notin F(E)$. *Then we have* $I^{(j,b')}_{(i,b)} \vee I^{(b',j)}_{(i,b)} \leq H^* - U_{ij}$.
Assume that $i,j \notin F(E)$. *Then*

$$I^{(j,b')}_{(i,b)} = H^* - U_{ij} \text{ iff } \begin{cases} (i,b),(j,b') \in \mathbf{E}_{H^*} \\ U(i) = U(j) \\ \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0 \end{cases}$$

and

$$I^{(b',j)}_{(i,b)} = H^* - U_{ij} \text{ iff } \begin{cases} (i,b),(b',j) \in \mathbf{E}_{H^*} \\ U(i) = U(j) \\ \mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) = 0 \ . \end{cases}$$

Moreover, if the condition $(C(E_{H^*}))$ *holds*

$$(C(E_{H^*}))\quad A_c(a,F(E)) > \sup_{f,f'\in F(E)} A_c(f,f');\ a\in E_{H^*},$$

then $I_{(i,b)}^{(b',j)} < H^* - U_{ij}$.

Proof. Let i,j,b and $b'\in E$. We know that

$$I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} \le \mathbf{A}_c((i,b),\mathbf{F}) \wedge \mathbf{A}_c((j,b'),\mathbf{F}) - \mathbf{U}(i,b) - \mathbf{U}(b',j)\ ,$$

and $\mathbf{A}_c((i,b),\mathbf{F}) \le (U(i) + A_c(b,F(E))) \vee (\sup_{f\in F(E)} A_c(i,f))$. Since the upper bound of $I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)}$ is symmetric in (i,b) and (j,b'), we can suppose that $U(b')\ge U(b)$. Hence,

$$\begin{aligned} I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} &\le (A_c(b,F(E)) - \mathbf{U}(j,b') - U(b)) \\ &\vee \left(\sup_{f\in F(E)} A_c(i,f) - \mathbf{U}(i,b) - \mathbf{U}(j,b')\right)\ . \end{aligned}$$

Since $A_c(b,F(E)) - U(b)\le H_0$, and $\sup_{f\in F(E)} A_c(i,f) - U(i)\le H_0$, we deduce immediately that

$$I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} \le (H_0 - U(j) - U(b')) \vee (H_0 - U(b) - U(j) - U(b'))\ .$$

So that the part (i) is proved.

Assume now that $i,j\notin F(E)$. Then $\sup_{f\in F(E)} A_c(i,f) - U(i)\le H^*$, and obviously $A_c(b,F(E)) - U(b)\le H^*$. Hence again

$$\begin{aligned} I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} &\le (H^* - U(j) - U(b')) \vee (H^* - U(b) - U(j) - U(b')) \\ &\le H^* - U_{ij}\ . \end{aligned} \tag{35}$$

Let us prove now the part (iii), and let $i,j\notin F(E)$. If $(b,b')\notin \mathbf{F}(\mathbf{E})$, we deduce from the inequality (35) and from the fact that $U(b')\ge U(b)$, that $I_{(i,b)}^{(j,b')} \vee I_{(i,b)}^{(b',j)} < H^* - U_{ij}$. Hence we deduce that b and b' belong to $F(E)$ so that

$$I_{(i,b)}^{(j,b')} \le A_c(i,b)\wedge A_c(j,b') - U(i) - U(j)\ .$$

Hence, if $I_{(i,b)}^{(j,b')} = H^* - U_{ij}$, then $(i,b),(j,b')\in \mathbf{E}_{H^*}$, $U(i)=U(j)$, and $A_c(i,b) = A_c(j,b')$. However in this case, we get

$$I_{(i,b)}^{(j,b')} = A_c(i,b) - 2U(i) - \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b'))\ ,$$

so that $\mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0$. Hence we have proved that if $I_{(i,b)}^{(j,b')} = H^* - U_{ij}$, then

$$(H)\begin{cases} (i,b),(j,b') \in \mathbf{E}_{H^*} \\ U(i) = U(j) \\ \mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0 \ . \end{cases}$$

Conversely, if (H) holds, we deduce easily that $I^{(j,b')}_{(i,b)} = H^* - U_{ij}$. The proof is the same for $I^{(b',j)}_{(i,b)}$. Similarly, if $I^{(b',j)}_{(i,b)} = H^* - U_{ij}$, then $(i,b),(b',j) \in \mathbf{E}_{H^*}$ and $U(i) = U(j)$. Using the Lemma 2, we deduce that, under condition $C(E_{H^*})$, $\mathbf{C}^*_{(\{(b',j)\}\cup\mathbf{F})^c}((i,b),(b',j)) > 0$. So that $I^{(b',j)}_{(i,b)} < H^* - U_{ij}$, and the proof is complete.

Now we can prove Theorem 3.

Proof. Let us use here the notations introduced in the proof of Theorem 2, in particular $\tilde{h}$, m_h, $m_{\tilde{h}}$ and $c_{\tilde{h}}$ as well as relations (31), (32) and (34).

