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Applications of sharp large deviations estimates to optimal cooling schedules

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ABSTRACT. — This is the second part of "Sharp large deviations estimates for simulated annealing algorithms". We give applications of our estimates focused on the problem of quasi-equilibrium. Is quasi-equilibrium maintained when the probability of being in the ground state at some finite large time is maximized? The answer is negative. Nevertheless the density of the law of the system with respect to the equilibrium law stays bounded in the "initial part" of the algorithm. The corresponding shape of the optimal cooling schedules is $1/T_n = d^{-1} \ln n + B + o(1)$ where d is Hajek's critical depth. The influence of variations of B on the law of the system and its density with respect to thermal equilibrium is studied: if B is above some critical value the density has an exponential growth and the rate of convergence can be made arbitrarily poor by increasing B. All these computations are made in the non-degenerate case when there is only one ground state and Hajek's critical depth is reached only once.

Key words : Simulated annealing, large deviations, non-stationary Markov chains, optimal cooling schedules.

RÉSUMÉ. — Cet article constitue le deuxième volet de notre étude des « Estimées précises de grandes déviations pour les algorithmes de recuit simulé ». Nous donnons ici des applications de ces estimées ayant trait à

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la question de l'équilibre thermique. Un quasi-équilibre thermique s'établit-il lorsque la suite des températures est choisie de façon à maximiser la probabilité pour que le système soit dans l'état fondamental à un instant lointain fixé? La réponse est négative. Néanmoins la densité de la loi du système par rapport à la loi d'équilibre reste bornée dans la partie initiale de l'algorithme. La forme correspondante des suites optimales de températures a un développement de la forme $1/T_n = d^{-1} \ln n + B + o(1)$ où d est la profondeur critique de Hajek. Nous étudions l'influence des variations de B sur la loi du système et sur sa densité par rapport à la loi d'équilibre : si B dépasse une certaine valeur critique, la densité a une croissance exponentielle avec le temps et la vitesse de convergence peut être rendue arbitrairement lente en augmentant B. Tous ces calculs sont menés dans le cas non dégénéré où il existe un unique état fondamental et où la profondeur de Hajek n'est pas atteinte plus d'une fois.

CONTENTS

INTRODUCTION

The study of cooling schedules of the type $1/T_n = A \ln n$ is the subject of most of the literature about annealing (D. Geman and S. Geman [9], Holley and Stroock [13], Hwang and Sheu [14], Chiang and Chow [6]). We investigate here for the first time the critical case $A = 1/d$ where d is Hajek's critical depth. We show that it is natural to introduce a second constant $1/T_n = d^{-1} \ln n + B$ and that quasi-equilibrium is never maintained in this case, but that the distance to quasi-equilibrium depends heavily on the choice of B.

These critical schedules are not merely a curiosity: when one fixes the simulation time *a priori* the "best" cooling schedules take this shape in their initial part. The final part of optimal schedules is beyond the scope of this paper and will be reported elsewhere.

This paper is the second part of "Sharp large deviations estimates for simulated annealing algorithms". We will assume that the reader is acquainted with the results and notations of the first part.

This work, as well as the preceding one, would not have come to birth without the incentive influence of R. Azencott, who has directed the thesis from which it is drawn, let him receive my sincere thanks again.

1. ESTIMATION OF THE PROBABILITY OF THE CRITICAL CYCLE

Our aim here is to study cooling schedules of the type $1/T_n = A \ln n + B$. The introduction of the non classical constant B will be justified when A takes its critical value.

We restrict ourselves to the case where there is only one global minimum and one deepest cycle not containing this global minimum. We will call this deepest cycle the criticle cycle, or Γ. We are interested in the case when the annealing algorithm converges. The condition for convergence is $A \leqq H(\Gamma)^{-1} = H'(E)^{-1}$.

When $A < H(\Gamma)^{-1}$, then $\sum_{k=m+1}^{n} e^{-H(\Gamma)/T_k}$ can be made large and $1/T_n - 1/T_m$ can be made small at the same time, and we can consider that temperature is almost constant. We will prove in that case that

$$\lim_{n \to +\infty} \frac{P(X_n = i)}{e^{-U_i/T_n}} = 1, \qquad i \in E.$$

The system remains in a state of quasi-equilibrium during the cooling process. This result is not new (*cf.* Hwang and Sheu [14], Chiang and Chow [6]).

When $A = H(\Gamma)^{-1}$ we can no more consider that temperature is almost constant. We have to study the behaviour of the system in the subdomain $E - (\{f\} \cup \Gamma)$ where f is the fundamental state (the global minimum). Indeed the probability to stay in $E - (\{f\} \cup \Gamma)$ during times m to n is of order

$$\prod_{k=m+1}^{n} (1 - a e^{-H(E - (\{f\} \cup \Gamma))/T_k}),$$

and $H(E-(\{f\}\cup\Gamma))<H(\Gamma)$. Thus during its life in $E-(\{f\}\cup\Gamma)$ the system can be considered to be at almost constant temperature. Studying the jumps of the system from f to Γ and back will give an estimate of $P(X_n\in\Gamma)$. From this estimate we will derive in a second step an equivalent of the law of X_n.

We will show that the influence of the second term B is decisive when $A=H(\Gamma)^{-1}=H'(E)^{-1}$ and that there is a value of B for which

$$P(X_n\in\Gamma)\simeq \min_{T_1,\ldots,T_n} P(X_n^T\in\Gamma).$$

We will need the following definitions throughout the discussion:

DEFINITION 1.1. – *Let* (E, U, q) be an energy landscape. An initial distribution $\mathscr{L}_0$ *will be called* γ*-uniform if*

$$\mathscr{L}_0(i)\geqq\gamma,\qquad i\in E. \tag{1}$$

DEFINITION 1.2. – *An energy landscape* (E, U, q) *will be said to be non-degenerate if:*

• *The energy* U *reaches its minimum on a single state of* E, *equivalently* $|F(E)|=1$.

• *There is in* $\mathscr{C}'$(E, U, q) *a single cycle of maximal depth, equivalently*

$$|\{C\in\mathscr{C}'(E):H(C)=H'(E)\}|=1. \tag{2}$$

We will call this cycle the critical cycle of (E, U, q).

1.1. A lower bound for any cooling schedule

The speed at which a cycle may be emptied will turn to be linked with the following quantity which we will call the "difficulty" of the cycle.

DEFINITION 1.3. – *Let* (E, U, q) *be any annealing framework. Let* C *be a cycle of* $\mathscr{C}'$(E) *which is maximal for inclusion. We define the difficulty of* C *to be the quantity*

$$\delta(C)=H(C)/U(C). \tag{3}$$

[*Let us remind that* $U(E)=0$ *by convention.*]

DEFINITION 1.4. – *Let* (E, U, q) *be a non-degenerate energy landscape. We introduce the second critical depth* S(E) *to be*

$$S(E)=\max\{H(C):C\in\mathscr{C}'(E),\ C\neq\Gamma\}, \tag{4}$$

where Γ *is the critical cycle of* E.

Let $\bar\Gamma$ be the natural context of Γ (that is the smallest cycle containing both Γ and f). Let $(G_k)_{k=1,\ldots,r}$ be the natural partition of $\bar\Gamma$. Assume that the G_ks are indexed according to decreasing depths, thus $f\in G_1$ and

$G_2=\Gamma$. Let Y be the Markov chain on the "abstract" space $\{1, \ldots, r\}$ with transitions

$$P(Y_{n+1}=k' \mid Y_n=k)=q(G_k, G_{k'})/q(G_k). \tag{5}$$

Let σ be the stopping time

$$\sigma=\inf\{n>0: Y_n \in \{1,2\}\}. \tag{6}$$

We define $\tilde{q}$ to be the critical communication rate

$$\tilde{q}=|F(\Gamma)|^{-(1+\delta(\Gamma))} q(\Gamma) P(Y_\sigma=1 \mid Y_0=2). \tag{7}$$

The introduction of the term $|F(\Gamma)|^{-(1+\delta)}$ is somewhat arbitrary. The meaning of $\tilde{q}$ will be clear from equation (34) in lemma 1.9. It is the multiplicative constant in the expression of the transitions between f and Γ viewed as two abstract states in a large scale of time.

We define also a critical communication kernel K on the abstract space $\{1,2\}$ by

$$K(m, n)=P(Y_\sigma=n \mid Y_0=m). \tag{8}$$

Let us notice that $K(2,2)\neq 0$ and $K(1,1)\neq 0$. $K(1,2)$ is the probability to jump from f into Γ knowing that the system has jumped out of $G_1 \ni f$.

PROPOSITION 1.5. — *There are positive constants* T_0, α *and* β *such that in the cooling framework* $\mathscr{G}(T_0, H(\Gamma))$, *for any initial distribution* $\mathscr{L}_0$, *putting* $\delta=\delta(\Gamma)$,

$$N_1=N(H(\Gamma), T_1, -\alpha, 0) \tag{9}$$

and

$$N_2=N(H(\Gamma), T_{N_1+1}, -\alpha, N_1), \tag{10}$$

we have

$$P(X_{N_2}\in\Gamma)^{-\delta}-P(X_{N_1}\in\Gamma)^{-\delta} \leq (1+\exp(-\beta/T_1))(1+\delta^{-1})^{-(1+\delta)}\tilde{q}(N_2-N_1). \tag{11}$$

Remark. — During times 0 to N_1 the chain X reaches a state of "partial equilibrium" where the memory of the initial distribution $\mathscr{L}_0$ is reduced to the quantity $\mathscr{L}_0(\Gamma)$ in a sens which the proof will make clear.

Proof of proposition 1.5. — It will require a succession of lemmas.

Let g be some state in $F(\Gamma)$ and let us put $E^{**}=E-\{f, g\}$. We begin with a formula.

LEMMA 1.6. — *We have*

$$P(X_{N_2}\in\Gamma)-P(X_{N_1}\in\Gamma)=\sum_{n=N_1+1}^{N_2}\sum_{m=0}^{n}P(X_m=g)\,M(E^{**},\Gamma)^{E,n}_{g,m}$$
$$+P(X_m=f)\,M(E^{**},\Gamma)^{E,n}_{f,m}-P(X_m=g)\,M(E^{**},E-\Gamma)^{E,n}_{g,m}$$
$$-P(X_m=f)\,M(E^{**},E-\Gamma)^{E,n}_{f,m}+\sum_{n=N_1+1}^{N_2}\sum_{j\in E^{**}}P(X_0=j)\,M(E^{**},\Gamma)^{E,n}_{j,0}$$
$$-P(X_0=j)\,M(E^{**},E-\Gamma)^{E,n}_{j,0}. \quad (12)$$

Proof. — We write

$$P(X_{N_2}\in\Gamma)-P(X_{N_1}\in\Gamma)$$
$$=\sum_{n=N_1+1}^{N_2}P(X_{n-1}\notin\Gamma,X_n\in\Gamma)-P(X_{n-1}\in\Gamma,X_n\notin\Gamma), \quad (13)$$

then we condition each term of this difference by the last visit to $\{f, g\}$.

End of the proof of lemma 1.6.

Let us state now to which class belong the GTKs of lemma 1.6. The results of proposition I.4.5 about the behaviour of annealing in restricted domains and the composition lemmas are leading to the following theorem:

LEMMA 1.7. — *There exist positive constants* T_0, *a and* α *such that in the cooling schedule* $\mathcal{G}(T_0, S(E))$

- *the kernel* $M(E^{**},\Gamma)^E_g$ *is of class*

$$\mathcal{E}(H(\Gamma), q(\Gamma)K(2,2), S(E), a), \quad (14)$$

- *the kernel* $M(E^{**},\Gamma)^E_f$ *is of class*

$$\mathcal{E}(H(\Gamma)+U(\Gamma), q(\Gamma)K(2,1), S(E), a), \quad (15)$$

- *the kernel* $M(E^{**},E-\Gamma)^{E,n}_{g,m}$ *is of class*

$$\mathcal{E}(H(\Gamma), q(\Gamma), S(E), a), \quad (16)$$

- *the kernel* $M(E^{**},E-\Gamma)^{E,n}_{f,m}$ *is of class*

$$\mathcal{E}(H(\Gamma)+\alpha, q(\Gamma), S(E), a), \quad (17)$$

- *for any* $i\in E^{**}$ *the kernels* $M(E^{**},\Gamma)^E_j$ *and* $M(E^{**},E-\Gamma)^E_j$ *are of class*

$$\mathcal{E}-(0, S(E)). \quad (18)$$

We deduce from this lemma the following proposition:

PROPOSITION 1.8. — *For any energy landscape with communications* (E, U, *q*), *there are positive constants* T_0 *and* β *such that in* $\mathcal{G}(T_0, H(\Gamma))$ *for any positive constant* $\alpha\leqq\beta$, *for* $N_1=N(H(\Gamma), T_1, -\alpha, 0)$ *and any*

$N_2 > N_1$, *we have*

$$P(X_{n_2} \in \Gamma) - P(X_{N_1} \in \Gamma) \geqq \left(1 - e^{-\alpha/T_1} - 2q(\Gamma) \sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}\right)$$
$$\times \left\{ (1 - e^{-\alpha/(4T_1)} - P(X_{N_1} \in \Gamma)) \sum_{n=N_1+1}^{N_2} e^{-(H(\Gamma)+U(\Gamma))/T_n} q(\Gamma) K(2,1) \right.$$
$$+ \frac{P(X_{N_1} \in \Gamma)}{|F(\Gamma)|} K(2,2) \left(1 - e^{-\alpha/(2T_1)} - 2q(\Gamma) \sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}\right)$$
$$\left. \times \left(q(\Gamma) \sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n} - e^{-\alpha/(2T_1)}\right)\right\}$$
$$- P(X_{N_1} \in \Gamma)\left((1 + e^{-\alpha/T_1}) \frac{q(\Gamma)}{|F(\Gamma)|} \sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n} + e^{-\alpha/T_1}\right). \quad (19)$$

Proof of proposition 1.8. – We have

$$P(X_{N_2} \in \Gamma) - P(X_{N_1} \in \Gamma)$$
$$= \sum_{n=N_1+1}^{N_2} P(X_{n-1} \notin \Gamma, X_n \in \Gamma) - P(X_{n-1} \in \Gamma, X_n \notin \Gamma), \quad (20)$$

moreover

$$\sum_{n=N_1+1}^{N_2} P(X_{n-1} \in \Gamma, X_n \notin \Gamma)$$
$$= \sum_{j \in \Gamma} \sum_{n=N_1+1}^{N_2} P(X_{N_1} = j) M(\Gamma, E - \Gamma)_{j, N_1}^{E, n}$$
$$+ \sum_{l=N_1+1}^{N_2} P(X_{l-1} \notin \Gamma, X_l = j) M(\Gamma, E - \Gamma)_{j, l}^{E, n}. \quad (21)$$

The second term in the right member of this equality is lower than

$$\sum_{l=N_1+1}^{N_2} \sum_{j \in \Gamma} P(X_{l-1} \notin \Gamma, X_l = j)\left(2q(\Gamma) \sum_{k=N_1+1}^{N_2} e^{-H(\Gamma)/T_k} + e^{-\alpha/T_{N_1}}\right) \quad (22)$$

and the first is lower than

$$P(X_{N_1} \in \Gamma)\left[(1 + e^{-\alpha/T_1}) \frac{q(\Gamma)}{|F(\Gamma)|} \sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n} + e^{-\alpha/T_1}\right]. \quad (23)$$

Moreover

$$\sum_{l=N_1+1}^{N_2} P(X_{l-1}\notin\Gamma, X_l\in\Gamma)\geqq \sum_{n=N_1+1}^{N_2}\sum_{m=0}^{n-1} P(X_m=f)\,M(E^{**},\Gamma)_{f,m}^{E,n} + P(X_m=g)\,M(E^{**},\Gamma)_{g,m}^{E,n}. \quad (24)$$

Let us put $N_{0.5}=N(H(\Gamma), T_1, -2\alpha, 0)$ and $N_{1.5}=N(H(\Gamma), T_1, -\alpha, N_1)$.

For any $m\in[N_{1.5}, N_2]$ (if any) we have

$$P(X_m=g)\geqq|F(\Gamma)|^{-1}P(X_{N_1}\in\Gamma)\times\left(1-2q(\Gamma)\sum_{n=N_1+1}^{N_2}e^{-H(\Gamma)/T_n}-e^{-\alpha/T_1}\right)(1-e^{-\alpha/T_1}) \quad (25)$$

because g is a concentration set of Γ.

For any $m\in[N_{0.5}, N_1]$

$$P(X_m=f)+P(X_m\in\Gamma)\geqq 1-e^{-\alpha/T_1} \quad (26)$$

as we can see from the fact that

$$H(E-(G_1\cup G_2))<H(G_1)\wedge H(G_2), \quad (27)$$

and the fact that f is a concentration set of G_1 and that $H'(G_1)<H(\Gamma)$.

Moreover

$$(1-e^{-\alpha/(2T_1)})P(X_m\in\Gamma)\leqq P(X_m\in\Gamma)\left(1-2q(\Gamma)\sum_{k=1}^{N_1}e^{-H(\Gamma)/T_k}-e^{-\alpha/T_1}\right)\leqq P(X_{N_1}\in\Gamma), \quad (28)$$

hence

$$P(X_m=f)\geqq 1-e^{-\alpha/T_1}-(1+e^{-\alpha/(3T_1)})P(X_{N_1}\in\Gamma)\geqq 1-e^{-\alpha/(3T_1)}-P(X_{N_1}\in\Gamma). \quad (29)$$

For $m\geqq N_1$

$$P(X_m=f)\geqq(1-e^{-\alpha/T_1})P(X_{N_1}=f)\geqq(1-e^{-\alpha/T_1})(1-P(X_{N_1}\in\Gamma)-e^{-\alpha/T_1}), \quad (30)$$

because $P(X_m=f\,|\,X_{N_1}=f)\geqq 1-e^{-\alpha/T_1}$, as can be seen from the fact that $\{f\}$ is a concentration set of E. This is true even for $m-N_1$ small, this can be seen by starting at time s sufficiently remote in the past (if necessary we start at a negative time, putting $T_l=T_1$ for $l\leqq 0$). Then (whatever the initial distribution) $P(X_m=f)\geqq 1-e^{-\alpha/T_1}$ and $P(X_{N_1}=f)\geqq 1-e^{-\alpha/T_1}$, hence

$$P(X_m=f\,|\,X_{N_1}=f)\geqq\frac{1-P(X_{N_1}\neq f)-P(X_m\neq f)}{P(X_{N_1}=f)}\geqq 1-2e^{-\alpha/T_1}.$$

Hence

$$\sum_{l=N_1+1}^{N_2} P(X_{l-1}\notin\Gamma, X_l\in\Gamma)$$

$$\geqq \sum_{n=N_1+1}^{N_2} e^{-(H(\Gamma)+U(\Gamma))/T_n} q(\Gamma) K(2,1)(1-e^{-\alpha/T_1})(1-e^{-\alpha/(3T_1)}-P(X_{N_1}\in\Gamma))$$

$$+\sum_{n=N_{1.75}}^{N_2} e^{-H(\Gamma)/T_n} q(\Gamma)\,|F(\Gamma)|^{-1}(1-e^{-\alpha/T_1})K(2,2)$$

$$\times P(X_{N_1}\in\Gamma)\left(1-2q(\Gamma)\sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}-e^{-\alpha/T_1}\right) \quad (31)$$

where $N_{1.75}=N(H(\Gamma), T_1, -\alpha, N_{1.5})$.