Assume first that there exists $f \in F(E)$ such that $h(f) \neq h(f_0)$. Then using Lemma 5 (i), we deduce that

$$m_{\tilde{h}} \leq K \exp(H_0\beta) \ .$$

Since h is not constant on $F(E)$, $c_{\tilde{h}}(0)$ is bounded from below by a strictly positive constant uniformly in β so that there exists $K > 0$ such that for any $\beta \geq 0$ we have

$$\rho_{\text{int},h} \leq K \exp(H_0\beta) \ .$$

Assume now that $h(f) = h(f_0),\ \forall f \in F(E)$. Then, using Lemma 5 (ii) and since there exists $c > 0$ such that $c_{\tilde{h}}(0) \geq c \exp(-U_h\beta)$ for any $\beta \geq 0$, we deduce that there exists $K > 0$ such that for any $\beta \geq 0$ we have

$$\rho_{\text{int},h} \leq K \exp(H^*\beta) \ .$$

Hence, parts (i) and (ii) (1) of the theorem are proved.

We turn now to the proof of part (ii) (2) and we assume that $h(f) = h(f_0),\ \forall f \in F(E)$.

Let us recall that we denote $U_h = \inf\{U(i) | \, h(i) \neq h(f_0)\}$. Assume first that for any $i \in E_{H^*}$ we have $U_h \neq U(i)$. Then, using Lemma 5 (iii), we deduce that there exists $H' < H^*$ and $K > 0$ such that for any $\beta \geq 0$ and any i, j such that $U(i) \wedge U(j) \geq U_h$, we have

$$|G_{ij}| \leq K \exp((H' - U_h)\beta) \ .$$

Hence, since again there exists $c > 0$ such that $c_{\tilde{h}}(0) \geq c \exp(-U_h\beta)$, we deduce that there exists $K > 0$ such that for any $\beta \geq 0$ we have

$$\rho_{\text{int},h} \leq K \exp(H'\beta) \ .$$

Assume now that there exists $i_* \in E_{H^*}$ such that $U(i_*) = U_h$, and that $C(E_{H^*})$ holds. Let $i, j \in E$ such that $U_{ij} =_{\text{def}} U(i) \wedge U(i) \geq U_h$. Using Lemma 5 (iii), we deduce that there exists $H' < H^*$ such that for any $b, b' \in E$, we have $I_{(i,b)}^{(b',j)} \leq H' - U_{ij}$. Hence there exists $K > 0$ such that for any $\beta \geq 0$

$$G_{ij}^2/c_h(0) \leq K \exp(H'\beta) \ .$$

Let us study now the behavior of the G_{ij}^1's. Let us note

$$A = \{(i,j) \in E_{H^*} \times E_{H^*} |\, U(i) = U(j) = U_h,\ C^*_{(\{j\}\cup F(E))^c}(i,j) = 0\} \ .$$

Since we assume that for any $(i,j) \in A$, we have $\tilde{h}(i)\tilde{h}(j) \geq 0$, we deduce that

$$\sum_{(i,j)\in A} \tilde{h}(i)\tilde{h}(j)G_{ij}^1 \geq \tilde{h}(i_*)\tilde{h}(i_*)G_{i_*i_*}^1 \ .$$

Now, since we assume that $(C(E_{H^*}))$ holds, we deduce from Lemma 3 that there exists $\beta_0 \geq 0$ and $K > 0$ such that, for all $\beta \geq \beta_0$,

$$G_{i_*i_*}^1/c_h(0) \geq K \exp(H^*\beta) \ .$$

Hence, to end the proof, it will be sufficient to prove that for any $(i,j) \notin A$, $U_{ij} \geq U_h$, there exists $K > 0$ and $H' < H^*$ such that for any $\beta \geq 0$ we have

$$G_{ij}^1/c_h(0) \leq K \exp(H'\beta) \ . \tag{36}$$

Moreover, to get (36) it is sufficient to prove that for any $b, b' \in E$, we have $I_{(i,b)}^{(j,b')} < H^* - U_h$. However, using Lemma 5, we get that if $I_{(i,b)}^{(j,b')} = H^* - U_h$ then $U(i) = U(j) = U_h$, $i, j \in E_{H^*}$ and $\mathbf{C}^*_{(\{(j,b')\}\cup\mathbf{F})^c}((i,b),(j,b')) = 0$. However, we deduce easily from Lemma 2 (ii) that $C^*_{(\{j\}\cup F(E))^c}(i,j) = 0$. This is in contradiction with the fact that $(i,j) \notin A$ so that (36) is proved and the proof of (ii) (3) is complete when $H^* > 0$.

When H^* is equal to 0, which implies that for any $i \notin F(E)$ and any $f \in F(E)$, $A_c(i,f) = U(i)$, using the same proof as in the case where $I^* + U_* = 0$ in Theorem 2, we get that there exists $\beta_0 > 0$ such that for all $\beta \geq \beta_0$, $\rho_{\text{int},h} \propto \exp(\beta H^*)$.

6. Concluding remarks

An interesting question is the existence of a true limit in β for $\ln(c_{\text{int},h}(\beta))/\beta$ as β tends to infinity. As a first remark, since $2c_{\text{int},h} = \mathscr{E}_{I-Q_\beta^* Q_\beta}(\psi_\beta, \psi_\beta)$, where ψ_β is the unique solution of the linear Poisson equation, we can deduce that if the components of Q_β are rational expressions in the variables $(e^{\alpha\beta})_{\alpha\in\mathbb{R}}$, $c_{\text{int},h}$ is also such a rational expression and the previous limit exists. However, in our larger framework of admissible families of Markov kernels, this limit may not exist and more importantly, even under the previous stronger assumptions, the limit may fail to depend only on the communication costs. As a counter-example, let us consider the three points configurations space $E = \{i, j, k\}$ and the following family of Markov kernels defined by

$$Q_\beta = \begin{pmatrix} \frac{1}{2} - \epsilon(\beta) & \frac{1}{2} + \epsilon(\beta) & 0 \\ \frac{1}{2} & \frac{1-e^{-H\beta}}{2} & \frac{e^{-H\beta}}{2} \\ 0 & \frac{e^{-\beta(H+D)}}{2} & 1 - \frac{e^{-\beta(H+D)}}{2} \end{pmatrix}$$

where D and H are strictly positive constants and $0 \leq \epsilon(\beta) \leq 1/3$ for all $\beta \geq 0$.

Note that we deduce from our constraint on $\epsilon(\beta)$ that $(Q_\beta)_{\beta\geq 0}$ is an admissible family. The virtual energy can be explicitly computed and we get $U(i) = U(j) = D$ and $U(k) = 0$. Moreover, one easily get that $I = I^* = H - D$ and $E_{I^*} = \{i, j\}$. Now, let h be the observable defined by $h(i) = -1$, $h(j) = 1$ and $h(k) = 0$. Solving explicitly the linear system (4), we can prove with a little piece of work, that

$$\frac{1}{\beta}\ln(c_{\text{int},h}(\beta)) = \left(\frac{2\ln(\epsilon(\beta))}{\beta} + H\right)^+ - D + O\left(\frac{1}{\beta}\right) .$$

Now, rewriting $\epsilon(\beta) = \frac{1}{3}e^{\frac{\beta}{2}(A(\beta)-H)}$ with $A(\beta) \leq H$, we get

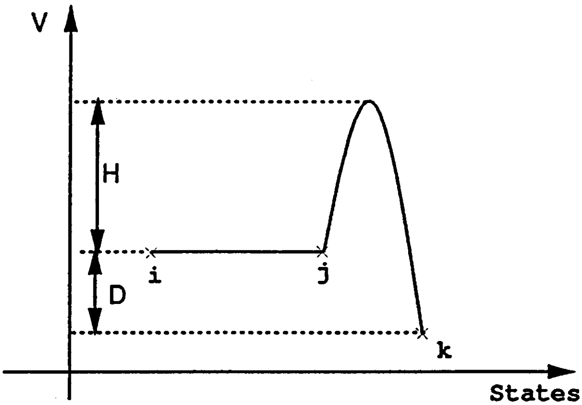

Fig. 1. Configurations space and communication costs

$$\frac{1}{\beta}\ln(c_{\text{int},h}(\beta)) = A(\beta)^+ - D + O\left(\frac{1}{\beta}\right) \; .$$

Since the constraint on $A(\beta)$ is very weak, the limit of $\ln(c_{\text{int},h}(\beta))/\beta$ exists iff $A(\beta)^+$ has a limit in β. As a consequence, without sharp constraints on the variations $\epsilon(\beta)$, the limit of $\frac{1}{\beta}\ln(c_{\text{int},h}(\beta))$ fails to exist. Moreover, this limit, when it exists, depends strongly on the variations of $\epsilon(\beta)$ and not only on the communication costs. This surprising result comes from the fact that the hypothesis of Theorem 2 is not fulfilled here since $(h(i) - h(k))(h(j) - h(k)) < 0$ (this shows that the positivity assumption can not be removed in Theorem 2). The key of this particular behaviour is hidden in the fact that for $\epsilon(\beta) = 0$, $Q_\beta(i,j) = Q_\beta(j,i) = 1/2$. Hence the averaged value of h for the process conditioned to stay in the cycle $\{i,j\}$ is negligible so that, roughly speaking, the fluctuations of $S_n(h)$ for the process within the cycle $\{i,j\}$ are of order $O(1/\sqrt{n})$ with *no* drift. However, for $\epsilon(\beta) > 0$, the symmetry between $Q_\beta(i,j)$ and $Q_\beta(j,i)$ is broken so that a non zero drift appears in the fluctuations of $S_n(h)$ within the cycle $\{i,j\}$ which may increase at an exponential order (in β) the value of $c_{\text{int},h}$. From this point of view, $\epsilon = 0$ is a critical point for our observable. As a consequence, our results stand in a sense in the largest set of observables for which one can expect a control of $\frac{1}{\beta}\ln(c_{\text{int},h}(\beta))$ independently of the bounded fluctuations of $Q_\beta(a,b)e^{\beta V(a,b)}$. For more precise results, one should clearly deal with a sharp estimate of the previous quantity which will take a part in the asymptotic behaviour of the integrated correlation time.

A. Appendix

The main result of this appendix is a general lemma which gives an exponential lower bound for the cumulated mass in a fixed point i before escaping from the largest cycle which contains i in its bottom.