Hence

$$\sum_{l=N_1+1}^{N_2} P(X_{l-1}\notin\Gamma, X_l\in\Gamma)$$

$$\geqq(1-e^{-\alpha/(4T_1)}-P(X_{N_1}\in\Gamma))\sum_{l=N_1+1}^{N_2} e^{-(H(\Gamma)+U(\Gamma))/T_l} q(\Gamma) K(2,1)$$

$$+\left(1-e^{-\alpha/(2T_1)}-2q(\Gamma)\sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}\right)\frac{P(X_{N_1}\in\Gamma)}{|F(\Gamma)|}$$

$$\times\left(q(\Gamma)\sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}-e^{-\alpha/(2T_1)}\right). \quad (32)$$

End of the proof of proposition 1.8.

We deduce from proposition 1.8 that

LEMMA 1.9. — *There is a positive constant* T_0 *such that in the cooling framework* $\mathcal{G}(T_0, H(\Gamma))$, *for any small enough constants* $\alpha_3<\alpha_2/2<\alpha_1/10$ *putting*

$$\left.\begin{aligned} N_1&=N(H(\Gamma), T_1, -\alpha_1, 0)\\ N_2&=N(H(\Gamma), T_1, -\alpha_2, 0)\end{aligned}\right\} \quad (33)$$

we have

$$P(X_{N_2}\in\Gamma)-P(X_{N_1}\in\Gamma)$$

$$\geqq\tilde{q}\,|F(\Gamma)|^{\delta}\left(|F(\Gamma)|(1-e^{-\alpha_3/T_1})\sum_{n=N_1+1}^{N_2} e^{-(H(\Gamma)+U(\Gamma))/T_n}\right.$$

$$\left.-(1+e^{-\alpha_3/T_1})P(X_{N_1}\in\Gamma)\sum_{n=N_1+1}^{N_2} e^{-H(\Gamma)/T_n}\right). \quad (34)$$

LEMMA 1.10. — *There are positive constants* T_0 *and* β *such that in the cooling framework* $\mathcal{G}(T_0, H(\Gamma))$ *we have*

$$P(X_{N_2}\in\Gamma)-P(X_{N_1}\in\Gamma) \geqq -(1+e^{-\alpha/T_1})\tilde{q}(N_2-N_1)(1+\delta^{-1})^{-(1+\delta)}\delta^{-1}P(X_{N_1}\in\Gamma)^{1+\delta}. \quad (35)$$

Proof of lemma 1.10. — The minimum of the function

$$T\mapsto\tilde{q}|F(\Gamma)|^{\delta}(|F(\Gamma)|(1-e^{-\alpha/T_1})e^{-(H+U)/T} -(1+e^{-\alpha/T_1})e^{-H/T}P(X_{N_1}\in\Gamma)) \quad (36)$$

is reached for

$$(H+U)|F(\Gamma)|(1-e^{-\alpha/T_1})e^{-U/T}=H(1+e^{-\alpha/T_1})P(X_{N_1}\in\Gamma). \quad (37)$$

End of the proof of lemma 1.10.

Continuation of the proof of proposition 1.5. — Let us put $P_1=P(X_{N_1}\in\Gamma)$, and $P_2=P(X_{N_2}\in\Gamma)$. If $P_2\leqq P_1$ we have

$$P_2^{-\delta}-P_1^{-\delta}\leqq\delta\frac{P_1-P_2}{P_2^{1+\delta}}\leqq(1+e^{-\alpha/T_1})\delta\frac{P_1-P_2}{P_1^{1+\delta}}, \quad (38)$$

from which we deduce proposition 1.5 with the help of lemma 1.10.

End of the proof of proposition 1.5.

PROPOSITION 1.11. — *For any energy landscape* (E, U, q), *there exist positive constants* T_0 *and* α *such that in* $\mathcal{F}(T_0)$, *for any* $\mathcal{L}_0$ *we have for any* $n\in\mathbb{N}$

$$P(X_n\in\Gamma)\geqq\{P(X_0\in\Gamma)\wedge|F(\Gamma)|e^{-U(\Gamma)/T_n}\}(1-e^{-\alpha/T_1}). \quad (39)$$

Proof of proposition 1.11. — Let us choose T_0 as in proposition 1.5. With the same notations in the framework $\mathcal{F}(T_0)$, if $N_1=+\infty$, for any n

$$P(X_n\in\Gamma)\geqq P(X_0\in\Gamma)\left(1-2\frac{q(\Gamma)}{|F(\Gamma)|}\sum_{k=1}^{n}e^{-H(\Gamma)/T_k}\right) \geqq P(X_0\in\Gamma)\left(1-2\frac{q(\Gamma)}{|F(\Gamma)|}e^{-\alpha_1/T_1}\right), \quad (40)$$

hence equation (39) is satisfied in this case.

If $N_1<+\infty$, we have in the same way for any $n\leqq N_1$

$$P(X_n\in\Gamma)\geqq P(X_0\in\Gamma)\left(1-2\frac{q(\Gamma)}{|F(\Gamma)|}e^{-\alpha_1/T_1}\right), \quad (41)$$

and equation (39) is satisfied for $0\leqq n\leqq N_1$.

Now putting $(u_k)_{k\in\mathbb{N}}=V(H(\Gamma), T_1, \alpha_1)$ it is easy to see that it is enough to prove equation (39) for $n=u_k$, $k\in\mathbb{N}$. We deduce from lemma 1.9 that if, for some $n>1$

$$P(X_{u_{k-1}}\in\Gamma)\leqq|F(\Gamma)|e^{-U(\Gamma)/T_{u_k}}\frac{1-e^{-\alpha_1/T_1}}{1+e^{-\alpha_1/T_1}}, \tag{42}$$

then

$$P(X_{u_k}\in\Gamma)\geqq P(X_{u_{k-1}}\in\Gamma). \tag{43}$$

Let us choose $\alpha_2>0$ such that

$$\frac{1-e^{-\alpha_1/T_0}}{1+e^{-\alpha_1/T_0}}\left(1-\frac{2q(\Gamma)}{|F(\Gamma)|}e^{-\alpha_1/T_0}\right)\geqq 1-e^{-\alpha_2/T_0}. \tag{44}$$

We are able now to show that equation (39) is true for $\alpha=\alpha_2$ and $n=u_k$, $k\in\mathbb{N}$ by induction on k. It is true for $k=0, 1$ according to equation (41). Assume that it is true for some $k\geqq 1$, then we can distinguish between two cases:

1.

$$P(X_{u_k}\in\Gamma)\leqq|F(\Gamma)|e^{-U(\Gamma)/T_{u_{k+1}}}\frac{1-e^{-\alpha_1/T_1}}{1+e^{-\alpha_1/T_1}} \tag{45}$$

hence

$$\begin{aligned}P(X_{u_{k+1}}\in\Gamma)&\geqq P(X_{u_k}\in\Gamma)\\&\geqq(P(X_0\in\Gamma)\wedge|F(\Gamma)|e^{-U(\Gamma)/T_{u_k}})(1-e^{-\alpha_2/T_1})\\&\geqq(P(X_0\in\Gamma)\wedge|F(\Gamma)|e^{-U(\Gamma)/T_{u_{k+1}}})(1-e^{-\alpha_2/T_1}).\end{aligned} \tag{46}$$

2.

$$P(X_{u_k}\in\Gamma)>|F(\Gamma)|e^{-U(\Gamma)/T_{u_{k+1}}}\frac{1-e^{-\alpha_1/T_1}}{1+e^{-\alpha_1/T_1}} \tag{47}$$

hence

$$\begin{aligned}P(X_{u_{k+1}}\in\Gamma)&\geqq P(X_{u_k}\in\Gamma)\left(1-\frac{2q(\Gamma)}{|F(\Gamma)|}e^{-\alpha_1/T_1}\right)\\&\geqq|F(\Gamma)|e^{-U(\Gamma)/T_{u_{k+1}}}(1-e^{-\alpha_2/T_1}).\end{aligned} \tag{48}$$

End of the proof of proposition 1.11.

THEOREM 1.12. – *For any positive constants* β *and* τ_0, *for any energy landscape* (E, U, q), *there exist positive constants* α *and* N *such that in the cooling framework* $\mathscr{F}(\tau_0)$, *for any initial distribution* $\mathscr{L}_0$ *satisfying*

$$\mathscr{L}_0(\Gamma)\geqq\beta, \tag{49}$$

we have for any $n\geqq N$

$$P(X_n\in\Gamma)\geqq(1-n^{-\alpha})(1+\delta^{-1})^{1+1/\delta}(\tilde{q}n)^{-1/\delta} \tag{50}$$

Proof.

LEMMA 1.13. — *For any positive constants* τ_0 *and* τ_1 *such that* $\tau_0 > \tau_1$, *any positive constant* β, *any initial distribution* $\mathscr{L}_0$ *such that* $\mathscr{L}_0(\Gamma) \geqq \beta$, *there is a positive constant* α_1 *such that putting*

$$N = \sup\{n > 0 \mid T_n > \tau_1\} \tag{51}$$

we have in the cooling framework $\mathscr{F}(\tau_0)$

$$P(X_N \in \Gamma) \geqq \alpha_1. \tag{52}$$

Remark. — Proposition 1.11 is sharper but works only for low temperatures.

Proof of lemma 1.13. — As q is symmetric irreducible, it is easy to see that p_{T_0} is recurrent aperiodic, hence we can consider

$$r = \inf\{n \geqq 0 \mid \inf_{i \in E} p_{T_0}^n(i, \Gamma) > 0\} < +\infty. \tag{53}$$

Let $\alpha_2 = \inf_{i \in E} p_{T_0}^r(i, \Gamma)$. As E is finite, $\alpha_2 > 0$. For any T such that $\tau_0 \geqq T \geqq \tau_1$, for $i, j \in E$

$$p_T(i, j) \geqq p_{\tau_0}(i, j) \exp\left(-\frac{\Delta}{\tau_1}\right), \tag{54}$$

where

$$\Delta = \sup\{U_j - U_i \mid i, j \in E, q(i, j) > 0\}. \tag{55}$$

Hence, if $N \geqq r$

$$P(X_N \in \Gamma) = \sum_{i \in E} P(X_{N-r} = i) P(X_N \in \Gamma \mid X_{N-r} = i) \geqq \alpha_2 \exp\left(-\frac{\Delta r}{\tau_1}\right). \tag{56}$$

If $N < r$, putting

$$\delta = \inf\{U_j - U_i \mid j \notin \Gamma, i \in \Gamma, q(i, j) > 0\} \tag{57}$$

we have

$$P(X_N \in \Gamma) \geqq P(X_0 \in \Gamma) e^{-r\delta/\tau_0}. \tag{58}$$

End of the proof of lemma 1.13.

With the notations of lemma 1.13 we put $u_0 = N$ and $u_{n+1} = N(H(\Gamma), T_{u_n+1}, -\alpha_2, u_n)$ where α_2 is the positive constant of proposition 1.5, and where τ_1 is the "T_0" of proposition 1.5. Hence we have

$$P(X_{u_{n+1}} \in \Gamma)^{-\delta} - P(X_{u_n} \in \Gamma)^{-\delta} \leqq K(u_{n+1} - u_n)(1 + e^{-\alpha_2/T_{u_{n-1}+1}}), \quad n > 0, \tag{59}$$

where $K = (1 + \delta^{-1})^{-(1+\delta)} \tilde{q}$.

Let us put

$$\hat{T}_n = H(\Gamma)\ln^{-1}\left(\frac{|F(\Gamma)|^{\delta}\tilde{q}n}{(1+\delta^{-1})^{(1+\delta)}}\right) \tag{60}$$

and

$$M = \inf\{m>0 \mid \alpha_1 \geqq |F(\Gamma)|\exp(-U(\Gamma)/\hat{T}_m) = (1+\delta^{-1})^{1+1/\delta}(\tilde{q}m)^{-1/\delta}\}. \tag{61}$$

For $n \geqq 1$ such that $u_{n+1} \geqq M$, we distinguish between two cases:

1.

$$1/T_{u_{n-1}} \leqq 1/\hat{T}_{u_{n+1}} - \ln 3/U(\Gamma), \tag{62}$$

in which case we deduce from proposition 1.11 that

$$P(X_{u_{n-1}} \in \Gamma)^{-\delta} \leqq \left(\frac{2}{3}\right)^{\delta} K\, u_{n+1}, \tag{63}$$

hence that

$$P(X_{u_{n+1}} \in \Gamma)^{-\delta} \leqq P(X_{u_{n-1}} \in \Gamma)^{-\delta}(1-e^{-\alpha_3/\tau_1}) \leqq K\, u_{n+1}. \tag{64}$$

2.

$$1/T_{u_{n-1}} \geqq 1/\hat{T}_{u_{n+1}} - \ln 3/U(\Gamma), \tag{65}$$

in which case, putting $\alpha_4 = \dfrac{\alpha_2}{2H(\Gamma)}$, we have

$$P(X_{u_{n+1}} \in \Gamma)^{-\delta} - P(X_{u_n} \in \Gamma)^{-\delta} \leqq K(u_{n+1}-u_n)(1+1/u_{n+1}^{\alpha_4}), \tag{66}$$

provided that τ_1 has been chosen small enough. Lowering its value if necessary, we can assume that $\alpha_4 < 1$.

If $M \leqq N$, we deduce from 1 and 2 that for some $\alpha_4 > 0$

$$\begin{aligned} P(X_{u_n} \in \Gamma)^{-\delta} &\leqq K(u_n - u_1) + \sum_{k=2}^{n}(u_k - u_{k-1})\frac{1}{u_k^{\alpha_4}} + P(X_{u_1} \in \Gamma)^{-\delta} \\ &\leqq K\,u_n + \sum_{k=N}^{u_n} k^{-\alpha_4} + 2\alpha_1^{-\delta} \\ &\leqq K\,u_n + (1-\alpha_4)^{-1}u_n^{1-\alpha_4} + 2\alpha_1^{-\delta}. \end{aligned} \tag{67}$$

If $M > N$, putting

$$R = \inf\{k>0 \mid u_k \geqq M\} \tag{68}$$

we have for any n such that $n \geqq R+1$

$$P(X_{u_n} \in \Gamma) \leqq K(u_n - u_1) + \sum_{k=2}^{R_1}(u_k - u_{k-1})e^{-\alpha_2/\tau_1} + \sum_{k=R}^{n}(u_k - u_{k-1})u_k^{-\alpha_4} + P(X_{u_1} \in \Gamma). \tag{69}$$

Let us recall that M is a constant (contrary to N). We deduce from equation (69) that

$$P(X_{u_n}\in\Gamma)\leqq K\,u_n+M\,e^{-\alpha_2/\tau_1}+(1-\alpha_4)^{-1}\,u_n^{1-\alpha_4}+2\,\alpha_1^{-\delta}. \qquad (70)$$

We deduce from equation (67) that there exist positive constants M_2 and α_5 such that for any n such that $u_n\geqq M_2$

$$P(X_{u_n}\in\Gamma)^{-\delta}\leqq K\,u_n(1+u_n^{-\alpha_5}). \qquad (71)$$

Now let us consider some arbitrary $n\geqq M_2$. Let us distinguish between two cases:

1. In case $n\geqq N$, let us consider k such that $u_k\leqq n<u_{k+1}$. We have for some positive α_6 and α_7

$$P(X_n\in\Gamma)^{-\delta}\leqq P(X_{u_k}\in\Gamma)^{-\delta}(1+e^{-\alpha_6/T_{u_k}})$$
$$\leqq K\,u_k(1+u_k^{-\alpha_7})\leqq K\,n(1+n^{-\alpha_7}). \qquad (72)$$

2. In case $M\leqq M_2\leqq n<N$

$$P(X_n\in\Gamma)^{-\delta}\leqq(2\,\alpha_1)^{-\delta}\leqq K\,n. \qquad (73)$$

Thus we have proved that for any $n\geqq M_2$

$$P(X_n\in\Gamma)^{-\delta}\leqq K\,n(1+n^{-\alpha_7}), \qquad (74)$$

hence for some positive α_8 and M_3 we have

$$P(X_n\in\Gamma)\geqq(K\,n)^{-1/\delta}(1-n^{-\alpha_8}), \qquad n\geqq M_3. \qquad (75)$$

End of the proof of theorem 1.12.

1.2. The critical feedback cooling schedule

Our aim will be now to prove that theorem 1.12 is sharp. We have a lower bound for $P(X_n\in\Gamma)$ whatever the cooling schedule may be. We will now be looking for a cooling schedule of the type $1/T_n=A\ln n+B$ for which $P(X_n\in\Gamma)$ is equivalent to this lower bound. We will thus prove that there exist values of A and B for which $1/T_n=A\ln n+B$ is asymptotically minimizing $P(X_n\in\Gamma)$.

We will not study directly the closed form $1/T_n=A\ln n+B$, instead we will define $1/T_n$ by a feedback relation of the type

$$\frac{1}{T_n}=\frac{1}{U(\Gamma)}\ln\left(\frac{c}{P(X_{n-1}\in\Gamma)}\right).$$

It is easy to guess from lemma 1.9 what the optimal value of the constant c should be. Solving this optimal feedback relation, we find

$1/T_n = H(\Gamma)^{-1} \ln n + B + \varepsilon_n$ with $|\varepsilon_n| \leqq n^{-\alpha}$ for n large and accordingly

$$\frac{P(X_n \in \Gamma)}{\min\limits_{T_1, \ldots, T_n} P(X_n \in \Gamma)} \leqq 1 + \frac{1}{n^\alpha}. \tag{76}$$

Then we show that $P(X_n \in \Gamma)$ is stable with respect to small perturbations of $1/T_n$ and conclude that equation (76) still holds when $1/T_n = H(\Gamma)^{-1} \ln n + B$ with the "optimal" B.

Cooling schedules of the type $1/T_n = H(\Gamma)^{-1} \ln n + B$ with non optimal B are studied in the same way through suboptimal feedback relations.

DEFINITION 1.14. – *Let* $(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0), \mathscr{X})$ *be a simple annealing framework. We define the critical feedback annealing algorithm to be the annealing algorithm* $(E, U, q, \mathscr{L}_0, \tilde{T}, \tilde{X})$ *defined by*

$$1/\tilde{T}_n = U(\Gamma)^{-1} \ln \frac{(1+\delta^{-1}) |F(\Gamma)|}{P(X_{n-1} \in \Gamma)} \vee 1/\tilde{T}_{n-1}, \qquad n > 0, \tag{77}$$

where we have put $\tilde{T}_0 = T_0$.

PROPOSITION 1.15. – *For any energy landscape* (E, U, q), *there is a positive constant* T_{-1} *such that for any simple cooling framework* $\mathscr{F}(T_0)$ *such that* $T_0 \leqq T_{-1}$, *there are positive constants* N *and* α *such that for any initial distribution* $\mathscr{L}_0$ *we have*

$$\left.\begin{aligned} |P(\tilde{X}_n \in \Gamma) - (1+\delta^{-1})^{(1+1/\delta)} (\tilde{q} n)^{-1/\delta}| \leqq n^{-\alpha} P(\tilde{X}_n \in \Gamma), \\ n \geqq N. \end{aligned}\right\} \tag{78}$$

COROLLARY. – *With the notions of the proposition, for any constants* $\beta > 0$, $T_{-1} > 0$, *there exist positive constants* N *and* α *such that for any* $\mathscr{L}_0$, $\mathscr{F}(T_0)$ *such that* $\mathscr{L}_0(\Gamma) > \beta$ *and* $T_0 \leqq T_{-1}$, *we have*

$$\left| \tilde{T}_n^{-1} - \frac{1}{H(\Gamma)} \ln \left(\frac{|F(\Gamma)|^\delta \tilde{q} n}{(1+\delta^{-1})} \right) \right| \leqq n^{-\alpha}, \qquad n \geqq N. \tag{79}$$

Proof of proposition 1.15. – In all this proof we will forget the tildes on the Ts.

For some positive constant α to be chosen later on, let us put $u_0 = 0$ and

$$u_{n+1} = N(H(\Gamma), T_{u_n}, -\alpha, u_n), \tag{80}$$

We have for any $n \geqq 0$

$$P(X_{u_{n+1}} \in \Gamma) \geqq P(X_{u_n} \in \Gamma) \left(1 - 2q(\Gamma) \sum_{k=u_n}^{u_{n+1}-1} e^{-H(\Gamma)/T_k} \right), \tag{81}$$

hence

$$\frac{1}{T_{u_{n+1}}}-\frac{1}{T_{u_n}}\leqq U(\Gamma)^{-1}\left(e^{U(\Gamma)(1/T_{u_{n+1}}-1/T_{u_n})}-1\right)$$

$$\leqq U(\Gamma)^{-1}\left(\frac{P(X_{u_n-1}\in\Gamma)}{P(X_{u_{n+1}-1}\in\Gamma)}-1\right)$$

$$\leqq U(\Gamma)^{-1}\quad\frac{1}{1-2q(\Gamma)\displaystyle\sum_{k=u_n}^{u_{n+1}-1}e^{-H(\Gamma)/T_k}}-1\ ,\qquad(82)$$

Hence there exists a positive constant K such that in $\mathscr{G}(T_0, H(\Gamma))$ we have

$$\frac{1}{T_{u_{n+1}}}-\frac{1}{T_{u_n}}\leqq Ke^{-\alpha/T_{u_n}}.\qquad(83)$$

We start with the rough inequalities: for any m

$$P(X_m=g)\leqq P(X_m\in\Gamma),\qquad(84)$$

for any $m\geqq N(H(\Gamma), T_{u_{n-1}}, -2\alpha, u_{n-1})$, $m\leqq u_{n+1}$,

$$P(X_m=g)\geqq|F(\Gamma)|^{-1}P(X_{u_{n-1}}\in\Gamma)(1-e^{-\beta/T_{u_n}}),\qquad(85)$$

$$P(X_m=f)\leqq 1,\qquad(86)$$

$$\sup_{k\in[u_{n-1},u_{n+1}]}P(X_k\in\Gamma)\leqq\left(1+2q(\Gamma)\sum_{l=u_{n-1}}^{u_{n+1}}e^{-H(\Gamma)/T_l}\right)P(X_{u_{n+1}}\in\Gamma)$$
$$\leqq(1+3q(\Gamma)e^{-\alpha/T_{u_n}})P(X_{u_{n+1}}\in\Gamma),\qquad(87)$$

hence for some constant K

$$P(X_m=g)\leqq(1+Ke^{-\alpha/T_{u_n}})P(X_{u_{n+1}}\in\Gamma).\qquad(88)$$

With the help of these inequalities we deduce from lemma 1.6 that

$$P(X_{u_{n+1}}\in\Gamma)-P(X_{u_n}\in\Gamma)\leqq P(X_{u_{n+1}}\in\Gamma)(1+Ke^{-\alpha/T_{u_n}})(1+e^{-\beta/T_{u_n}})$$
$$\times(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}}q(\Gamma)K(2,2)|F(\Gamma)|^{-1}$$
$$+(1+e^{-\beta/T_{u_n}})(u_{n+1}-u_n)e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}}q(\Gamma)K(2,1)$$
$$-|F(\Gamma)|^{-1}P(X_{u_{n-1}}\in\Gamma)(1-e^{-\beta/T_{u_n}})q(\Gamma)(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}}$$
$$+(1+b)\exp(-a(u_n-u_{n-1})e^{S(E)/T_{u_n}}).\qquad(89)$$

It is easy to see that if α and T_{-1} are small enough, then the last term is negligeable before $(u_{n+1}-u_n)e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}}$, indeed for

$\alpha \leqq (H(\Gamma) - S(E))/2$ we have

$$(1+b)\exp(-a(u_{n+1}-u_n)e^{-S(E)/T_{u_n}})$$
$$\leqq (1+b)\exp(-a e^{-\alpha/T_{u_n}} e^{(H(\Gamma)-S(E))/T_{u_n}})$$
$$\leqq (1+b)\exp(-a e^{(H(\Gamma)-S(E))/(2T_{u_n})})$$
$$\leqq \exp\left(-\frac{\beta+H(\Gamma)+U(\Gamma)}{T_{u_n}}\right). \quad (90)$$

Hence we have, omitting the negative term as well, for some positive constant K

$$P(X_{u_{n+1}} \in \Gamma) - P(X_{u_n} \in \Gamma)$$
$$\leqq K(u_{n+1}-u_n)(e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}} + P(X_{u_{n+1}} \in \Gamma) e^{-H(\Gamma)/T_{u_n}}). \quad (91)$$

Thus there is a positive constant k such that

$$P(X_{u_{n+1}} \in \Gamma) \leqq K(u_{n+1}-u_n) e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}}$$
$$+ (1+K e^{-\alpha/T_{u_n}}) P(X_{u_n} \in \Gamma). \quad (92)$$

This enables us to sharpen our rough inequalities of the beginning: for $m \geqq N(H(\Gamma), T_{u_{n-1}}, -2\alpha, u_{n-1})$, $m \leqq u_{n+1}$

$$P(X_m = g) \leqq |F(\Gamma)|^{-1} P(X_{u_{n-1}} \in \Gamma)(1+e^{-\beta/T_{u_n}})$$
$$+ K(u_{n+1}-u_n)(e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}} + P(X_{u_{n+1}} \in \Gamma) e^{-H(\Gamma)/T_{u_n}})$$
$$\leqq (1+e^{-\beta/T_{u_n}} + K e^{-\alpha/T_{u_n}}) |F(\Gamma)|^{-1} P(X_{u_n} \in \Gamma)$$
$$+ K'(u_{n+1}-u_n)(e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}} + P(X_{u_n} \in \Gamma) e^{-H(\Gamma)/T_{u_n}})$$
$$\leqq (1+e^{-\beta'/T_{u_n}}) |F(\Gamma)|^{-1} P(X_{u_n} \in \Gamma)$$
$$+ K'(u_{n+1}-u_n)(e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}} + P(X_{u_n} \in \Gamma) e^{-H(\Gamma)/T_{u_n}}). \quad (93)$$

On the other side, also for $m \geqq N(H(\Gamma), T_{u_{n-1}}, -2\alpha, u_{n-1})$, $m \leqq u_{n+1}$ we have

$$P(X_m = g) \geqq |F(\Gamma)|^{-1} P(X_{u_{n-1}} \in \Gamma)(1-e^{-\beta/T_{u_n}})$$
$$\geqq (1-K e^{-\alpha/T_{u_n}}) P(X_{u_n} \in \Gamma) |F(\Gamma)|^{-1} (1-e^{-\beta/T_{u_n}})$$
$$- K(u_n - u_{n-1}) e^{-(H(\Gamma)+U(\Gamma))/T_{u_{n-1}}} \quad (94)$$

for some positive constants k and β.

Hence, comming back to lemma 1.6, we get that

$$
\begin{aligned}
P(X_{u_{n+1}}\in\Gamma)-P(X_{u_n}\in\Gamma)&\\
\leqq(1+e^{-\beta/T_{u_n}})\,|F(\Gamma)|^{-1}P(X_{u_n}\in\Gamma)K(2,2)q(\Gamma)&\\
\times(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}}+K(u_{n+1}-u_n)^2&\\
\times(e^{-(2H(\Gamma)+U(\Gamma))/T_{u_n}}+P(X_{u_n}\in\Gamma)e^{-2H(\Gamma)/T_{u_n}})&\\
+(1+e^{-\beta/T_{u_n}})(u_{n+1}-u_n)K(2,1)q(\Gamma)e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}}&\\
-(1-e^{-\beta/T_{u_n}})P(X_{u_n}\in\Gamma)q(\Gamma)\,|F(\Gamma)|^{-1}(u_{u+1}-u_n)e^{-H(\Gamma)/T_{u_n}}&\\
+K(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}}(u_n-u_{n-1})e^{-(H(\Gamma)+U(\Gamma))/T_{u_{n-1}}}.&\qquad(95)
\end{aligned}
$$

Noticing that

$$(u_n-u_{n-1})e^{-H(\Gamma)/T_{u_{n-1}}}\leqq 2(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}},\qquad(96)$$

we deduce from this last inequality that there are positive constants T_0 and β such that in $\mathcal{G}(T_0, H(\Gamma))$

$$
\begin{aligned}
P(X_{u_{n+1}}\in\Gamma)-P(X_{u_n}\in\Gamma)&\\
\leqq(1+e^{-\beta/T_{u_n}})(u_{n+1}-u_n)e^{-(H(\Gamma)+U(\Gamma))/T_{u_n}}\tilde{q}\,|F(\Gamma)|^{1+\delta}&\\
-(1-e^{-\beta/T_{u_n}})P(X_{u_n}\in\Gamma)(u_{n+1}-u_n)e^{-H(\Gamma)/T_{u_n}}\tilde{q}\,|F(\Gamma)|^{\delta}.&\qquad(97)
\end{aligned}
$$

Let us recall now that

$$\frac{1}{T_n}\geqq U(\Gamma)^{-1}\ln\left(\frac{(1+\delta^{-1})\,|F(\Gamma)|}{P(X_{n-1}\in\Gamma)}\right)\qquad(98)$$

hence we see from the preceding inequality that

$$P(X_{u_{n+1}}\in\Gamma)<P(X_{u_n}\in\Gamma).\qquad(99)$$

On the other hand we know from the study of the chain at constant temperature that for fixed small enough T_0 there is some constant N such that

$$\inf\{n\,|\,P(X_n\in\Gamma)<(1+\delta^{-1})\,|F(\Gamma)|\,e^{-U(\Gamma)/T_0}\}<N.\qquad(100)$$

From these remarks we deduce that for any small enough positive choice of T_0 there are positive constants N, β, such that for $n\geqq N$

$$\frac{1}{T_n}\leqq U(\Gamma)^{-1}\ln\left(\frac{(1+\delta^{-1})\,|F(\Gamma)|}{P(X_{n-1}\in\Gamma)}\right)(1+P(X_{n-1}\in\Gamma)^{\beta})\qquad(101)$$

or

$$e^{-U(\Gamma)/T_n}\geqq(1+\delta^{-1})^{-1}\,|F(\Gamma)|^{-1}P(X_{n-1}\in\Gamma)(1-P(X_{n-1}\in\Gamma)^{\beta}).\qquad(102)$$

Let us put $p_n = \mathrm{P}(\mathrm{X}_n \in \Gamma)$, we get that for any $n > 1$

$$p_{u_{n+1}} - p_{u_n} \leqq (u_{n+1} - u_n)\tilde{q}\,|\mathrm{F}(\Gamma)|^{\delta}\left((1+p_{u_n}^{\beta})\,|\mathrm{F}(\Gamma)|\left(\frac{p_{u_n}}{(1+\delta^{-1})\,|\mathrm{F}(\Gamma)|}\right)^{1+\delta}\right.$$
$$\left. - (1-p_{u_n}^{\beta})\left(\frac{p_{u_n}}{(1+\delta^{-1})\,|\mathrm{F}(\Gamma)|}\right)^{\delta} p_{u_n}\right)$$
$$\leqq (u_{n+1} - u_n)\,\tilde{q} p_{u_n}^{1+\delta}(1+\delta^{-1})^{-\delta}((1+p_{u_n}^{\beta})(1+\delta^{-1})^{-1} - 1 + p_{u_n}^{\beta})$$
$$\leqq (u_{n+1} - u_n)\,\tilde{q} p_{u_n}^{1+\delta}(1+\delta^{-1})^{-\delta}(2p_{u_n}^{\beta} - (1+\delta)^{-1}), \quad (103)$$

hence for $u_n > \mathrm{N}$

$$p_{u_{n+1}}^{-\delta} - p_{u_n}^{-\delta} \geqq \delta \frac{p_{u_n} - p_{u_{n+1}}}{p_{u_n}^{1+\delta}}$$
$$\geqq (u_{n+1} - u_n)\,\tilde{q}\,(1+\delta^{-1})^{-(\delta+1)}(1 - 2(1+\delta)p_{u_n}^{\beta}). \quad (104)$$

We know that for $u_n > \mathrm{N}$

$$p_{u_n} \leqq (1+\delta^{-1})\,|\mathrm{F}(\Gamma)|\,e^{-\mathrm{U}(\Gamma)/\mathrm{T}_0}, \quad (105)$$

hence choosing T_0 small enough we have

$$1 - 2(1+\delta)p_{u_n}^{\beta} \leqq \frac{1}{2}, \quad (106)$$

hence putting

$$n_0 = \inf\{n \mid u_n > \mathrm{N}\}$$

we have

$$p_{u_n}^{-\delta} \geqq p_{u_{n_0}}^{-\delta} + (u_n - u_{n_0})\frac{1}{2}\tilde{q}\,(1+\delta^{-1})^{-(\delta+1)} \geqq \mathrm{K}\,(u_n - u_{n_0}). \quad (107)$$

Hence for some positive constant K, $\beta > 0$, putting $\chi = \tilde{q}\,(1+\delta^{-1})^{-(1+\delta)}$, we have

$$p_{u_n}^{-\delta} \geqq p_{u_{n_0}}^{-\delta} + \chi\,(u_n - u_{n_0}) - \sum_{k=n_0+1}^{n} \mathrm{K}\,(u_k - u_{n_0})^{-\beta}(u_k - u_{k-1}), \quad (108)$$

but

$$(u_k - u_{n_0})^{-\beta}(u_k - u_{k-1}) \leqq \frac{1}{1-\beta}((u_k - u_{n_0})^{1-\beta} - (u_{k-1} - u_{n_0})^{1-\beta}) \quad (109)$$

hence

$$p_{u_n}^{-\delta} \geqq p_{u_{n_0}}^{-\delta} + \chi\,(u_n - u_{n_0}) - \mathrm{K}\,(u_n - u_{n_0})^{1-\beta}. \quad (110)$$

Moreover $(u_{n_0} - u_{n_0-1}) \leqq 2\,e^{(\mathrm{H}(\Gamma)-\alpha)/\mathrm{T}_0}$ and

$$p_{u_{n_0}}^{-\delta} \geqq (1+\delta^{-1})^{-\delta}\,|\mathrm{F}(\Gamma)|^{-\delta}\,e^{\mathrm{H}(\Gamma)/\mathrm{T}_0} \geqq \chi\,(u_{n_0} - u_{n_0-1}) \quad (111)$$

for T_0 small enough. Hence

$$p_{u_n}^{-\delta} \geqq \chi (u_n - u_{n_0-1}) - K (u_n - u_{n_0-1})^{1-\beta}$$
$$\geqq \chi (u_n - N) - K (u_n - N)^{1-\beta} \geqq \chi u_n (1 - u_n^{-\beta/2}) \quad (112)$$

for u_n large enough.

Now for $u_n \leqq k < u_{n+1}$ we have

$$p_{u_n} (1 - K e^{-\alpha/T_{u_n}}) \leqq p_k \leqq (1 + K e^{-\alpha/T_{u_n}}) p_{u_{n+1}}, \quad (113)$$

hence there is a positive β such that for any large enough n

$$p_n^{-\delta} \geqq \chi n (1 - n^{-\beta}). \quad (114)$$

End of the proof of proposition 1.15.

1.3. Other feedback relations

As we have already explained at the beginning of the last section, changing the constants in the feedback relation leads to cooling schedules $1/T_n = A \ln n + B$ with critical A and non-critical B. One relatively innocuous change is to play with constant ρ in

$$\rho e^{-U(\Gamma)/T_n} = P(X_{n-1} \in \Gamma). \quad (115)$$

In order to get a decreasing sequence T_n we should have $\rho > |F(\Gamma)|$, because $P(X_{n-1} \in \Gamma) = |F(\Gamma)| e^{-U(\Gamma)/T_n}$ is the asymptotical thermal equilibrium equation for cycle Γ at low temperatures. For ρ ranging in $)|F(\Gamma)|, +\infty($, we get $1/T_n \simeq H(\Gamma)^{-1} \ln n + B + o(1)$ with B ranging in $)-\infty, B_0($ where B_0 is a critical value which can be computed [*cf.* equation (135)]. A more drastic move away from thermal equilibrium is to change in (115) the potential $U(\Gamma)$ of Γ to some lower value h. As the influence of a change in ρ compared with a change of h is minor, we chose the relation:

$$e^{-h/T_n} = P(X_{n-1} \in \Gamma), \quad (116)$$

with $h < U(\Gamma)$. With this relation, we find $1/T_n = H(\Gamma)^{-1} \ln n + B + o(1)$, B ranging in $)B_0, +\infty($.