Let $\Pi \in \mathscr{C}(E)$ be a cycle. Assume that that $\Pi \neq E$. Let γ be an element not in E, and denote $\widetilde{E} = \Pi \cup \{\gamma\}$. Now define, for $\alpha > 0$ small enough, $\widetilde{Q}_\beta : \widetilde{E} \times \widetilde{E} \to \mathbb{R}_+$ by

$$\begin{cases} \widetilde{Q}_\beta(i,j) &= Q_\beta(i,j) \text{ if } i,j \in \Pi, \\ \widetilde{Q}_\beta(i,\gamma) &= \sum_{j \notin \Pi} Q_\beta(i,j) \text{ if } i \in \Pi, \\ \widetilde{Q}_\beta(\gamma,j) &= \alpha \exp(\beta A_c(\Pi,\Pi^c)) \sum_{i \notin \Pi} \mu_\beta(i) Q_\beta(i,j) \text{ if } j \in \Pi \; , \\ \widetilde{Q}_\beta(\gamma,\gamma) &= 1 - \sum_{j \in \Pi} \widetilde{Q}_\beta(\gamma,j) \quad . \end{cases}$$

Lemma 6. *There exists* $\alpha > 0$ *such that for any* $\beta \geq 0$, $\widetilde{Q}_\beta$ *is an irreducible Markov kernel with unique invariant probability measure* $\widetilde{\mu}_\beta$ *defined on* $\widetilde{E}$ *by* $\widetilde{\mu}_\beta(i) = v_\beta(i)/v_\beta(\widetilde{E})$, *where*

$$v_\beta(i) = \begin{cases} \mu_\beta(i) \text{ if } i \in \Pi, \\ \alpha^{-1} \exp(-\beta A_c(\Pi, \Pi^c)) \text{ if } i = \gamma \end{cases} .$$

Let now $\widetilde{X}$ *be a Markov chain on* $\widetilde{E}$ *with transition kernel* $\widetilde{Q}$. *Then, there exists* $M > 0$ *and* $\beta_0 \geq 0$ *such that for all* $\beta \geq \beta_0$, *and all* $f \in F(\Pi)$,

$$E\left(\widetilde{\tau}_e\left(\widetilde{E}\backslash\{f\}\right) | \widetilde{X}_0 = f\right) \leq M \ .$$

Proof. For any $i \notin \Pi$ and any $j \in \Pi$, there exists $K_{i,j} \geq 0$ such that for all $\beta \geq 0$

$$\mu_\beta(i) Q_\beta(i,j) \leq K_{i,j} \mathrm{e}^{-(U(i)+V(i,j))\beta} \leq K_{i,j} \mathrm{e}^{-A_c(\Pi,\Pi^c)\beta} \ .$$

Hence, there exists $K > 0$ such that for any $\beta \geq 0$, $\widetilde{Q}_\beta(\gamma, j) \leq K\alpha$. Hence there exists $\alpha > 0$ such that $\widetilde{Q}_\beta$ is a Markov kernel on $\widetilde{E} \times \widetilde{E}$ for all $\beta \geq 0$. The irreducibility of $\widetilde{Q}_\beta$ follows easily from the irreducibility of Q_β. We easily check that for all $i \in \widetilde{E}$, $\sum_{j \in \widetilde{E}} v_\beta(j) \widetilde{Q}_\beta(j, i) = v_\beta(i)$. Hence the probability measure $\widetilde{\mu}_\beta$ is the unique invariant probability measure of $\widetilde{Q}_\beta$. Moreover, since $v(\gamma) \propto \mathrm{e}^{-A_c(\Pi,\Pi^c)\beta}$ and $v(j) \propto \mathrm{e}^{-U(j)\beta}$ for all $j \in \Pi$, we get that there exists $\beta_0 \geq 0$ and $c > 0$ such that for all $f \in F(\Pi)$, $\widetilde{\mu}_\beta(f) \geq c$ for all $\beta \geq \beta_0$. Since for any Markov chain $\widetilde{X}$ on $\widetilde{E}$ with transition probability $\widetilde{Q}_\beta$ $E\left(\widetilde{\tau}_e\left(\widetilde{E}\backslash\{f\}\right) | \widetilde{X}_0 = f\right) = 1/\widetilde{\mu}_\beta(f)$, the proof is complete.

Notation 8. Let $i \in E\backslash F(E)$ and denote Π_i the greatest cycle (for the inclusion order) among all the cycles Π such that $i \in F(\Pi)$. We denote $H_i = H_e(\Pi_i)$.

Lemma 7. *Let* $i \in E\backslash F(E)$. *Then for any* $0 \leq H \leq H_i$, *there exists* $R_0 > 0$ *and* $\beta_0 \geq 0$ *such that for all* $0 < R < R_0$ *there exists* $c > 0$ *which satisfies*

$$\sum_{k=0}^{[R\mathrm{e}^{H\beta}]} P(X_k = i,\ T_e(\Pi_i) > k | X_0 = i) \geq c\mathrm{e}^{H\beta}\ \forall\, \beta \geq \beta_0 \ . \tag{37}$$

Remark 7. Let $G_i(m) = \sum_{k=0}^{m} \mathbf{1}_{X_k = i}$ be the occupation time in i until time m. The lemma 7 states that $E(G_i([R\mathrm{e}^{H\beta}] \wedge T_e(\Pi_i))) \geq c\mathrm{e}^{H\beta}$. Quite precise results, in the continuous time setting, have been proved in [9] on the asymptotic law of $G_i(T_e(\Pi_i))$ after adequate time normalization. However, those results do not apply directly for $G_i([R\mathrm{e}^{H\beta}] \wedge T_e(\Pi_i))$ so that we give below an elementary proof of our lemma.