The conclusion is that the thermal quasi-equilibrium equation for cycle Γ can be deeply affected by a change of the additive constant B only, eventhough the multiplicative constant A is kept to the critical value.

DEFINITION 1.16. – *Let* $(E, U, q, \mathscr{L}_0)$ *be an energy landscape with communications. For any positive constant* T_0, *for any real numbers* $\rho > |F(\Gamma)|$ *and* h, $0 < h < U(\Gamma)$, *we define the subcritical annealing algorithms* $\mathscr{A}_1(E, U, q, T_0, \mathscr{L}_0, \rho)$ *and* $\mathscr{A}_2(E, U, q, T_0, \mathscr{L}_0, h)$ *by*

- $\mathcal{A}_1(\mathrm{E}, \mathrm{U}, q, \mathrm{T}_0, \mathcal{L}_0, \rho) = (\mathrm{E}, \mathrm{U}, q, \mathcal{L}_0, \mathrm{T}, \mathrm{X})$ *with*

$$\mathrm{T}_n^{-1} = \frac{1}{\mathrm{U}(\Gamma)} \ln\left(\frac{\rho}{\mathrm{P}(\mathrm{X}_{n-1} \in \Gamma)}\right) \vee \mathrm{T}_{n-1}, \qquad n > 0. \tag{117}$$

- $\mathcal{A}_2(\mathrm{E}, \mathrm{U}, q, \mathrm{T}_0, \mathcal{L}_0, h) = (\mathrm{E}, \mathrm{U}, q, \mathcal{L}_0, \mathrm{T}, \mathrm{X})$ *with*

$$\mathrm{T}_n^{-1} = -\frac{\ln \mathrm{P}(\mathrm{X}_{n-1} \in \Gamma)}{h} \vee \mathrm{T}_{n-1}, \qquad n > 0. \tag{118}$$

PROPOSITION 1.17. — *Let* (E, U, q) *be an energy landscape. For any* $\rho > |\mathrm{F}(\Gamma)|$, *any positive* γ *and any small enough positive* T_0, *there exist positive constants* N *and* α *such that for any initial distribution* $\mathcal{L}_0$ *such that* $\mathcal{L}_0(\Gamma) > \gamma$, *the annealing algorithm*

$$(\mathrm{E}, \mathrm{U}, q, \mathcal{L}_0, \mathrm{T}, \mathrm{X}) = \mathcal{A}_1(\mathrm{E}, \mathrm{U}, q, \mathrm{T}_0, \mathcal{L}_0, \rho)$$

satisfies

$$\begin{aligned} |\mathrm{P}(\mathrm{X}_n \in \Gamma) - \rho(\delta\tilde{q}\,|\mathrm{F}(\Gamma)|^{1+\delta}(|\mathrm{F}(\Gamma)|^{-1} - \rho^{-1})n)^{-1/\delta}| \\ \leqq \mathrm{P}(\mathrm{X}_n \in \Gamma)\, n^{-\alpha}, \\ n > \mathrm{N}. \end{aligned} \tag{119}$$

Consequently there is N (*the same*) *and a positive* α *such that*

$$\begin{aligned} |\mathrm{T}_n^{-1} - \mathrm{H}(\Gamma)^{-1} \ln(\delta\tilde{q}\,|\mathrm{F}(\Gamma)|^{1+\delta}(|\mathrm{F}(\Gamma)|^{-1} - \rho^{-1})n)| \leqq n^{-\alpha}, \\ n > \mathrm{N}. \end{aligned} \tag{120}$$

Proof of proposition 1.17. — It is an easy adaptation of the proof of proposition 1.15:
putting $u_0 = 0$ and

$$u_{n+1} = \mathrm{N}(\mathrm{H}(\Gamma), \mathrm{T}_{u_n}, -\alpha, u_n), \tag{121}$$

we have in the same way for some positive constants K and T_0 in the framework $\mathcal{G}(\mathrm{T}_0, \mathrm{H}(\Gamma))$

$$\frac{1}{\mathrm{T}_{u_{n+1}}} - \frac{1}{\mathrm{T}_{u_n}} \leqq \mathrm{K}\, e^{-\alpha/\mathrm{T}_{u_n}}, \tag{122}$$

from which we deduce that there are positive constants β, T_0 such that in $\mathcal{G}(\mathrm{T}_0, \mathrm{H}(\Gamma))$, putting

$$\begin{aligned} a_n &= (u_{n+1} - u_n)\, e^{-(\mathrm{H}(\Gamma) + \mathrm{U}(\Gamma))/\mathrm{T}_{u_n}} \tilde{q}\,|\mathrm{F}(\Gamma)|^{1+\delta}, \\ b_n &= (u_{n+1} - u_n)\, e^{-\mathrm{H}(\Gamma)/\mathrm{T}_{u_n}} \tilde{q}\,|\mathrm{F}(\Gamma)|^{\delta}, \end{aligned} \tag{123}$$

we have for $n > 0$

$$\left|\frac{\mathrm{P}(\mathrm{X}_{u_{n+1}} \in \Gamma) - \mathrm{P}(\mathrm{X}_{u_n} \in \Gamma)(1 - b_n) - a_n}{a_n + \mathrm{P}(\mathrm{X}_{u_n} \in \Gamma)\, b_n}\right| \leqq e^{-\beta/\mathrm{T}_{u_n}}. \tag{124}$$

The end of the proof are elementary calculations stemming from this formula and will not be detailed.

End of the proof of proposition 1.17.

PROPOSITION 1.18. – *Let* (E, U, q) *be an energy landscape. For any positive constants* γ *and* $h < U(\Gamma)$, *for any small enough* T_0, *there exist positive constants* N *and* α *such that for any initial distribution* $\mathscr{L}_0$ such that $\mathscr{L}_0(\Gamma) \geqq \gamma$, *the annealing algorithm*

$$(E, U, q, \mathscr{L}_0, T, X) = \mathscr{A}_2(E, U, q, T_0, \mathscr{L}_0, h)$$

satisfies

$$\left| P(X_n \in \Gamma) - \left(\frac{H(\Gamma)}{h} \tilde{q} \,|\, F(\Gamma) \,|^\delta n\right)^{-h/H(\Gamma)} \right| \leqq n^{-\alpha}. \tag{125}$$

Consequently there exist N (*the same*) *and a positive* α *such that*

$$\left| T_n^{-1} - H(\Gamma)^{-1} \ln\left(\frac{H(\Gamma)}{h} \tilde{q} \,|\, F(\Gamma) \,|^\delta n\right) \right| \leqq n^{-\alpha}. \tag{126}$$

Remarks. – *The feedbacks* $\mathscr{A}_1$ *are not too far the critical one, in the sens that* $P(X_n \in \Gamma)$ *decreases according to the same power of n, but for the feedbacks* $\mathscr{A}_2$ *the power of n is changed and tends to* 0 *when the parameter h tends to* 0. *This shows that in the class of cooling schedules of the parametric form*

$$T_n^{-1} = \frac{1}{H(\Gamma)} \ln n + B, \tag{127}$$

the rate of convergence of $P(X_n \in \Gamma)$ *towards* 0, *and hence the rate of convergence of* $P(U(X_n) = U(E))$ *towards* 1 *is strongly dependent on the choice of the constant term* B. *This fact does not appear in the existant literature and is worth being noticed.*

Proof of proposition 1.18. – It follows again the same lines as the proof of proposition 1.15.

We choose α such that $M(\Gamma, E-\Gamma)_i^j$, $i \in \Gamma$, $j \in \tilde{B}(\Gamma)$, and $M(\Gamma, E-\Gamma)_i^E$ are α-adjacent to $\dfrac{q(\Gamma)}{|F(\Gamma)|} \mathscr{I}(H(\Gamma))$. We have

$$\begin{aligned} \frac{1}{T_{u_{n+1}}} - \frac{1}{T_{u_n}} \leqq \frac{1}{h}\left(\exp\left(h\left(\frac{1}{T_{u_{n+1}}} - \frac{1}{T_{u_n}}\right)\right) - 1\right) &\leqq h^{-1}\left(\frac{P(X_{u_{n-1}} \in \Gamma)}{P(X_{u_n} \in \Gamma)} - 1\right) \\ &\leqq h^{-1}\left(\frac{1}{1 - 2q(\Gamma)e^{-\alpha/T_{u_n}}} - 1\right). \end{aligned} \tag{128}$$

Hence there exists a positive constant K such that

$$\frac{1}{T_{u_{n+1}}}-\frac{1}{T_{u_n}}\leqq K e^{-\alpha/T_{u_n}} \tag{129}$$

from which we deduce estimation (124) as in the proof of proposition 1.15.

We see in the same way that there is some constant N independent of $\mathscr{L}_0$ and some positive β such that

$$\frac{1}{T_n}\leqq\frac{-\ln P(X_{n-1}\in\Gamma)}{h}(1+P(X_{n-1}\in\Gamma)^{\beta}) \tag{130}$$

or

$$e^{-h/T_n}\geqq P(X_{n-1}\in\Gamma)(1-P(X_{n-1}\in\Gamma)^{\beta}). \tag{131}$$

Hence we deduce that, putting $p_n=P(X_n\in\Gamma)$, we have

$$\begin{aligned} p_{u_{n+1}}-p_{u_n}&=(u_{n+1}-u_n)\tilde{q}\,|F(\Gamma)|^{\delta}\\ &\quad\times((1+\eta_n)\,|F(\Gamma)|\,p_{u_n}^{(H(\Gamma)+U(\Gamma))/h}-(1-\eta_n)\,p_{u_n}^{1+H(\Gamma)/h})\\ &=-(1+\eta_n')\,p_{u_n}^{1+H(\Gamma)/h}\,\tilde{q}\,|F(\Gamma)|^{\delta}(u_{n+1}-u_n). \end{aligned} \tag{132}$$

with $|\eta_n|,\ |\eta_n'|\leqq p_{u_n}^{\beta}$. Hence

$$p_{u_{n+1}}^{-H/h}-p_{u_n}^{H/h}\leqq-(1+\eta_n)\,\tilde{q}\,|F(\Gamma)|^{\delta}\frac{H}{h}(u_{n+1}-u_n) \tag{133}$$

with $|\eta_n|\leqq p_{u_n}^{\beta}$.

The end of the proof is as the end of the proof of proposition 1.15.

End of the proof of proposition 1.18.

1.4. Stability under small perturbations of the cooling schedule

In the preceding section we have built feedback cooling schedules with asymptotics

$$T_n^{-1}=H(\Gamma)^{-1}\ln n+B+\varepsilon_n, \tag{134}$$

with $\lim_{n\to\infty}\varepsilon_n=0$ and

$$B\neq B_0=H(\Gamma)^{-1}\ln(\delta\tilde{q}\,|F(\Gamma)|^{\delta}). \tag{135}$$

A natural question is then to ask for the behaviour of small perturbations of these cooling schedules, *i.e.* to study the asymptotics of $P(X_n\in\Gamma)$ when we modify the sequence ε_n. The present section is answering this question.

PROPOSITION 1.19. – *Let* (E, U, q) *be an energy landscape. Let* B *be a real constant such that* $B<B_0$ *where* B_0 *is defined by equation* (135). *Let* ρ

be the positive real constant defined by

$$B=H(\Gamma)^{-1}\,ln(\delta\tilde{q}\,|F(\Gamma)|^{(1+\delta)}(|F(\Gamma)|^{-1}-\rho^{-1})). \tag{136}$$

Let $\mathscr{L}_0$ *be an initial distribution on* E. *Let* $\tilde{T}$ *be the cooling schedule and let* $\tilde{X}$ *be the Markov chain of the feedback annealing algorithm* $\mathscr{A}_1(E, U, q, \mathscr{L}_0, \rho)$. *Let* $(\varepsilon_n)_{n\in\mathbb{N}^*}$ *be a sequence of real numbers satisfying*

$$\lim_{n\to\infty}\varepsilon_n=0 \tag{137}$$

and

$$T_n^{-1}=H(\Gamma)^{-1}\ln n+B+\varepsilon_n \tag{138}$$

is a cooling schedule (i.e. *is decreasing, in fact the reader will easily see that this condition is not necessary). Then for the annealing algorithm* $(E, U, q, \mathscr{L}_0, T, X)$ *we have*

$$\lim_{n\to\infty}\frac{P(X_n\in\Gamma)}{P(\tilde{X}_n\in\Gamma)}=1 \tag{139}$$

uniformly in $\mathscr{L}_0$. *Moreover if there exist positive constants* N *and* α *such that*

$$|T_n^{-1}-\tilde{T}_n^{-1}|\leqq n^{-\alpha},\qquad n\geqq N, \tag{140}$$

then there exist positive constants N′ *and* β such that for any initial distribution $\mathscr{L}_0$

$$\left|\frac{P(X_n\in\Gamma)}{P(\tilde{X}_n\in\Gamma)}-1\right|\leqq n^{-\beta},\qquad n\geqq N'. \tag{141}$$

Consequently there exist positive constants N *and* α *such that for any initial distribution* $\mathscr{L}_0$ *the annealing algorithm* $(E, U, q, \mathscr{L}_0, T, X)$ *associated with the cooling schedule*

$$T_n^{-1}=H(\Gamma)\ln n+B \tag{142}$$

satisfies

$$|P(X_n\in\Gamma)-\rho(\delta\tilde{q}\,|F(\Gamma)|^{(1+\delta)}(|F(\Gamma)|^{-1}-\rho^{-1})\,n)^{-1/\delta}|\leqq n^{-\alpha},\quad n\geqq N. \tag{143}$$

Proposition 1.20. – *Let* $(E, U, q, \mathscr{L}_0)$ *be an energy landscape with initial distribution* $\mathscr{L}_0$ *satisfying* $\mathscr{L}_0(\Gamma)>0$. *Let* B *be a real constant such that* $B>B_0$. *Let h be defined by*

$$B=H(\Gamma)^{-1}\ln\left(\frac{H(\Gamma)\,\tilde{q}\,|F(\Gamma)|^{\delta}}{h}\right). \tag{144}$$

[*which implies that* $0 < h < \mathrm{U}(\Gamma)$.] *Let* $(\varepsilon_n)_{n \in \mathbb{N}^*}$ *be a sequence of real numbers such that for some positive* α *and* N *and any* $n \geqq \mathrm{N}$

$$|\varepsilon_n| \leqq \frac{1}{n^\alpha} \tag{145}$$

and such that

$$\mathrm{T}_n^{-1} = \mathrm{H}(\Gamma)^{-1} \ln n + \mathrm{B} + \varepsilon_n \tag{146}$$

is increasing.

Let $(\mathrm{E}, \mathrm{U}, q, \mathscr{L}_0, \tilde{\mathrm{T}}, \tilde{\mathrm{X}})$ *be the feedback annealing* $\mathscr{A}_2(\mathrm{E}, \mathrm{U}, q, \mathrm{T}_0, \mathscr{L}_0, h)$ *where* T_0 *is as in proposition* 1.18.

There exists a positive constant λ *such that*

$$\lim_{n \to +\infty} \frac{\mathrm{P}(\mathrm{X}_n \in \Gamma)}{\mathrm{P}(\tilde{\mathrm{X}}_n \in \Gamma)} = \lambda. \tag{147}$$

Moreover, if we have only

$$\lim_{n \to +\infty} \varepsilon_n = 0 \tag{148}$$

we have still

$$\lim_{n \to +\infty} \frac{\ln \mathrm{P}(\mathrm{X}_n \in \Gamma)}{\ln \mathrm{P}(\tilde{\mathrm{X}}_n \in \Gamma)} = 1. \tag{149}$$

Remark. — *The limit ratio* λ *depends on the sequence* ε *of perturbations and on the initial distribution* $\mathscr{L}_0$.

In conclusion we can say that the feedback algorithms of type $\mathscr{A}_1$ are stable under small perturbations whereas the feedback algorithms of type $\mathscr{A}_2$ are stable only according to the logarithmic equivalent of $\mathrm{P}(\mathrm{X}_n \in \Gamma)$.

Proofs. — Let $\alpha > 0$ be chosen such that in some framework $\mathscr{G}(\mathrm{T}_0, \mathrm{H}(\Gamma))$ for any $i \in \Gamma$ and $j \in \tilde{\mathrm{B}}(\Gamma)$, $\mathrm{M}(\Gamma, \mathrm{E}-\Gamma)_i^j$ and $\mathrm{M}(\Gamma, \mathrm{E}-\Gamma)_i^{\mathrm{E}}$ are α-adjacent to $\dfrac{q(\Gamma)}{|\mathrm{F}(\Gamma)|} \mathscr{I}(\mathrm{H}(\Gamma))$. Let us put $u_0 = 0$ and

$$u_{k+1} = \mathrm{N}(\mathrm{H}(\Gamma), \mathrm{T}_{u_k}, -\alpha, u_k). \tag{150}$$

Let us put $p_k = \mathrm{P}(\mathrm{X}_k \in \Gamma)$ and $\tilde{p}_k = \mathrm{P}(\tilde{\mathrm{X}}_k \in \Gamma)$. We have as in the proofs of propositions 1.15, 1.17 and 1.18

$$\frac{1}{\mathrm{T}_{u_{n+1}}} - \frac{1}{\mathrm{T}_{u_n}} \leqq \varepsilon_{u_{n+1}} - \varepsilon_{u_n} + \mathrm{K}\, e^{-\alpha/\mathrm{T}_{u_n}} \tag{151}$$

for some positive constant K.

We deduce from this that for any $k \geqq 1$

$$p_{u_{k+1}} = p_{u_k}(1 - b_k) + a_k \tag{152}$$

with

$$a_k = \tilde{q}\,|\,\mathrm{F}(\Gamma)\,|^{1+\delta} \sum_{n=u_k+1}^{u_{k+1}} e^{-(H(\Gamma)+\mathrm{U}(\Gamma))/\mathrm{T}_n}(1+\eta(k)),$$

$$b_k = \tilde{q}\,|\,\mathrm{F}(\Gamma)\,|^{\delta} \sum_{n=u_k+1}^{u_{k+1}} e^{-\mathrm{H}(\Gamma)/\mathrm{T}_n}(1-\eta(k)) \tag{153}$$

and $|\,\eta(k)\,| \leqq e^{-\beta/\mathrm{T}_{u_k}}$ for some positive constant β.

In the same way we have

$$\tilde{p}_{u_{k+1}} = \tilde{p}_{u_k}(1-\tilde{b}_k)+\tilde{a}_k, \tag{154}$$

with

$$\tilde{a}_k = \tilde{q}\,|\,\mathrm{F}(\Gamma)\,|^{1+\delta} \sum_{n=u_k+1}^{u_{k+1}} e^{-(\mathrm{H}(\Gamma)+\mathrm{U}(\Gamma))/\tilde{\mathrm{T}}_n}(1+\tilde{\eta}(k)),$$

$$\tilde{b}_k = \tilde{q}\,|\,\mathrm{F}(\Gamma)\,|^{\delta} \sum_{n=u_k+1}^{u_{k+1}} e^{-\mathrm{H}(\Gamma)/\tilde{\mathrm{T}}_n}(1-\tilde{\eta}(k)) \tag{155}$$

and $|\,\tilde{\eta}(k)\,| \leqq e^{-\beta/\mathrm{T}_{u_k}}$ for some positive constant β.

[We can use the same sequence u_n in both cases because for some positive constants K_1 and K_2, depending on $(\varepsilon_n)_{n\in\mathbb{N}^*}$, we have

$$\mathrm{K}_1 e^{-\alpha/\tilde{\mathrm{T}}_{u_k}} \leqq \sum_{n=u_k+1}^{u_{k+1}} \mathrm{e}^{-\mathrm{H}(\Gamma)/\tilde{\mathrm{T}}_n} \leqq \mathrm{K}_2 e^{-\alpha/\tilde{\mathrm{T}}_{u_k}} \tag{156}$$

and it is really all what we need about u_k.]

Let us put $\chi_k = p_{u_k}/\tilde{p}_{u_k}$. We have for $k \geqq 1$

$$\frac{p_{u_{k+1}}}{\tilde{p}_{u_{k+1}}} = \frac{p_{u_k}}{\tilde{p}_{u_k}}\left(\frac{\tilde{p}_{u_k}}{\tilde{p}_{u_{k+1}}} - \frac{\tilde{p}_{u_k}}{\tilde{p}_{u_{k+1}}} b_k\right) + \frac{a_k}{\tilde{p}_{u_{k+1}}} \tag{157}$$

and

$$\frac{\tilde{p}_{u_k}}{\tilde{p}_{u_{k+1}}} = \frac{1}{1-\tilde{b}_k+(\tilde{a}_k/\tilde{p}_{u_k})} = 1+\left(\tilde{b}_k - \frac{\tilde{a}_k}{\tilde{p}_{u_k}}\right)(1+\rho(k)) \tag{158}$$

with

$$|\,\rho(k)\,| \leqq \mathrm{K}\left(\tilde{b}_k - \frac{\tilde{a}_k}{\tilde{p}_{u_k}}\right) \leqq \mathrm{K}'\, e^{-\alpha/\tilde{\mathrm{T}}_{u_k}} \leqq e^{-\beta/\tilde{\mathrm{T}}_{u_k}} \tag{159}$$

for $\beta = \alpha/2$ and T_0 small enough.

Hence

$$\chi_{k+1} = \chi_k(1-d_k)+e_k, \qquad k \geqq 1 \tag{160}$$

with

$$\left.\begin{aligned} d_k &= \left(-\tilde{b}_k + \frac{\tilde{a}_k}{\tilde{p}_{u_k}}\right)(1+\rho(k)) + b_k(1+\mu_0(k)),\\ |\mu_0(k)| &\leqq e^{-\beta/\tilde{T}_{u_k}},\\ e_k &= \frac{a_k}{\tilde{p}_{u_k}}(1+\mu_1(k)),\\ |\mu_1(k)| &\leqq e^{-\beta/\tilde{T}_{u_k}}. \end{aligned}\right\} \tag{161}$$

Let us distinguish at this point between proposition 1.19 and 1.20.

CASE OF PROPOSITION 1.19. – We have

$$\left.\begin{aligned} \frac{\tilde{a}_k}{\tilde{p}_{u_k}} &= \frac{|F(\Gamma)|}{\rho}(1+\mu_2(k))\,\tilde{b}_k,\\ |\mu_2(k)| &\leqq e^{-\beta/\tilde{T}_{u_k}} \end{aligned}\right\} \tag{162}$$

and

$$\lim_{n \to +\infty} \frac{b_k}{\tilde{b}_k} = 1, \tag{163}$$

hence

$$d_k = \frac{|F(\Gamma)|}{\rho}\tilde{b}_k(1+\mu_3(k)), \tag{164}$$

with

$$\lim_{n \to +\infty} \mu_3(k) = 0. \tag{165}$$

In the same way

$$\lim_{n \to +\infty} \frac{a_k}{\tilde{a}_k} = 1 \tag{166}$$

hence

$$e_k = \frac{|F(\Gamma)|}{\rho}\tilde{b}_k(1+\mu_4(k)) \tag{167}$$

with

$$\lim_{k \to +\infty} \mu_4(k) = 0. \tag{168}$$

From equation (160) we deduce that

$$\chi_n = \sum_{k=1}^{n-1} e_k \prod_{l=k+1}^{n-1} (1-d_l) + \chi_1 \prod_{l=1}^{n-1} (1-d_l)$$
$$= \sum_{k=1}^{n-1} \frac{e_k}{d_k} d_k \prod_{l=k+1}^{n-1} (1-d_l) + \chi_1 \prod_{l=1}^{n-1} (1-d_l), \quad (169)$$

and from

$$\prod_{l=1}^{+\infty} (1-d_l) = 0 \quad (170)$$

and

$$\sum_{k=1}^{n-1} d_k \prod_{l=k+1}^{n-1} (1-d_l) + \prod_{l=1}^{n-1} (1-d_l) = 1 \quad (171)$$

we deduce that

$$\lim_{n \to +\infty} \chi_n = 1. \quad (172)$$

Now if for some $N>0$ and any $n>N$

$$\left| \frac{1}{T_n} - \frac{1}{\tilde{T}_n} \right| \leqq e^{-\beta/\tilde{T}_n} \quad (173)$$

then for $u_k > N$ we have for some positive β

$$|\mu_3(k)| \leqq e^{-\beta/\tilde{T}_{u_k}}, \quad (174)$$

and

$$|\mu_4(k)| \leqq e^{-\beta/\tilde{T}_{u_k}}, \quad (175)$$

hence for some $\beta > 0$

$$e_k = d_k (1 + \mu_5(k)) \quad (176)$$

with $|\mu_5(k)| \leqq e^{-\beta/\tilde{T}_{u_k}}$.

Hence

$$\chi_n = \sum_{k=1}^{n-1} d_k \prod_{l=k+1}^{n-1} (1-d_l) + \chi_1 \prod_{l=1}^{n-1} (1-d_l) + \sum_{k=1}^{n-1} \mu_5(k) d_k \prod_{l=k+1}^{n-1} (1-d_l)$$
$$= 1 + (\chi_1 - 1) \prod_{l=1}^{n-1} (1-d_l) + \sum_{k=1}^{n-1} \mu_5(k) d_k \prod_{l=k+1}^{n-1} (1-d_l). \quad (177)$$

Now there is $N>0$ such that for any $u_l \geqq N$

$$d_l \geqq \frac{\tilde{q} |F(\Gamma)|^\delta}{2B} \sum_{n=u_l+1}^{u_{l+1}} \frac{1}{n} \quad (178)$$

hence for $N < u_k < u_n$

$$\prod_{l=k}^{n-1} (1-d_l) \leqq \left(\frac{u_k}{u_n}\right)^{\tilde{q} \mid F(\Gamma) \mid^\delta / 4B}. \tag{179}$$

As $\mu_5(k)$ is bounded we can put

$$M = \sup_{k \in \mathbb{N}^*} |\mu_5(k)|. \tag{180}$$

We have

$$\sum_{k=1}^{n-1} |\mu_5(k)| d_k \prod_{l=k+1}^{n-1} (1-d_l)$$
$$\leqq M \prod_{l \mid \sqrt{u_n} \leqq u_l \leqq u_{n-1}} (1-d_l) + \sup_{u_k \geqq \sqrt{u_n}} |\mu_5(k)| \leqq M\, u_n^{-(\tilde{q} \mid F(\Gamma) \mid^\delta / 8B)} + u_n^{-\beta/2} \tag{181}$$

if $\sqrt{u_n} > N$ and $|\mu_5(k)| \leqq u_k^{-\beta}$ for $u_k > N$.

Hence for $u_n > N^2$

$$|\chi_n - 1| \leqq u_n^{-\beta} \tag{182}$$

for some $\beta > 0$.

This ends the case of proposition 1.19.

Case of proposition 1.20. – Here for some $\beta > 0$

$$\frac{\tilde{a}_k}{\tilde{p}_{u_k}} \leqq e^{-\beta/\tilde{T}_{u_k}} \tilde{b}_k \tag{183}$$

hence in case $|\varepsilon_n| < e^{-\beta/\tilde{T}_n}$, for n large enough

$$\sum_{k=1}^{+\infty} e_k < +\infty, \tag{184}$$

and

$$\sum_{k=1}^{+\infty} |d_k| < +\infty \tag{185}$$

(we do not know any more the sign of d_k). Hence the infinite product

$$\prod_{n=1}^{+\infty} (1-d_n) \tag{186}$$

is convergent towards some strictly positive value,

$$\lim_{n \to +\infty} \prod_{k=n}^{+\infty} (1-d_k) = 1 \tag{187}$$

and χ_n converges towards

$$\sum_{k=1}^{+\infty} e_k \sum_{l=k+1}^{+\infty} (1-d_l)+\chi_1 \prod_{l=1}^{+\infty} (1-d_l). \tag{188}$$

In case we have only

$$\lim_{n \to +\infty} \varepsilon_n=0 \tag{189}$$

we do not know whether $\Sigma |d_k| < +\infty$ or not. However we have the rougher estimates

$$\lim_{n \to +\infty} \frac{\sum_{k=1}^{n} |d_k|}{\sum_{k=1}^{n} \tilde{b}_k}=0 \tag{190}$$

because

$$\sum_{k=1}^{+\infty} \tilde{b}_k=+\infty. \tag{191}$$

On the other hand we know that

$$\sum_{k=1}^{+\infty} e_k<+\infty, \tag{192}$$

hence we have

$$\begin{aligned}\chi_n \leqq \sum_{k=1}^{n-1} \mathrm{e}_k \prod_{l=k+1}^{n-1} (1+|d_k|)+\chi_1 \prod_{l=1}^{n-1} (1+|d_k|) \\ \leqq \left(\chi_1+\sum_{k=1}^{+\infty} e_k\right) \prod_{l=1}^{n-1} (1+|d_k|),\end{aligned} \tag{193}$$

but

$$\tilde{p}_n=\tilde{p}_1 \prod_{k=1}^{n-1} (1-\tilde{b}_k(1+\eta(k))) \tag{194}$$

with $|\eta(k)| \leqq e^{-\beta/\tilde{T}_{u_k}}$, hence

$$\limsup_{n \to +\infty} \frac{\ln \chi_n}{-\ln \tilde{p}_{u_n}} \leqq 0. \tag{195}$$

In the same way

$$\chi_n \geqq \sum_{k=1}^{n-1} e_k \prod_{l=k+1}^{n-1} (1-|d_l|) + \chi_1 \prod_{l=1}^{n-1} (1-|d_l|)$$

$$\geqq \left(\sum_{k=1}^{n-1} e_k + \chi_1 \right) \prod_{l=1}^{n-1} (1-|d_l|) \quad (196)$$

hence

$$\liminf_{n \to +\infty} \frac{\ln \chi_n}{-\ln \tilde{p}_{u_n}} \geqq 0. \quad (197)$$

Hence

$$\lim_{n \to +\infty} \frac{\ln \chi_n}{\ln \tilde{p}_{u_n}} = 0 \quad (198)$$

and

$$\lim_{n \to +\infty} \frac{\ln p_{u_n}}{\ln \tilde{p}_{u_n}} = 1 \quad (199)$$

from which it is easy to end the proof of proposition 1.20.

End of the proofs of the section.

2. ASYMPTOTICS OF THE LAW OF THE SYSTEM

In this section we draw the conclusions of the last section concerning the law of the system. We consider again converging cooling schedules of the type $1/T_n = A \ln n + B$ and non-degenerate energy landscapes. We study the behaviour of the system in the domain obtained by removing from the states space the ground state and one point in the bottom of the critical cycle. In this domain temperature can be considered to be almost constant. Therefore it is straightforward to derive an equivalent of the law of the system from an equivalent of the probability to be in any one state of the bottom of the critical cycle.

We will consider cooling schedules of the following types

DEFINITION 2.1. — *Let* A, B *and* α *be positive constants, let* N *be a positive integer. We define the cooling framework* $\mathcal{H}$ (A, B, α, N) *to be the set of cooling schedules satisfying the following assertion: for any* $n \geqq N$ *we have*

$$|T_n^{-1} - A^{-1} \ln n - B| \leqq n^{-\alpha}. \quad (200)$$

We will look for an equivalent of the law of X_n in parametric cooling frameworks $\mathscr{H}$ in which the annealing algorithm converges. We will sometimes make the asumption that the energy landscape (E, U, q) is non-degenerate in the sens of definition 1.2.

This study can be compared with results in Holley and Stroock [13], Chiang and Show [6] and Hwang and Sheu [15]. Theorem 2.2 is proved in [6] as well as in [15]. The introduction of the constant B is new. It plays an important role in theorems 2.4 and 2.5. These theorems show that Hwang and Sheu's claim that results for $A > H'(E)$ extend to the case $A = H'(E)$ is wrong (*cf.* [15] th. 4.2.).

THEOREM 2.2. – *Let* (E, U, q) *be any energy landscape* (*non necessarly non degenerate*). *Let* A *and* B *be real constants. Assume that*

$$A > H'(E). \tag{201}$$

Let α *be any positive constant, let* N_1 *be a positive integer. Then there exist positive constants* N_2 *and* β *such that for any initial law* $\mathscr{L}_0$, *in the annealing framework* (E, U, q, $\mathscr{L}_0$, $\mathscr{H}(A, B, \alpha, N_1)$, $\mathscr{X}$) *we have for any* $i \in E$

$$\left| \frac{n^{-U_i/A} \exp(-U_i B)}{|F(E)| P(X_n = i)} - 1 \right| \leqq n^{-\beta}, \qquad n \geqq N_2. \tag{202}$$

Proof of theorem 2.2. – We write for $i \in E$ and some $f \in F(E)$

$$\begin{aligned} P(X_n = i) = \sum_{l < m \leqq n} P(X_l = f) M(E - \{f\}, \{i\})_{f, l}^{E, m} P(\tau(\{i\}, m) > n \mid X_m = i) \\ + \sum_{j \in E - \{f\}} \sum_{m=1}^{n} P(X_0 = j) \\ \times M(E - \{f\}, \{i\})_{j, 0}^{i, m} P(\tau(\{i\}, m) > n \mid X_m = i). \end{aligned} \tag{203}$$

We will need the following lemma:

LEMMA 2.3. – *For any energy landscape* (E, U, q), *for any* $f \in F(E)$, *any cycle* $C \subset \bar{C} \in \mathscr{M}(E - \{f\})$, *there are positive constants* T_0, α *such that in the cooling framework* $\mathscr{G}(T_0, H(E - \{f\}))$, *the* GTK

$$M(E - \{f\}, C)_{f, m}^{E, n} e^{-(H(\bar{C}) + U(\bar{C}) - H(C) - U(C))/T_n}$$

is of class

$$\mathscr{E}^l(H(\bar{C}) + U(\bar{C}), q(C), H(E - \{f\}), \alpha).$$

Proof of lemma 2.3. – Let us examine first the case when $C \in \mathscr{M}(E - \{f\})$. Let G be the smallest cycle containing f and C.

We know from the proof of $\mathscr{P}_1$ in theorem I.2.25 that $M(G - \{f\}, C)_f^E$ is of class

$$\mathscr{E}^l(H(C) + U(C), q(C), H(E - \{f\}), \alpha).$$

Moreover

$$\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})_f^{\mathrm{E}} = \mathrm{M}(\mathrm{G}-\{f\}, \mathrm{C})_f^{\mathrm{E}} + \{\mathrm{M}(\mathrm{G}-\{f\}, \mathrm{E}-\mathrm{G})\,\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})\}_f^{\mathrm{E}}, \quad (204)$$

$\mathrm{M}(\mathrm{G}-\{f\}, \mathrm{E}-\mathrm{G})$ is of class $\mathscr{E}_-^l(\mathrm{H}(\mathrm{G}), \mathrm{H}(\mathrm{E}-\{f\}))$ and for any $j \in \mathrm{E}-\mathrm{G}$, the kernel $\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})_j^{\mathrm{E}}$ is of class $\mathscr{E}_-^l(0, \mathrm{H}(\mathrm{E}-\{f\}))$ (from proposition I.4.5), hence by the composition lemmas $\{\mathrm{M}(\mathrm{G}-\{f\}, \mathrm{E}-\mathrm{G})\,\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})\}_f^{\mathrm{E}}$ is of class $\mathscr{E}_-^l(\mathrm{H}(\mathrm{G}), \mathrm{H}(\mathrm{E}-\{f\}))$. But $\mathrm{H}(\mathrm{G}) > \mathrm{H}(\mathrm{C}) + \mathrm{U}(\mathrm{C})$, hence $\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})_f^{\mathrm{E}}$ is itself of class $\mathscr{E}^l(\mathrm{H}(\mathrm{C}) + \mathrm{U}(\mathrm{C}), q(\mathrm{C}), \mathrm{H}(\mathrm{E}-\{f\}), \alpha)$.