Proof. If $H = 0$, then (37) is straightforward. Assume that $H > 0$, so that $H_i > 0$. Then, from Theorem 1 (iii), there exists $\beta_0 \geq 0$, $R_0 > 0$ and $\delta > 0$ such that for any $R \leq R_0$, and all $\beta \geq \beta_0$, we have

$$P(T_e(\Pi_i) > \mathrm{Re}^{H\beta} \mid X_0 = i) \geq \delta \ .$$

Let now $T_1 = \tau_e(E \setminus \{i\})$ and define recursively $T_{k+1} = \inf\{n > T_k; X_n = i\}$. Let us define, for any $A > 0$,

$$H_A = P\Big(T_{[A\mathrm{e}^{H\beta}]} \leq \mathrm{Re}^{H\beta} < T_e(\Pi_i) | \ X_0 = i\Big) \ .$$

Let us consider the Markov Kernel $\widetilde{Q}$ and the Markov chain $\widetilde{X}$ associated with Π_i as in Lemma 6 (since $i \notin F(E)$, Π_i is different from E). Since H_A is also equal to $P(\widetilde{T}_{[A\mathrm{e}^{H\beta}]} \leq \mathrm{Re}^{H\beta} < \widetilde{T}_e(\Pi_i) | \ \widetilde{X}_0 = i)$, we deduce that

$$\begin{aligned} H_A &\geq P\Big(\widetilde{T}_{[A\mathrm{e}^{H\beta}]} \leq \mathrm{Re}^{H\beta} | \ \widetilde{X}_0 = i\Big) - P\Big(\mathrm{Re}^{H\beta} \geq \widetilde{T}_e(\Pi_i) | \ \widetilde{X}_0 = i\Big), \\ &\geq 1 - P\Big(\widetilde{T}_{[A\mathrm{e}^{H\beta}]} > \mathrm{Re}^{H\beta} | \ \widetilde{X}_0 = i\Big) - (1-\delta) \ . \end{aligned}$$

Applying at first Bienaymé-Chebyshev inequality, and then Markov property and Lemma 6 we get that

$$\begin{aligned} P\Big(\widetilde{T}_{[A\mathrm{e}^{H\beta}]} > \mathrm{Re}^{H\beta} | \ \widetilde{X}_0 = i\Big) &\leq E\Big(\widetilde{T}_{[A\mathrm{e}^{H\beta}]} | \ \widetilde{X}_0 = i\Big) / (\mathrm{Re}^{H\beta}) \\ &\leq \frac{[A\mathrm{e}^{H\beta}]}{\mathrm{Re}^{H\beta}} M \ \leq \frac{AM}{R} \ , \end{aligned}$$

so that $H_A \geq \delta - AM/R$. If we take $A = \delta R/2M$, we get $H_A \geq \delta/2$. Now, since

$$\begin{aligned} &\sum_{k=0}^{[\mathrm{Re}^{H\beta}]} P(X_k = i, \ T_e(\Pi_i) > k | \ X_0 = i) \\ &\qquad \geq 1 + \sum_{k=1}^{[\mathrm{Re}^{H\beta}]} P(X_k = i, \ T_e(\Pi_i) > \mathrm{Re}^{H\beta} | \ X_0 = i), \end{aligned}$$

and since

$$\sum_{k=1}^{[\mathrm{Re}^{H\beta}]} P(X_k = i, \ T_e(\Pi_i) > \mathrm{Re}^{H\beta} | \ X_0 = i) \geq [A\mathrm{e}^{H\beta}] H_A,$$

we get that $\sum_{k=0}^{[\mathrm{Re}^{H\beta}]} P(X_k = i, \ T_e(\Pi_i) > k | \ X_0 = i) \geq (A\delta/2)\mathrm{e}^{H\beta} = (\delta^2 R/2M)\mathrm{e}^{H\beta}$, and the proof is complete.

B. Appendix

This appendix is devoted to the statement of Lemmas 9 and 11 which link the localized costs to the communication altitude. Lemma 8 is used in the proof of Lemma 9, and Lemma 10 in the proof of Lemma 11.

Lemma 8. *Let $j \in \mathscr{E}$, $B \subset \mathscr{E}$ such that $j \in B$, and $q \in B^c$. Then*

$$C^*_{B\setminus\{j\}}(j,q) \leq C^*_B(j,q) + A_c(j,B^c) - \mathscr{U}(j) \ . \tag{38}$$

Proof. The proof will be done by induction on the size of B.