The case of a general $\mathrm{C} \subset \mathrm{E}-\{f\}$ is by induction: Assume that the lemma is true for some cycle $\mathrm{G} \subset \mathrm{E}$. We will show it is still true for any $\mathrm{C} \in \mathscr{N}(\mathrm{G})$ (the natural partition of G). For this purpose we write

$$\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})_f^{\mathrm{E}} = \mathrm{M}(\mathrm{E}-\{f\}, \mathrm{G})_f^{\mathrm{C}} + [\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{G})\,\mathrm{M}(\mathrm{G}, \mathrm{C})]_f^{\mathrm{C}} \quad (205)$$

and for any $i \in \mathrm{G}$, g being some point of $\mathrm{F}(\mathrm{G})$,

$$\mathrm{M}(\mathrm{G}, \mathrm{C})_{i,m}^{\mathrm{E},n} = \mathbf{1}_{i \neq g}\,\mathrm{M}(\mathrm{G}-\{g\}, \mathrm{C})_{i,m}^{\mathrm{E},n} + \sum_{k=m}^{n-1} \mathrm{P}(\mathrm{X}_k = g, \tau(\mathrm{G}, m) > k \mid \mathrm{X}_m = i)\,\mathrm{M}(\mathrm{G}-\{g\}, \mathrm{C})_{g,k}^{\mathrm{E},m} \quad (206)$$

(for $i = g$ there is only the second term).

This formula shows that

$$\mathrm{M}(\mathrm{G}, \mathrm{C})_{i,m}^{\mathrm{E},n} \exp(-\mathrm{H}(\mathrm{G})/\mathrm{T}_{m+1})$$

is of class

$$\mathscr{E}^l(\mathrm{H}(\mathrm{C}) + \mathrm{U}(\mathrm{C}) - \mathrm{U}_g, q(\mathrm{C})/q(\mathrm{G}), \mathrm{H}(\mathrm{E}-\{f\}), \alpha)$$

for some positive α in some $\mathscr{G}(\mathrm{T}_0, \mathrm{H}(\mathrm{E}-\{f\}))$. [The first term is negligeable because $\mathrm{H}(\mathrm{G}) > \mathrm{H}(\mathrm{C}) + \mathrm{U}(\mathrm{C}) - \mathrm{U}_g$.]

Hence we deduce from equation (205) (where the first term is again negligeable because $\mathrm{H}(\mathrm{G}) + \mathrm{U}(\mathrm{G}) > \mathrm{H}(\mathrm{C}) + \mathrm{U}(\mathrm{C})$) that

$$\mathrm{M}(\mathrm{E}-\{f\}, \mathrm{C})_{f,m}^{\mathrm{E},n}\, e^{-(\mathrm{H}(\bar{\mathrm{C}}) + \mathrm{U}(\bar{\mathrm{C}}) - \mathrm{H}(\mathrm{C}) - \mathrm{U}(\mathrm{C}))/\mathrm{T}_n}$$

is of class

$$\mathscr{E}^l(\mathrm{H}(\bar{\mathrm{C}}) + \mathrm{U}(\bar{\mathrm{C}}), q(\mathrm{C}), \mathrm{H}(\mathrm{E}-\{f\}, \alpha)$$

for some positive contant α in some $\mathscr{G}(\mathrm{T}_0, \mathrm{H}(\mathrm{E}-\{f\}))$.

End of the proof of lemma 2.3.

Let us come back to equation (203). Let us assume that $H'(E)N^{-\alpha} \leqq 1/2$. For $m<n$ we have

$$\frac{B^{-H'/A}}{1-H'/A}((n+1)^{1-H'/A}-(m+1)^{1-H'/A})(1-H'(m+1)^{-\alpha})$$
$$\leqq \sum_{k=m+1}^{n} e^{-H'/T_k}$$
$$\leqq \frac{B^{-H'/A}}{1-H'/A}(n^{1-H'/A}-m^{1-H'/A})(1+2H(m+1)^{-\alpha}). \quad (207)$$

Hence for n large enough there are $N \leqq L_1 < L_2$ such that

$$\left.\begin{aligned} (n+1)^{(1-H'/A)/2} &\leqq \sum_{k=L_2+1}^{n} e^{-H'/T_k} \leqq 2(n+1)^{(1-H'/A)/2}, \\ (n+1)^{(1-H'/A)/2} &\leqq \sum_{k=L_1+1}^{L_2} e^{-H'/T_k} \leqq 2(n+1)^{(1-H'/A)/2}. \end{aligned}\right\} \quad (208)$$

Putting

$$K = \frac{B^{-H'/A}}{8(1-H'/A)} \quad (209)$$

we have

$$K((n+1)^{1-H'/A}-(L_1+1)^{1-H'/A}) \leqq (n+1)^{(1-H'/A)/2}. \quad (210)$$

Hence

$$(L_1+1) \geqq (n+1)\left(1-\frac{1}{K(1-H'/A)}(n+1)^{-(1-H'/A)/2}\right), \quad (211)$$

hence for n large enough, putting

$$K' = \frac{1}{2K(1-H'/A)} \quad (212)$$

we have

$$\left|\frac{1}{T_n}-\frac{1}{T_{L_2}}\right| \leqq K' n^{-(1-H'/A)/2} + 2^{1+\alpha} n^{-\alpha}. \quad (213)$$

Hence there exist positive constants N and β_1 such that for $n>N$

$$\left|\frac{1}{T_n}-\frac{1}{T_{L_1}}\right| \leqq n^{-\beta_1}. \quad (214)$$

Thus, as f is a concentration set of E, we have for some positive β_2 and any $l \geqq L_2$,

$$\left| P(X_l = f) - \frac{1}{|F(E)|} \right| \leqq n^{-\beta_2}. \tag{215}$$

Thus there are positive constants a and b such that, for $n > N$ and some positive β_3

$$P(X_n = i) \geqq \sum_{l=L_2}^{n} P(X_l = f) M(E - \{f\}, \{i\})_{f,l}^{i,m} P(\tau(\{i\}, m) > n \mid X_m = i)$$

$$\geqq |F(E)|^{-1} \left(1 - \frac{1}{3} n^{-\beta_3}\right) \left(1 - (1+b) \prod_{l=L_2+1}^{n} (1 - a e^{-H'/T_l})\right) e^{-U_i/T_n}, \tag{216}$$

but

$$(1+b) \prod_{l=L_2+1}^{n} (1 - a e^{-H'/T_l}) \leqq (1+b) \exp(-a n^{(1-H'/A)/2}) \leqq \frac{1}{3} n^{-\beta_3} \tag{217}$$

for n large enough, hence

$$P(X_n = i) \geqq |F(E)|^{-1} (1 - n^{-\beta_3}) e^{-U_i/T_n}. \tag{218}$$

On the other hand for n large enough and some positive a, b, β_4 and β_5

$$P(X_n = i) \leqq \sum_{l=L_2}^{n} P(X_l = f) M(E - \{f\}, \{i\})_{f,l}^{i,m} P(\tau(\{i\}, m) > n \mid X_m = i)$$

$$+ (1+b) \prod_{l=L_2+1}^{n} (1 - a e^{-H'/T_l})$$

$$\leqq |F(E)|^{-1} (1 + n^{\beta_4}) e^{-U_i/T_{L_2+1}} + (1+b) \exp(-a n^{(1-H'/A)/2})$$

$$\leqq |F(E)|^{-1} (1 + n^{-\beta_5}) e^{-U_i/T_n}. \tag{219}$$

End of the proof of theorem 2.2.

THEOREM 2.4. – *Let* (E, U, q) *be a non-degenerate energy landscape. Let* B *be a real constant satisfying*

$$B < B_0, \tag{220}$$

where B_0 *is given by equation* (135). *Let* ρ *be defined by equation* (136). *There exist positive constants* $(\gamma_i)_{i \in E}$ *such that for any positive constants* N_1 *and* α, *there are positive constants* N_2 *and* β *such that for any initial law* $\mathscr{L}_0$ *in the annealing framework* (E, U, q, $\mathscr{L}_0$, $\mathscr{H}(H(\Gamma), B, \alpha, N_1)$, $\mathscr{X}$) *we have*

$$\left| \frac{\gamma_i \exp(-U_i/T_n)}{P(X_n = i)} - 1 \right| \leqq \exp(-\beta/T_n), \qquad n \geqq N_2. \tag{221}$$

Moreover we have

$$\gamma_i \geqq 1, \qquad i \in E. \tag{222}$$

Substituting T_n with its asymptotic expression in equation (221) gives the following corollary:

COROLLARY. – *With the notations of theorem* 2.4 *there exist positive constants* N_2 *and* α *such that*

$$|\gamma_i \exp(U_i B) n^{-U_i/H(\Gamma)}/P(X_n \in i) - 1| \leqq n^{-\alpha}. \tag{223}$$

THEOREM 2.5. – *Let* (E, U, q) *be a non-degenerate energy landscape. Let* B *be a real constant satisfying*

$$B > B_0, \tag{224}$$

where B_0 *is given by equation* (135). *There exist positive or null constants* $(W_i)_{i \in E}$ *such that for any positive constants* N_1 *and* α, *any initial law* $\mathscr{L}_0$ *in the annealing framework* (E, U, q, $\mathscr{L}_0$, $\mathscr{H}(H(\Gamma), B, \alpha, N_1)$, $\mathscr{X}$) *there exist real numbers* $L_i(T)$ *such that*

$$\lim_{n \to \infty} \exp(-W_i/T_n)/P(X_n = i) = L_i(T) \tag{225}$$

Moreover we have

$$W_i \leqq U_i, \qquad i \in E, \tag{226}$$

and the inequality is strict for $i \in \Gamma$.

Proof of theorem 2.4 *and theorem* 2.5. – Let $F(E) = \{f\}$ and let g be some point of $F(\Gamma)$. We write for $i \in E - \{f\}$, putting $E^{**} = E - \{f, g\}$,

$$\begin{aligned} P(X_n = i) = \sum_{l=0}^{n-1} \sum_{h \in \{f, g\}} P(X_l = h) M(E^{**}, \{i\})_{f, l}^{E, m} P(\tau(\{i\}, m) > n \mid X_m = i) \\ + \sum_{j \in E^{**}} P(X_0 = j) M(E^{**}, \{i\})_{j, 0}^{E, m} P(\tau(\{i\}, O) > n \mid X_m = i). \end{aligned} \tag{227}$$

As in the proof of the previous theorem, we will introduce a lemma giving estimates of some interesting GTKs:

LEMMA 2.6. – *For any non-degenerate energy landscape* (E, U, q), *there are positive* α, T_0 *such that for any* $g \in F(\Gamma)$, *any cycle* $C \subset \bar{C} \in \mathscr{M}(E - \{f, g\})$, *there are constants* $\gamma(f, C) \geqq 0$, $\gamma(g, C) \geqq 0$, $H(f, C)$ *and* $H(g, C)$ *such that in the cooling framework* $\mathscr{G}(T_0 H(E - \{f, g\}))$ *the kernels*

$$M(E - \{f, g\}, C)_{h, m}^{E, n} e^{-(H(\bar{C}) + U(\bar{C}) - H(C) - U(C))/T_n},$$

$h = f, g$ *are of class* $\mathscr{E}^l(H(h, C), \gamma(h, C), H(E - \{f, g\}, \alpha))$. *Moreover*

$$H(h, C) \geqq (H(\bar{C}) + U(\bar{C}) - U_h)^+, \qquad h = f, g, \tag{228}$$

and

$$\sum_h \gamma(h, C)\,\mathbf{1}(H(h, C) = (H(\bar{C}) + U(\bar{C}) - U_h)^+) = q(C). \tag{229}$$

Proof of lemma 2.6. – In case $C \in \mathcal{M}(E - \{f, g\})$, the only sharpening from proposition I.4.5 is to get rid of the $\exp(-H(E - \{f, g\})/T_{m+1})$ before the GTKs. For this purpose, let G be the largest cycle containing f and not Γ. Let us put $A = E - \{f, g\}$.

If $C \subset G$ then $M(G - \{f\}, C)_f^E$ is of class $\mathcal{E}^l(H(C) + U(C), q(C), H(A), \alpha)$ from the proof of $\mathcal{P}_1$ of theorem I.2.25, and

$$M(A, C) = M(G - \{f\}, C) + M(G - \{f\}, A - G)\,M(A, C). \tag{230}$$

In this equation, the second term is of class $\mathcal{E}^-(H(G), H(A))$, moreover $H(G) > H(C) + U(C)$.

If $C \cap G = \varnothing$ we have again

$$M(A, C) = M(G - \{f\}, A - G)\,M(A, C) + M(G - \{f\}, C), \tag{231}$$

$M(G - \{f\}, A - G)_f^j$ is of class $\mathcal{E}(H(G), q(G, j), H(A), \alpha)$ for $j \in B(G)$ and $\exp(-H(A)/T_{m+1})\,M(A, C)_{j, m}^{C, n}$ is of class $\mathcal{E}(H(A) + H(j, C), \delta(j, C), H(A), \alpha)$ for some appropriate constants in some framework $\mathcal{G}(T_0, H(A))$. Moreover $H(G) > H(A)$, hence composition lemmas show that $M(A, C)$ is of class $\mathcal{E}^l(H(f, C), \gamma(f, C), H(A), \alpha)$.

Evaluating $M(A, C)_g^E$ can be done in the same way, treating separately the case $C \subset \Gamma$ and the case $C \cap \Gamma = \varnothing$.

Now it remains to prove that

$$H(h, C) \geqq (H(\bar{C}) + U(\bar{C}) - U_h)^+ \tag{232}$$

and that

$$\sum_h \gamma(h, C)\,\mathbf{1}(H(h, C) = (H(\bar{C}) + U(\bar{C}) - U_h)^+) = q(C), \tag{233}$$

but it is easily seen to be a necessity from the case of annealing at constant low temperature T, $\mathcal{L}_0$ being the invariant probability measure: the equation to be considered is

$$\begin{aligned} P(X_m = C) = &\sum_{h \in \{f, g\}} \sum_{l=0}^{n-1} P(X_l = h) \\ &\times M(E - \{f, g\}, C)_{h, l}^{j, m}\,P(\tau(C, m) > n \mid X_m = j) \\ + &\sum_{h \in E - \{f, g\}} P(X_0 = h)\,M(E - \{f, g\}, C)_{h, 0}^{j, m}\,P(\tau(C, m) > n \mid X_m = j). \end{aligned} \tag{234}$$

This ends the proof when C is maximal, the remaining part of the proof is the same as in lemma 2.3.

End of the proof of lemma 2.6.

Proving theorems 2.4 and 2.5 from equation (227) and lemma 2.6 is no more difficult than proving theorem 2.2 from lemma 2.3 and will not be detailed.

End of the proof of theorem 2.4 *and theorem* 2.5.

3. TRIANGULAR COOLING SCHEDULES

This section is mainly descriptive. It introduces the optimization problem we will be interested in. Subsection 3.1 shows that the probability to be in any state which is not a global ground state cannot be smaller than what it is at thermal equilibrium. Subsection 3.2 formulates the optimization problem. We still work with the assumption that the energy landscape is non-degenerate.

3.1. A rough upper bound for the convergence rate

PROPOSITION 3.1. – *Let* (E, U, q) *be an energy landscape. For any positive constant* γ, *for any* γ*-uniform initial distribution* $\mathscr{L}_0$, *for any annealing algorithm* (E, U, q, $\mathscr{L}_0$, T, X) *we have*

$$P(X_n = i) \geqq \gamma \exp(-U_i/T_n), \qquad i \in E. \tag{235}$$

Proof of proposition 3.1. – The proof is by induction on n. Let $n>0$ and assume that

$$P(X_{n-1} = i) \geqq \gamma \exp(-U_i/T_{n-1}), \qquad i \in E, \tag{236}$$

then

$$P(X_{n-1} = i) \geqq \gamma \exp(-U_i/T_n), \qquad i \in E. \tag{237}$$

Hence we have

$$\begin{aligned} P(X_n = i)\exp(U_i/T_n) &= \sum_{j \in E} P(X_{n-1} = j)\exp(U_j/T_n)\, p_{T_n}(j, i)\exp((U_i - U_j)/T_n) \\ &= \sum_{j \in E} p_{T_n}(i, j)\, P(X_{n-1} = j)\exp(U_j/T_n) \geqq \gamma. \end{aligned} \tag{238}$$

End of the proof of proposition 3.1.

3.2. Description of the optimization problem

We will be interested in non-degenerate energy landscapes. If f is the ground state and N the time of the end of the simulation, we measure the quality of convergence by the quantity $P(X_N=f)$. Our optimization problem is $\max_{T_i, \ldots, T_N} P(X_N=f)$. There is no reason why the optimal solutions $(T_1^N, T_2^N, \ldots, T_N^N)$ should not depend on N. Thus the proper framework to study our optimization problem is to consider "triangular" annealing algorithms where we are given for each N a finite sequence $(T_1^N, \ldots, T_N^N)$ and the corresponding finite Markov chain $(X_0^N, \ldots, X_N^N)$.

DEFINITION 3.2. — *A triangular cooling schedule is a family* $(T_n^N)_{0<n\leqq N}$ *indexed by increasing couples of integers with values in* $\mathbb{R}_+$ *such that for any* $N\in\mathbb{N}$, $(T_n^N)_{0<n\leqq N}$ *is a decreasing sequence relatively to n:*

$$T_{n+1}^N \leqq T_n^N, \qquad 0<n<N.$$

DEFINITION 3.3. — *We define a triangular annealing algorithm to be* $(E, U, q, \mathscr{L}_0, T, X)$ *where:*

• $(E, U, q, \mathscr{L}_0)$ *is an energy landscape with communications and initial distribution;*

• T *is a triangular cooling schedule;*

• *and* X *is the family of finite Markov chains* X^N, *where* X^N *is the chain* $(X_n^N)_{0\leqq n\leqq N}$ *with initial distribution* $\mathscr{L}_0$ *and transitions*

$$P(X_n^N=j \mid X_{n-1}^N=i)=p_{T_n^N}(i, j), \qquad 0<n\leqq N. \tag{239}$$

Notice that we do not specify any stochastic link between the X^N*'s: we define them on different probability spaces. We will call* X *a "triangular Markov chain".*

DEFINITION 3.4. — *We define a triangular cooling framework to be any set of triangular cooling schedules.*

We define a triangular annealing framework to be $(E, U, q, \mathscr{L}_0, \mathscr{F}, \mathscr{X})$ *where* $(E, U, q, \mathscr{L}_0)$ *is an energy landscape with communications and initial distribution,* $\mathscr{F}$ *is a triangular cooling framework and* $\mathscr{X}$ *is the family of triangular Markov chains* X *such that there exists some* $T\in\mathscr{F}$ *such that* $(E, U, q, \mathscr{L}_0, T, X)$ *is a triangular annealing algorithm.*

Let us introduce now the optimization problem we are going to be interested in:

DEFINITION 3.5. — *Let* T_0 *be a positive constant. Let* $(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0), \mathscr{X})$ *be a simple triangular annealing framework*

$$[\mathscr{F}(T_0)=\{(T_k^N)_{1\leqq k\leqq N} \mid T_{k+1}^N \leqq T_k^N,\ k\leqq 1,\ \textit{and}\ T_1^N\leqq T_0\}].$$

We will say that the cooling schedule $\hat{T}$ *is optimal in* $\mathscr{F}(T_0)$ *for* $\mathscr{L}_0$ *for* $\mathscr{L}_0$ *and write*

$$\hat{T}\in\mathscr{T}(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0)) \tag{240}$$

if the triangular Markov chain $\hat{X}$ *associated with* $\hat{T}$ *satisfies for any* $N \in \mathbb{N}$

$$P(\hat{X}_N^N \in F(E)) = \sup_{X \in \mathscr{X}} P(X_N^N \in F(E)). \tag{241}$$

We are interested in the asymptotical behaviour of $\hat{T}_n^N$ when N is large.

4. THE OPTIMIZATION PROBLEM FAR FROM THE HORIZON

The probability to be in the ground state moves slower than the probability to be in any other state: if the cooling schedule is convergent this probability is almost equal to one for large times, hence almost constant. Then comes the probability to be in any state in the bottom of the critical cycle Γ, because Γ is the deepest cycle not containing the ground state. Hence if there is a sufficient stretch of time between the time k we examine and the time N of the end of simulation, the law of the system at time N will depend almost exclusively on $P(X_k \in \Gamma)$ and $P(X_k = f)$. Hence we expect the solutions $(\hat{T}_1^N, \ldots, \hat{T}_N^N)$ of $\max_{T_1, \ldots, T_N} P(N_N = f)$ and the solutions $(\tilde{T}_1^M, \ldots, \tilde{T}_N^M)$ of $\min_{T_1, \ldots, T_M} P(X_M \in \Gamma)$ to be close as long as $(N - M)$ is large enough. For technical considerations, we will prove that

$$\frac{1}{\hat{T}_k^N} \leqq \frac{1}{\tilde{T}_k^M} + \frac{1}{k^\alpha}$$

for k large enough and $N - M$ large enough, and that roughly speaking $\sup(1/\hat{T}^N, 1/\tilde{T}^N)$ is almost optimal.

We will prove elsewhere that $\tilde{T}^N$ is far to be even an approximated solution to $\max_{T_1, \ldots, T_N} P(X_N = f)$.

THEOREM 4.1. – *Let* T_0, γ *be any positive constants. Let* $(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0), \mathscr{X})$ *be a simple annealing framework such that* $\mathscr{L}_0$ *is* γ*-uniform. For any* $T \in \mathscr{T}(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0))$ *there exist positive constants* K *and* α *such that we have for any* $k \geqq K$

$$\limsup_{N \to \infty} (T_k^N)^{-1} \leqq H(\Gamma)^{-1} \left(\ln k + \ln \frac{\tilde{q} \,|\, F(\Gamma) \,|^\delta}{(1 + \delta^{-1})} \right) + k^{-\alpha}. \tag{242}$$

Remark. – *More precisely, inequality* (242) *holds for couples* (k, N) *satisfying*

$$\sum_{l = k+1}^{N} \exp(-H(\Gamma)/T_l^N) \geqq \exp(-\alpha/T_k^N), \tag{243}$$

for some positive constant α.

In [2] we had given a lower bound as well. Unfortunately the proof concerning that lower bound has revealed to be uncomplete. However we will show the following slightly weaker result:

THEOREM 4.2. – *Let* T_0 *and* γ *be any positive constants. Let* $(E, U, q, \mathscr{L}_0)$ be a non-degenerate energy landscape with γ-uniform initial distribution $\mathscr{L}_0$. *There is a triangular cooling schedule* $T \in \mathscr{F}(T_0)$ *and positive constants* β *and* M *such that for* $\tilde{T} \in \mathscr{T}(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0))$ *we have*

$$P(X_N^N \neq f) - P(\tilde{X}_N^N \neq f) \leqq P(\tilde{X}_N^N \neq f)^{1+\beta}, \qquad N \geqq M, \tag{244}$$

and such that for any k

$$\liminf_{N \to +\infty} \frac{1}{T_k^N} \geqq \frac{1}{H(\Gamma)} \ln\left(\frac{|F(\Gamma)|^\delta \tilde{q}n}{1+\delta^{-1}}\right). \tag{245}$$

Remark. – *Equation* (244) *implies that for some positive constants* α *and* M

$$P(X_N^N \neq f) - P(\tilde{X}_N^N \neq f) \leqq \frac{1}{N^\alpha} P(\tilde{X}_N^N \neq f), \qquad N \geqq M, \tag{246}$$

Proof of theorem 4.1. – During the course of this proof, T will be in $\mathscr{T}(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0))$, that is, will be some optimal triangular cooling schedule, and

$$(E, U, q, \mathscr{L}_0, \hat{T}, \hat{X})$$

will be the critical feedback annealing algorithm for $(E, U, q, \mathscr{L}_0)$.

We begin with the following lemma:

LEMMA 4.3. – *We have for any* $k \in \mathbb{N}$

$$\lim_{N \to +\infty} \sum_{l=k+1}^{N} \exp(-H(\Gamma)/T_l^N) = +\infty. \tag{247}$$

Proof. – It is enough to give the proof for any $k \geqq M$ for some constant M (it would even be enough to give a proof for some fixed k).

According to theorem 1.12, there are positive constants M_1 and K_1 such that for any $k \geqq M_1$, for any $N \geqq k$

$$P(X_k^N \in \Gamma) \geqq K_1 k^{-1/\delta(\Gamma)}. \tag{248}$$

Let us choose some positive constant τ such that we can apply theorem I.2.25 to Γ with $\tau = T_0$.

- If $T_k^N > \tau$, putting

$$M_2 = \sup\{m \geqq k \mid T_m^N > \tau\}, \tag{249}$$

we have

$$P(X_{M_2}^N \in \Gamma) \geqq \gamma |F(\Gamma)| e^{-U(\Gamma)/\tau}. \tag{250}$$

Hence putting

$$K_2 = \gamma\,|F(\Gamma)|\,e^{-U(\Gamma)/\tau}, \tag{251}$$

we have

$$\begin{aligned} P(X_N^N \in \Gamma) &\geqq K_2 \prod_{l=M_2+1}^{N} \left(1 - 2\frac{q(\Gamma)}{|F(\Gamma)|} e^{-H(\Gamma)/T_l^N}\right) \\ &\geqq K_2 \exp\left(-4\frac{q(\Gamma)}{|F(\Gamma)|} \sum_{l=m_2+1}^{N} e^{-H(\Gamma)/T_l^N}\right) \\ &\geqq K_2 \exp\left(-4\frac{q(\Gamma)}{|F(\Gamma)|} \sum_{l=k+1}^{N} e^{-H(\Gamma)/T_l^N}\right). \end{aligned} \tag{252}$$

- If $T_k^N \leqq \tau$ we have, according to equation (248)

$$P(X_N^N \in \Gamma) \geqq K_1 k^{-1/\delta} \exp\left(-4\frac{q(\Gamma)}{|F(\Gamma)|} \sum_{l=k+1}^{N} e^{-H(\Gamma)/T_l^N}\right). \tag{253}$$

Hence there exist some positive function of k only $f(k)$ such that for any $k > M_1$

$$P(X_N^N \in \Gamma) \geqq f(k) \exp\left(-4\frac{q(\Gamma)}{|F(\Gamma)|} \sum_{l=k+1}^{N} e^{-H(\Gamma)/T_l^N}\right). \tag{254}$$

As

$$\lim_{N \to +\infty} P(X_N^N \in \Gamma) = 0, \tag{255}$$

we deduce lemma 4.3 from equation (254).

End of the proof of lemma 4.3.

DEFINITION 4.4. – *Let* $(E, U, q, \mathscr{L}_0, \mathscr{F}, \mathscr{X})$ *be an annealing framework. An initial differential distribution is defined to be any signed measure* ρ_0 *on* E *such that*

$$\sum_{i \in E} \rho_0(i) = 0 \quad \textit{and} \quad \sum_{i \in E} (\rho_0(i))^+ \leqq 1. \tag{256}$$

We will note ρ_0^+ *the measure* $\rho_0^+(i) = (\rho_0(i))^+$, $i \in E$ *and* ρ_0^- *the measure* $\rho_0^-(i) = (-\rho_0(i))^+$, $i \in E$. *We have* $\rho_0 = \rho_0^+ - \rho_0^-$. *We will also put* $|\rho_0| = \rho_0^+ + \rho_0^-$.

For any initial distribution ρ_0, *we define the differential distribution at time* n, ρ_n, *to be*

$$\rho_n(i) = \sum_{j \in E} \rho_0(j) P(X_n = i \mid X_0 = j), \qquad i \in E. \tag{257}$$

(*It depends on the cooling schedule* T.)

PROPOSITION 4.5. — *For any energy landscape* (E, U, q) *there exist constants* $T_0>0$, $\alpha>0$, *and constants* $K_i \geqq 0$, $i \in E$, *such that in* $\mathscr{G}(T_0, H(\Gamma))$, *putting*

$$N = N(H(\Gamma), T_1, -\alpha, 0) \tag{258}$$

we have

$$\left.\begin{array}{c} P(X_N=f \mid X_0=i) \geqq K_i(1-e^{-\alpha/T_1}), \\ P(X_N=g \mid X_0) \geqq |F(\Gamma)|^{-1}(1-K_i)(1-e^{-\alpha/T_1}), \\ g \in F(\Gamma). \end{array}\right\} \tag{259}$$

Moreover for $i \in \Gamma$, $K_i=0$ *and for* $i \in G_1$, *the maximal cycle containing* f *and not* Γ, $K_i=1$.

DEFINITION 4.6. — *We define two "principal valleys"* V_1 *and* V_2 *in the following way:*

- V_1 *is the function* $i \to K_i$;
- $V_2 = 1 - V_1$ *is the function* $i \to 1-K_i$.

For any measure $\lambda \in M(E)$ *we put*

$$\lambda(V_1) = 1 - \lambda(V_2) = \sum_{i \in E} K_i \lambda(i). \tag{260}$$

Proof of proposition 4.5. — Let g be a point of $F(\Gamma)$. We put $A = E - \{f, g\}$. We have

$$P(X_N=f \mid X_0=i) = \sum_{l=1}^{N} M(A, \{f\})_{i,0}^{E,l} P(X_N=f \mid X_l=f) + \sum_{l=1}^{N} M(A, \{g\})_{i,0}^{E,l} P(X_N=f \mid X_l=g) \tag{261}$$

and in the same way for any $g \in F(\Gamma)$

$$P(X_N=g \mid X_0=i) = \sum_{l=1}^{N} M(A, E-A)_{i,0}^{g,l} P(X_N=g \mid X_l=g) + \sum_{l=1}^{N} M(A, E-A)_{i,0}^{f,l} P(X_N=g \mid X_l=f). \tag{262}$$

From proposition I.4.5 we deduce that there are positive constants T_0, β, and constants $(K_i)_{i \in E}$ in the intervall [0, 1], such that the GTKs $M(A, E-A)_i^f$ and $M(A, E-A)_i^g$ are respectively of class $\mathscr{E}^r(0, K_i, H(A), \alpha)$ and $\mathscr{E}^r(0, 1-K_i, H(A), \alpha)$ in $\mathscr{G}(T_0, H(A))$. [We see moreover that $K_i=1$ if $i \in G_1$ and $K_i=0$ if $i \in \Gamma$, the convention for $\mathscr{E}^r(H_1, 0, H_2, \alpha)$ is $\mathscr{E}^r_-(H_1+\gamma, H_2)$ for some positive γ.]

Moreover for $l \in [1, N]$, f being a concentration set of E, there exists a positive β such that

$$P(X_N=f \mid X_l=f) \geqq 1 - e^{-\beta/T_1} \tag{263}$$

and, putting

$$M=N(H(\Gamma), T_1, -2\alpha, 0), \tag{264}$$

for $l\in[1, M]$ we have

$$P(X_N=g\,|\,X_l=g)\geqq |F(\Gamma)|^{-1}(1-e^{-\beta/T_1}), \tag{265}$$

g being a concentration set of Γ, as soon as, say, $\alpha\leqq(H(\Gamma)-H(A))/2$.

We have thus

$$P(X_N=f\,|\,X_0=i)\geqq\left(1-(1+b)\prod_{l=1}^{N}(1-a\,e^{-H(A)/T_l})\right)K_i(1-e^{-\beta/T_1}). \tag{266}$$

In the same way

$$P(X_N=g\,|\,X_0=i)\geqq\left(1-(1+b)\prod_{l=1}^{M}(1-a\,e^{-H(A)/T_l})\right)\times(1-K_i)\,|F(\Gamma)|^{-1}(1-e^{-\beta/T_1}). \tag{267}$$

From these two inequalities we deduce proposition 4.5 for $\alpha=(H(\Gamma)-H(A))/4$.

End of the proof of proposition 4.5.

PROPOSITION 4.7. — *For any non-degenerate energy landscape* (E, U, q), *for any positive constant* α_1 *there exist positive constants* T_0 *and* α_2 *such that in* $\mathscr{F}(T_0)$ *for any initial differential distribution* ρ_0 *such that,*

$$\left.\begin{aligned}\rho_0^-(g)&\geqq(1-e^{-\alpha_1/T_1})\,\rho_0^+(E)/|F(\Gamma)|, \qquad g\in F(\Gamma),\\ \rho_0^+(f)&\geqq(1-e^{-\alpha_1/T_1})\,\rho_0^+(E)\end{aligned}\right\} \tag{268}$$

we have for any $n\in\mathbb{N}$

$$\left.\begin{aligned}\rho_n^-(g)&\geqq(1-e^{-\alpha_2/T_1})\,\rho_n^+(E)/|F(\Gamma)|, \qquad g\in F(\Gamma),\\ \rho_n^+(f)&\geqq(1-e^{\alpha_2/T_1})\,\rho_n^+(E).\end{aligned}\right\} \tag{269}$$

Proof of proposition 4.7. — We will prove first the following:

LEMMA 4.8. — *Let us choose* α *as in proposition* 4.5. *Let* $u_0=0$ *and*

$$u_{k+1}=N(H(\Gamma), T_1, -\alpha, u_k), \tag{270}$$

For any small enough positive β, *there is a positive constant* T_0 *such that if* $T_1\leqq T_0$, *and if*

$$\left.\begin{aligned}\rho_0^-(F(\Gamma))&\geqq(1-e^{-\beta/T_1})\,\rho_0^+(E),\\ \rho_0^+(f)&\geqq(1-e^{-\beta/T_1})\,\rho_0^+(E),\end{aligned}\right\} \tag{271}$$

then for any $k>0$ *the same inequalities are true:*

$$\left.\begin{aligned}\rho_{u_k}^-(F(\Gamma))&\geqq(1-e^{-\beta/T_1})\,\rho_0^+(E),\\ \rho_{u_k}^+(f)&\geqq(1-e^{-\beta/T_1})\,\rho_0^+(E).\end{aligned}\right\} \tag{272}$$

Proof of lemma 4.8. – The proof is by induction on k. Let us put $A=E-(\{f\}\cup F(\Gamma))$.

From proposition I.4.5 we see that there is a positive α_1 such that

$$\rho^+_{u_{k+1}}(A)\leqq e^{-\alpha_1/T_1}\rho^+_{u_k}(E) \tag{273}$$

and

$$\rho^-_{u_{k+1}}(A)\leqq e^{-\alpha_1/T_1}\rho^+_{u_k}(E). \tag{274}$$

Now it is easy to see that $\rho^+_{u_{k+1}}(F(\Gamma))=0$ and that $\rho^-_{u_{k+1}}(f)=0$. Indeed there is $\alpha_2>0$ such that

$$\left.\begin{aligned}\sum_{i\in E}\rho^+_{u_k}(i)P(X_{u_{k+1}}=f\,|\,X_{u_k}=i)\geqq(1-e^{-\alpha_2/T_1})\rho^+_{u_k}(E),\\ \sum_{j\in E}\rho^-_{u_k}(i)P(X_{u_{k+1}}=g\,|\,X_{u_k}=i)\geqq(1-e^{-\alpha_2/T_1})\,|F(\Gamma)|^{-1}\rho^+_{u_k}(E)\end{aligned}\right\} \tag{275}$$

(because of the induction hypothesis and the fact that f and g are concentration sets). Hence

$$\rho_{u_{k+1}}(f)\geqq(1-2e^{-\alpha_2/T_1})\rho^+_{u_k}(E)>0, \tag{276}$$

$$\rho_{u_{k+1}}(g)\geqq(1-(|F(\Gamma)|+1)e^{-\alpha_2/T_1})\,|F(\Gamma)|^{-1}\rho^+_{u_k}(E)>0. \tag{277}$$

[Let us remind that $\rho^+(E)=\rho^-(E)$.]

From this we deduce that

$$\rho^+_{u_{k+1}}(A)=\rho^+_{u_{k+1}}(E)-\rho^+_{u_{k+1}}(f) \tag{278}$$

and that

$$\rho^-_{u_{k+1}}(A)=\rho^-_{u_{k+1}}(E)-\rho^-_{u_{k+1}}(F(\Gamma)), \tag{279}$$

hence from inequalities (273) and (274) we have

$$\left.\begin{aligned}\rho^+_{u_{k+1}}(f)\geqq(1-e^{-\alpha_1/T_1})\rho^+_{u_k}(E),\\ \rho^+_{u_{k+1}}(F(\Gamma))\geqq(1-e^{-\alpha_1/T_1})\rho^+_{u_k}(E)\end{aligned}\right\} \tag{280}$$

(let us lay the stress on the fact that α_1 is independent of β; only α_2 is dependent on β).

Hence for $\beta\leqq\alpha_1$ the induction step is proved.

End of the proof of lemma 4.8.

It is an easy matter to deduce proposition 4.7 from lemma 4.8, using inequalities of the kind of (276) and (277).

End of the proof of proposition 4.7.