Let $B = \{j\}$, and $q \neq j$. Since $C^*_{\{j\}}(j,q) = \mathscr{U}(j) + \mathscr{V}(j,q) - A_c(j,\{j\}^c)$ and $C^*_\emptyset(j,q) = \mathscr{V}(j,q)$, we get the inequality (38) and the proof is complete for $B = \{j\}$.

Assume now that the lemma is proved for $|B| \leq n$. Let B be a set which contains j of size $n+1$ and Π_j be the unique cycle in $\mathscr{M}_*(B)$ containing j. Let $q \in B^c$, $g \in \mathrm{Pth}_B(j,q)$ such that $C_B(g) = C^*_B(j,q)$ and $k_0 = \sup\{k \geq 0 |\ g_k \in \Pi_j\}$. Since there exists $g' \in \mathrm{Pth}_{\Pi_j}(j, g_{k_0})$ such that $C_{\Pi_j}(g') = 0$, we can suppose that for all $k \leq k_0$, $g_k \in \Pi_j$. Let us denote now $m^1 = (g_0, \ldots, g_{k_0+1})$, and $m^2 = (g_{k_0+1}, \ldots, g_{n_g})$.

Let $a \in \Pi_j$. If B is a cycle, then $A_c(a, \Pi_j^c) = \mathscr{U}(B) + H_m(B) \leq A_c(a, B^c) = \mathscr{U}(B) + H_e(B)$ and

$$C_{\Pi_j}(a,b) = \begin{cases} C_B(a,b) & \text{if } b \in B \\ C_B(a,b) + H_e(B) - H_m(B) & \text{if } b \in B^c \end{cases}, \text{ so that}$$

$$C_{\Pi_j}(m^1) = C_B(m^1) + (H_e(B) - H_m(B))\mathbf{1}_{g_{k_0+1}\notin B} \ . \tag{39}$$

If B is not a cycle, then $A_c(a, \Pi_j^c) = A_c(a, B^c)$ so that $C_B(a,b) = C_{\Pi_j}(a,b)$ for any $b \in \mathscr{E}$ and

$$C_{\Pi_j}(m^1) = C_B(m^1) \ . \tag{40}$$

Indeed, we already have that $A_c(a,B^c) \geq A_c(a,\Pi_j^c)$. Let us assume now that $A_c(a,\Pi_j^c) < A_c(a,B^c)$, and let $\Pi'_j = \{c \in \mathscr{E} |\ A_c(a,c) \leq A_c(a,\Pi_j^c)\}$. The set Π'_j is a cycle and satisfies $\Pi_j \subset \Pi'_j \subset B$. Since B is not a cycle, and since $\Pi'_j \neq \Pi_j$, we obtain a contradiction with the definition of Π_j.

Assume first that $k_0 = n_g - 1$ i.e. $m^1 = g$ and m^2 is empty. Then, if B is a cycle, we deduce from the induction hypothesis and (39) that

$$\begin{aligned} C^*_{B\setminus\{j\}}(j,q) &\leq C^*_{\Pi_j\setminus\{j\}}(j,q) \leq C^*_{\Pi_j}(j,q) + A_c(j,\Pi_j^c) - \mathscr{U}(j) \\ &\leq C_{\Pi_j}(m^1) + A_c(j,\Pi_j^c) - \mathscr{U}(j) \\ &= C_B(m^1) + (H_e(B) - H_m(B)) + A_c(j,\Pi_j^c) - \mathscr{U}(j) \\ &= C_B(m^1) + A_c(j,B^c) - \mathscr{U}(j) = C^*_B(j,q) + A_c(j,B^c) - \mathscr{U}(j) \ , \end{aligned}$$

so that inequality (38) is proved. If B is not a cycle, then we deduce from the induction hypothesis and (40) that

$$\begin{aligned} C^*_{B\setminus\{j\}}(j,q) &\le C^*_{\Pi_j\setminus\{j\}}(j,q) \le C^*_{\Pi_j}(j,q) + A_c(j,\Pi_j^c) - \mathscr{U}(j) \\ &\le C_B(m^1) + A_c(j,B^c) - \mathscr{U}(j) \\ &= C^*_B(j,q) + A_c(j,B^c) - \mathscr{U}(j)\ , \end{aligned}$$

so that inequality (38) is proved in this case.

Assume now that $k_0 + 1 < n_g$ i.e. $g_{k_0+1} \in B$ and m^2 is not empty. Let $a \in B \setminus \Pi_j$. If B is a cycle, then $A_c(a,\Pi_j) = \mathscr{U}(B) + H_m(B) \le A_c(a,B^c) = \mathscr{U}(B) + H_e(B)$ and

$$C_{B\setminus\Pi_j}(a,b) = \begin{cases} C_B(a,b) & \text{if } b \in B\setminus\Pi_j \\ C_B(a,b) + H_e(B) - H_m(B) & \text{if } b \in B^c \end{cases},$$

so that

$$C_{B\setminus\Pi_j}(m^2) = C_B(m^2) + H_e(B) - H_m(B)\ . \tag{41}$$

If B is not a cycle then $A_c(a,\Pi_j) \ge A_c(a,B^c)$ so that $C_B(a,b) = C_{B\setminus\Pi_j}(a,b)$ and

$$C_{B\setminus\Pi_j}(m^2) = C_B(m^2)\ . \tag{42}$$

Indeed, if we assume that $A_c(a,\Pi_j) < A_c(a,B^c)$, then considering the cycle $\Pi' = \{c \in \mathscr{E} |\ A_c(a,c) \le A_c(a,\Pi_j)\}$, we deduce that Π' is a cycle included in B and containing a and Π_j. Since B is not a cycle, $\Pi' \ne B$, which is in contradiction with $\Pi_j \in \mathscr{M}_*(B)$.

From (39), (41) and the induction hypothesis, we deduce that if B is a cycle, then

$$\begin{aligned} C^*_{B\setminus\{j\}}(j,q) &\le C^*_{B\setminus\{j\}}(j,g_{k_0+1}) + C^*_{B\setminus\{j\}}(g_{k_0+1},q) \\ &\le C^*_{\Pi_j\setminus\{j\}}(j,g_{k_0+1}) + C^*_{B\setminus\Pi_j}(g_{k_0+1},q) \\ &\le C^*_{\Pi_j}(j,g_{k_0+1}) + (A_c(j,\Pi_j^c) - \mathscr{U}(j)) + C_{B\setminus\Pi_j}(m^2) \\ &\le C_{\Pi_j}(m^1) + (A_c(j,\Pi_j^c) - \mathscr{U}(j)) \\ &\quad + C_B(m^2) + (H_e(B) - H_m(B)) \\ &\le C_B(g) + (A_c(j,B^c) - \mathscr{U}(j)) \\ &\le C^*_B(j,q) + A_c(j,B^c) - \mathscr{U}(j)\ , \end{aligned}$$

so that inequality (38) is proved in this case. Now, if B is not a cycle, we deduce from (40), (42) and the induction hypothesis that

$$\begin{aligned}
C^*_{B\setminus\{j\}}(j,q) &\le C^*_{B\setminus\{j\}}(j,g_{k_0+1}) + C^*_{B\setminus\{j\}}(g_{k_0+1},q) \\
&\le C^*_{\Pi_j\setminus\{j\}}(j,g_{k_0+1}) + C^*_{B\setminus\Pi_j}(g_{k_0+1},q) \\
&\le C^*_{\Pi_j}(j,g_{k_0+1}) + (A_c(j,\Pi_j^c) - \mathscr{U}(j)) + C_{B\setminus\Pi_j}(m^2) \\
&\le C_{\Pi_j}(m^1) + (A_c(j,B^c) - \mathscr{U}(j)) + C_B(m^2) \\
&\le C^*_B(j,q) + (A_c(j,B^c) - \mathscr{U}(j)) \ ,
\end{aligned}$$

so that the proof is complete.

Lemma 9. *Let F be a subset of $F(\mathscr{E})$ and let $j \in \mathscr{E}$. We have the following relation between the localized costs and the communication altitude*

$$C^*_{(F\cup\{j\})^c}(j,F) = A_c(j,F) - \mathscr{U}(j) \ . \tag{43}$$

Proof. If j belongs to F, the result is clear. Let then $j \notin F$. Let Π_j be the unique cycle in $\mathscr{M}(F^c)$ containing j (note that we do not impose here Π_j to be strictly included in F^c). Let us prove the inequality

$$C^*_{(F\cup\{j\})^c}(j,F) \ge A_c(j,F) - \mathscr{U}(j) \ .$$

Let $a \in \Pi_j$. Since $A_c(a,j) \le A_c(a,\Pi_j^c) \le A_c(a,F)$ we deduce that for any $b \in \mathscr{E}$, $C_{(F\cup\{j\})^c}(a,b) = C_{\Pi_j\setminus\{j\}}(a,b)$ and

$$C^*_{(F\cup\{j\})^c}(j,\Pi_j^c) = C^*_{\Pi_j\setminus\{j\}}(j,\Pi_j^c) \ . \tag{44}$$

However, we have $C^*_{\Pi_j\setminus\{j\}}(j,\Pi_j^c) = \mathscr{U}(\Pi_j) + H_e(\Pi_j) - \mathscr{U}(j)$ (cf Lemma 3.5 in [12]). Since from the definition of Π_j we get $\mathscr{U}(\Pi_j)+H_e(\Pi_j) = A_c(j,\Pi_j^c) = A_c(j,F)$, we deduce

$$C^*_{(F\cup\{j\})^c}(j,F) \ge C^*_{(F\cup\{j\})^c}(j,\Pi_j^c) = A_c(j,F) - \mathscr{U}(j) \ .$$

Let us prove now the inequality

$$C^*_{(F\cup\{j\})^c}(j,F) \le A_c(j,F) - \mathscr{U}(j).$$

Since $C^*_{F^c}(j,F) = 0$, there exists then $f \in F$ such that $C^*_{F^c}(j,f) = 0$. Applying Lemma 8, we deduce that $C^*_{F^c\setminus\{j\}}(j,f) \le A_c(j,F) - \mathscr{U}(j)$ ($j \in F^c$). Hence the proof of Lemma 9 is complete.

Lemma 10. *Let Π be a cycle, $i \in \Pi$, and $f \in F(\Pi)$. Then, we have*

$$C^*_{\Pi\setminus\{f\}}(i,\Pi^c) \ge A_c(i,\Pi^c) - A_c(i,f) \ .$$

Proof. Let $B = \Pi \setminus \{f\}$ and $q \in \Pi^c$. Using Lemma 8 we get

$$\begin{aligned}
C^*_{\Pi\setminus\{i\}}(i,\Pi^c) \le C^*_{B\setminus\{i\}}(i,\Pi^c) &\le C^*_{B\setminus\{i\}}(i,q) \\
&\le C^*_B(i,q) + A_c(i,B^c) - \mathscr{U}(i).
\end{aligned}$$

Hence $C^*_{\Pi\setminus\{i\}}(i,\Pi^c) \leq C_{\Pi\setminus\{f\}}(i,\Pi^c) + A_c(i,B^c) - \mathcal{U}(i)$. Since $A_c(i,\ \{f\} \cup \Pi^c) = A_c(i,f)$ and $C^*_{\Pi\setminus\{i\}}(i,\Pi^c) = A_c(i,\Pi^c) - \mathcal{U}(i)$ ([12]), we get $C^*_{\Pi\setminus\{f\}}(i,\Pi^c) \geq A_c(i,\Pi^c) - A_c(i,f)$.

Lemma 11. *Let $i \in \mathcal{E}$, $j \in \mathcal{E}$, and F a subset of $F(\mathcal{E})$. If we have $A_c(i,F) < A_c(j,F)$, then $C^*_{(F\cup\{j\})^c}(i,j) \geq A_c(j,F) - A_c(i,F)$.*

Proof. We claim first that $A_c(j,F) \leq A_c(i,j)$. Let indeed $f \in F$ such that $A_c(i,f) = A_c(i,F)$. Since $A_c(j,f) \leq A_c(i,j) \vee A_c(i,f)$, and since $A_c(i,F) < A_c(j,F)$, we deduce that $A_c(i,F) < A_c(j,f) \leq A_c(i,j)$, and our statement is proved.

Let now Π_{ij} be the smallest cycle which contains i and j, and $f \in F$ satisfying $A_c(i,f) = A_c(i,F)$. Note that $f \in \Pi_{ij}$ $(A_c(i,f) < A_c(i,j))$. Let us denote $\Pi_i \in \mathcal{M}_*(\Pi_{ij})$ containing i. Since $(F \cup \{j\})^c \subset \{f\}^c$, we have

$$C^*_{(F\cup\{j\})^c}(i,j) \geq C^*_{\{f\}^c}(i,j)\ .$$

Now, since $j \notin \Pi_i$, $C^*_{\{f\}^c}(i,j) \geq C^*_{\{f\}^c}(i,\Pi_i^c)$. Checking that $C^*_{\{f\}^c}(i,\Pi_i^c) = C^*_{\Pi_i\setminus\{f\}}(i,\Pi_i^c)$ and using Lemma (10), we get

$$C^*_{(F\cup\{j\})^c}(i,j) \geq A_c(i,\Pi_i^c) - A_c(i,f)\ .$$

Since $A_c(i,\Pi_i^c) = A_c(i,j) \geq A_c(j,F)$, and $A_c(i,f) = A_c(i,F)$, the proof is complete.

Acknowledgement. We thank very much the referee for his careful reading and helpful suggestions (especially those concerning the link with Poisson equation) which improve the final version.

References

1. Billingsley, P.: Convergence of Probability Measures. John Wiley &Sons, (1968)
2. Catoni,O.: Sharp large deviations estimates for simulated annealing algorithms. Ann. Inst. H. Poincaré Probab. Statist., **27**(3), 291–383 (1991)
3. Catoni, O.: Rough large deviation estimates for simulated annealing. Application to exponential schedules. Ann. Probab., **20**, 1109–1146 (1992)
4. Freidlin, M.I., Wentzell, A.D.: Random Perturbations of Dynamical Systems, volume 260. Springer-Verlag (1984)
5. Gaudron, I.: Rate of convergence of the Swendsen-Wang dynamics in image segmentation problems: a theoretical and experimental study. ESAIM: Probability and Statistics, Vol. 1, 259–284, (1997)
6. Lindvall, T.: Lectures on the coupling methods. Wiley Series in Probability and Mathematical Statistics. Wiley (1992)
7. Miclo, L.: Comportement de spectre d'opérateur de Schrödinger à basse température. Bull. Sc. math., **119**, 529–553 (1995)
8. Miclo, L.: Remarques sur l'ergodicité des algorithmes de recuit simulé sur un graphe. Stochastic Process. Appl. 58, n°2, 329–360 (1995)

9. Miclo, L.: Sur les temps d'occupations des processus de Markov finis inhomogènes à basse température Preprint (1995), to appear in Stochastics and Stochastics Reports.
10. Sokal, A.D.: Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms. Cours de Troisième cycle de la Physique en Suisse Romande (1989)
11. Trouvé, A.: Parallélisation massive du recuit simulé. PhD thesis, Université d'Orsay, Jan (1993)
12. Trouvé, A.: Rough large deviation estimates for the optimal convergence speed exponent of generalized simulated annealing algorithm. Ann. Inst. H. Poincaré. Probab. Statist., **32**(2) (1996)