LEMMA 4.9. – *Let* T_0, γ *be any positive constants. Let* $(E, U, q, \mathscr{L}_0, \mathscr{F}(T_0), \mathscr{X})$ *be a non-degenerate simple annealing framework such that* $\mathscr{L}_0$ *is* γ*-uniform. For any positive constant* σ_3 *there exist positive constants* K,

σ_1, σ_2 *such that for any* $k>\mathrm{K}$, *for any cooling schedule* $\mathrm{T}\in\mathcal{F}(\mathrm{T}_0)$ *satisfying*

$$\mathrm{T}_k^{-1}\geqq\hat{\mathrm{T}}_k^{-1}+e^{-\sigma_1/\hat{\mathrm{T}}_k} \tag{281}$$

where $\hat{\mathrm{T}}$ *is defined by*

$$\hat{\mathrm{T}}_n^{-1}=\frac{1}{\mathrm{H}(\Gamma)}\ln\left(\frac{|\mathrm{F}(\Gamma)|^{\delta}\tilde{q}n}{(1+\delta^{-1})}\right)\vee\mathrm{T}_0^{-1},\qquad n>0, \tag{282}$$

we have, putting $n=k+[e^{(\mathrm{H}(\Gamma)-\sigma_2)/\hat{\mathrm{T}}_k}]$

$$\mathrm{P}(\mathrm{X}_n\in\Gamma)\geqq\mathrm{P}(\hat{\mathrm{X}}_n\in\Gamma)(1+e^{-\sigma_3/\hat{\mathrm{T}}_n}). \tag{283}$$

Proof. – According to theorem 1.12 there are positive constants α_1, K such that in $\mathcal{F}(\mathrm{T}_0)$, for any $k\geqq\mathrm{K}$,

$$\mathrm{P}(\mathrm{X}_k\in\Gamma)\geqq\mathrm{P}(\hat{\mathrm{X}}_k\in\Gamma)(1-e^{-\alpha_1}/\hat{\mathrm{T}}_k). \tag{284}$$

Let us put

$$\mathrm{K}_1=\frac{2q(\Gamma)}{|\mathrm{F}(\Gamma)|}. \tag{285}$$

We are led to distinguish between two cases:

1. Case (1):

$$\mathrm{P}(\mathrm{X}_k\in\Gamma)\geqq 2\,\mathrm{P}(\hat{\mathrm{X}}_k\in\Gamma). \tag{286}$$

In this case

$$\begin{aligned}\mathrm{P}(\mathrm{X}_n\in\Gamma)&\geqq\left(1-2\frac{q(\Gamma)}{|\mathrm{F}(\Gamma)|}\sum_{l=k+1}^{n}e^{-\mathrm{H}(\Gamma)/\mathrm{T}_l}\right)\mathrm{P}(\mathrm{X}_k\in\Gamma)\\&\geqq\frac{3}{4}\mathrm{P}(\mathrm{X}_k\in\Gamma)\geqq\frac{3}{2}\mathrm{P}(\hat{\mathrm{X}}_k\in\Gamma)\end{aligned} \tag{287}$$

provided that k is large enough.

2. Case (2):

$$\mathrm{P}(\mathrm{X}_k\in\Gamma)\leqq 2\,\mathrm{P}(\hat{\mathrm{X}}_k\in\Gamma) \tag{288}$$

Let us call τ the constant named T_0 in lemma 1.9. We can assume that K has been chosen large enough such that

$$\hat{\mathrm{T}}_{\mathrm{K}}^{-1}-\frac{\ln 9}{\mathrm{U}(\Gamma)}>\tau. \tag{289}$$

Let us put

$$\mathrm{M}=\sup\left\{m\,|\,\mathrm{T}_m^{-1}<\hat{\mathrm{T}}_k^{-1}-\frac{\ln 9}{\mathrm{U}(\Gamma)}\right\}\vee\mathrm{K} \tag{290}$$

then

$$2\,P(\hat{X}_k\in\Gamma)\geqq P(X_k\in\Gamma)$$
$$\geqq P(X_M\in\Gamma)\left(1-K_1\sum_{l=M+1}^{k}e^{-H(\Gamma)/T_l}\right)$$
$$\geqq\frac{1}{2}P(\hat{X}_M\in\Gamma)\left(1-K_1\sum_{l=M+1}^{k}e^{-H(\Gamma)/T_l}\right)$$
$$\geqq 4\,P(\hat{X}_k\in\Gamma)\left(1-K_1\sum_{l=M+1}^{k}e^{-H(\Gamma)/T_l}\right)$$
$$\geqq 4\,P(\hat{X}_k\in\Gamma)\left(1-K_1\sum_{l=M+1}^{k}e^{-H(\Gamma)/T_l}\right),\quad (291)$$

hence

$$\sum_{l=M+1}^{k}e^{-H(\Gamma)/T_l}\geqq\frac{1}{2K_1}.\quad (292)$$

Thus we can apply proposition 1.8. There are positive constants α_2 and K such that for any $k>K$ and any cooling schedule T such that $T_k^{-1}\geqq\hat{T}_k^{-1}$, for any $\sigma_2>0$ we have for $n=k+[e^{(H-\sigma_2)/\hat{T}_k}]$

$$P(X_n\in\Gamma)-P(X_k\in\Gamma)\geqq(1-e^{-\sigma_2/(2\hat{T}_k)})\,q(\Gamma)\,K(2,1)\sum_{l=k+1}^{n}e^{-(H(\Gamma)+U(\Gamma))/T_l}$$
$$-(1+e^{-\sigma_2/(2\hat{T}_k)})\,P(X_k\in\Gamma)\,q(\Gamma)\,|F(\Gamma)|^{-1}K(2,1)$$
$$\times\left(e^{\alpha_2/\hat{T}_k}+\sum_{l=k+1}^{n}e^{-H(\Gamma)/T_l}\right).\quad (293)$$

Thus, using equation (284) and noticing that

$$\sum_{l=k+1}^{n}e^{-H(\Gamma)/T_l}\leqq(n-k)\,e^{-H(\Gamma)/\hat{T}_k}\leqq e^{-\sigma_2/\hat{T}_k}\quad (294)$$

choosing K such that

$$2\,q(\Gamma)\,K(2,1)\,|F(\Gamma)|^{-1}(e^{-\sigma_2/\hat{T}_k}+e^{-\alpha_2/\hat{T}_k})\leqq 1,\quad (295)$$

we have

$$P(X_n\in\Gamma)\geqq P(\hat{X}_k\in\Gamma)\,(1-e^{-\alpha_1/\hat{T}_k})$$
$$\times\left(1-(1+e^{-\sigma_2/(2\hat{T}_k)})\,q(\Gamma)\,K(2,1)\right.$$
$$\left.\times|F(\Gamma)|^{-1}\left(e^{-\alpha_2/\hat{T}_k}+\sum_{l=k+1}^{n}e^{-H(\Gamma)/T_l}\right)\right)$$
$$+(1-e^{-\sigma_2/(2\hat{T}_k)})\,q(\Gamma)\,K(2,1)\sum_{l=k+1}^{n}e^{-(H(\Gamma)+U(\Gamma))/T_l}.\quad (296)$$

Using the fact that

$$1-x+\frac{x^2}{2}-\frac{x^3}{6}\leqq e^{-x}\leqq 1-x+\frac{x^2}{2} \tag{297}$$

and putting

$$1/\tilde{T}_k=\frac{1}{U(\Gamma)}\left\{\ln\left(\frac{|F(\Gamma)|(H(\Gamma)+U(\Gamma))}{P(\hat{X}_k\in\Gamma)H(\Gamma)}\right)+\ln\left(\frac{(1-e^{-\alpha_1/\hat{T}_k})(1+e^{-\sigma_2/(2\hat{T}_k)})}{1-e^{-\sigma_2/(2\hat{T}_k)}}\right)\right\} \tag{298}$$

we deduce from (296) that for

$$T_k^{-1}\geqq\tilde{T}_k^{-1}+h \tag{299}$$

we have

$$\begin{aligned}P(X_n\in\Gamma)\geqq{}&P(\hat{X}_k\in\Gamma)(1-e^{-\alpha_1/\hat{T}_k})\\&\times\left\{1-(1+e^{-\sigma_2/(2\hat{T}_k)})\frac{q(\Gamma)K(2,1)}{|F(\Gamma)|(1+\delta^{-1})}(n-k)e^{-H(\Gamma)/\tilde{T}_k}\right\}\\&-P(\hat{X}_k\in\Gamma)q(\Gamma)K(2,1)|F(\Gamma)|^{-1}(1-e^{-\alpha_1/\hat{T}_k})e^{-\alpha_2/\hat{T}_k}+R\end{aligned} \tag{300}$$

with

$$\begin{aligned}R={}&(1-e^{-\sigma_2/(2\hat{T}_k)})q(\Gamma)K(2,1)(n-k)e^{-(H(\Gamma)+U(\Gamma))/\tilde{T}_k}h^2\\&\times\left(\frac{(H(\Gamma)+U(\Gamma))^2}{2}-\frac{(U(\Gamma)+H(\Gamma))^3}{6}h\right)\\&-P(\hat{X}_k\in\Gamma)(1-e^{-\alpha_1/\hat{T}_k})(1+e^{-\sigma_2/(2\hat{T}_k)})\\&\frac{q(\Gamma)K(2,1)}{|F(\Gamma)|}(n-k)e^{-H(\Gamma)/\tilde{T}_k}\frac{H(\Gamma)^2}{2}h^2\\&=P(\hat{X}_k\in\Gamma)(1-e^{-\alpha_1/\hat{T}_k})(1+e^{-\sigma_2/(2\hat{T}_k)})\\&\frac{q(\Gamma)K(2,1)}{|F(\Gamma)|}(n-k)e^{-H(\Gamma)/\tilde{T}_k}H(\Gamma)\\&\times\left(\frac{U(\Gamma)}{2}-\frac{(H(\Gamma)+U(\Gamma))^2}{6}h\right)h^2.\end{aligned} \tag{301}$$

On the other hand we see that for σ_2 small enough

$$P(\hat{X}_n\in\Gamma)\leqq P(\hat{X}_k\in\Gamma)\left(1-\frac{q(\Gamma)K(2,1)}{|F(\Gamma)|(1+\delta^{-1})}\times(n-k)e^{-H(\Gamma)/\hat{T}_k}(1-e^{-\sigma_2/(2\hat{T}_k)})\right) \tag{302}$$

and that

$$|\hat{T}_k^{-1}-\tilde{T}_k^{-1}|\leqq e^{-\sigma_2/(3\hat{T}_k)}, \tag{303}$$

hence

$$\begin{aligned}P(X_n \in \Gamma) \geqq P(\hat{X}_n \in \Gamma) - e^{-\alpha_1/\hat{T}_k} P(\hat{X}_k \in \Gamma)\\ \times \left(1 - (1 + e^{-\sigma_2/(2\hat{T}_k)}) \frac{q(\Gamma) K(2, 1)}{|F(\Gamma)|(1+\delta^{-1})} (n-k) e^{-H(\Gamma)/\tilde{T}_k}\right)\\ - e^{-\sigma_2/(2\hat{T}_k)} \frac{q(\Gamma) K(2, 1)}{(1+\delta^{-1})|F(\Gamma)|} (n-k) e^{-H(\Gamma)/\tilde{T}_k} P(\hat{X}_k \in \Gamma)\\ - e^{-\sigma_2/(2\hat{T}_k)} \frac{q(\Gamma) K(2, 1)}{(1+\delta^{-1})|F(\Gamma)|} (n-k) e^{-H(\Gamma)/\hat{T}_k} P(\hat{X}_k \in \Gamma)\\ - P(\hat{X}_k \in \Gamma)(1 - e^{-\alpha_1/\hat{T}_k}) e^{-\alpha_2/\hat{T}_k} + R. \quad (304)\end{aligned}$$

We can choose σ_1 and σ_2 such that

$$\left.\begin{aligned}\frac{3}{2}\sigma_2 < \alpha_1 \wedge \alpha_2 \wedge \frac{3}{4}\sigma_3,\\ \sigma_2 + 2\sigma_1 < \frac{3}{2}\sigma_2 \wedge \frac{\sigma_3}{2}.\end{aligned}\right\} \quad (305)$$

For example we can take

$$\left.\begin{aligned}\sigma_1 = \frac{\alpha_1 \wedge \alpha_2}{24} \wedge \frac{\sigma_3}{16},\\ \sigma_2 = \frac{\alpha_1 \wedge \alpha_2}{3} \wedge \frac{\sigma_3}{2}.\end{aligned}\right\} \quad (306)$$

With these choices we see that for $1/\hat{T}_k$ large enough, that is for k large enough, and for some positive constant a

$$\begin{aligned}P(X_n \in \Gamma) \geqq P(\hat{X}_n \in \Gamma) + P(\hat{X}_k \in \Gamma)\, a e^{-(\sigma_2 + 2\sigma_1)/\hat{T}_k}\\ \geqq P(\hat{X}_n \in \Gamma) + a e^{-\sigma_3/(2\hat{T}_k)} P(\hat{X}_k \in \Gamma)\\ \geqq P(\hat{X}_n \in \Gamma)(1 + e^{-\sigma_3/\hat{T}_n}). \quad (307)\end{aligned}$$

End of the proof of lemma 4.9.

Let us call α_7 the constant α of proposition 4.5. Let us put

$$u_0 = N(H(\Gamma), \hat{T}_k, -\sigma_2, k) \quad \text{and} \quad u_{n+1} = N(H(\Gamma), \hat{T}_k, -\alpha_7, u_n). \quad (308)$$

Let us consider the differential distributions

$$\rho_{u_0}(i) = P(\hat{X}_{u_0} = i) - P(X_{u_0} = i) \quad (309)$$

and for any $m > u_0$

$$\rho_m(i) = \sum_{j \in E} \rho_{u_0}(j) P(X_m = i \mid X_{u_0} = j). \quad (310)$$

Then ρ_m is the differential distribution starting from time u_0 of the annealing Markov chain X associated to T and the annealing Markov chain $\tilde{X}$ associated to the cooling schedule $\tilde{T}$ defined by

$$\left.\begin{aligned} \tilde{T}_m &= \hat{T}_m \quad \text{for} \quad m \leqq u_0, \\ \tilde{T}_m &= T_m \quad \text{for} \quad m > u_0. \end{aligned}\right\} \tag{311}$$

For any positive s we have

$$\begin{aligned} P(X_{u_s} \in \Gamma) &\geqq (1 - s K_1 e^{-\alpha_7/\hat{T}_k}) P(X_{u_0} \in \Gamma) \\ &\geqq (1 - s K_1 e^{-\alpha_7/\hat{T}_k})(1 + e^{-\sigma_3/\hat{T}_k}) P(\tilde{X}_{u_0} \in \Gamma) \\ &\geqq (1 - s K_1 e^{-\alpha_7/\hat{T}_k})(1 + e^{-\sigma_3/\hat{T}_k}) P(\tilde{X}_{u_s} \in \Gamma), \end{aligned} \tag{312}$$

hence as long as

$$s K_1 e^{-\alpha_7/\hat{T}_k} \leqq \frac{1}{3} e^{-\sigma_3/\hat{T}_k} \tag{313}$$

we have

$$P(X_{u_s} \in \Gamma) \geqq \left(1 + \frac{1}{2} e^{-\sigma_3/\hat{T}_k}\right) P(\tilde{X}_{u_s} \in \Gamma). \tag{314}$$

Moreover there are positive constants α_8, α_9 such that

$$\begin{aligned} \rho_{u_s}(V_2 - \Gamma) \leqq \rho^+(V_2 - \Gamma) &\leqq P(\tilde{X}_{u_s} \in E - (\Gamma \cup G_1)) \\ &\leqq e^{-(U(\Gamma) + \alpha_s)/\hat{T}_k} \leqq P(\tilde{X}_{u_s} \in \Gamma) e^{-\alpha_9/\hat{T}_k}, \end{aligned} \tag{315}$$

hence assuming that $\sigma_3 < \alpha_9$ and that K is large enough, we have

$$\left.\begin{aligned} \rho_{u_s}(V_2) &\leqq -\frac{1}{3} P(\tilde{X}_{u_s} \in \Gamma) e^{-\sigma_3/\hat{T}_k} \\ \rho_{u_s}(V_2) &\leqq -\frac{1}{4} P(\hat{X}_k \in \Gamma) e^{-\sigma_3/\hat{T}_k}. \end{aligned}\right\} \tag{316}$$

Then according to proposition 4.5, for any m such that

$$m K_1 e^{-\alpha_7/\hat{T}_k} \leqq \frac{1}{3} e^{-\sigma_3/\hat{T}_k} \tag{317}$$

we have

$$\frac{1}{2} |\rho_{u_m}|(E) \leqq \frac{1}{2} |\rho_{m-1}|(E) - (1 - e^{-\alpha_7/\hat{T}_k})(\rho^-_{u_{m-1}}(V_1) + \rho^+_{u_{m-1}}(V_2)). \tag{318}$$

But for any differential distribution ρ

$$\rho^-(V_1) + \rho^+(V_2) = \frac{1}{2} |\rho|(E) + \rho^+(V_2) - \rho^-(V_2) = \frac{1}{2} |\rho|(E) + \rho(V_2), \tag{319}$$

hence equation (318) becomes

$$\frac{1}{2} |\rho_{u_m}|(E) \leqq \frac{1}{2} |\rho_{u_{m-1}}|(E) e^{-\alpha_7/\hat{T}_k} - \rho_{u_{m-1}}(V_2)(1 - e^{-\alpha_7/\hat{T}_k}), \tag{320}$$

from which we deduce that

$$\frac{1}{2}|\rho_{u_m}|(\mathrm{E}) \leqq \frac{1}{2}|\rho_{u_0}|(\mathrm{E})\, e^{-m\alpha_7/\hat{\mathrm{T}}_k} + \sum_{s=0}^{m-1} -\rho_{u_s}(\mathrm{V}_2)\, e^{-(m-1-s)\,\alpha_7/\hat{\mathrm{T}}_k}. \quad (321)$$

In the same spirit as equation (312), we have or any s, m such that $s<m$ and $m\,\mathrm{K}_1\, e^{-\alpha_7/\hat{\mathrm{T}}_k} \leqq \frac{1}{3} e^{-\sigma_3/\hat{\mathrm{T}}_k}$

$$\begin{aligned} -\rho_{u_m}(\Gamma) &\geqq \mathrm{P}(\mathrm{X}_{u_s}\in\Gamma)(1-\mathrm{K}_1(m-s)\,e^{-\alpha_7/\hat{\mathrm{T}}_k}) - \mathrm{P}(\tilde{\mathrm{X}}_{u_s}\in\Gamma) \\ &\geqq -\rho_{u_s}(\Gamma) - \frac{1}{3} e^{-\sigma_3/\hat{\mathrm{T}}_k}\, \mathrm{P}(\mathrm{X}_{u_s}\in\Gamma), \end{aligned} \quad (322)$$

but from equation (314)

$$-\rho_{u_s}(\Gamma) \geqq \frac{1}{2}\mathrm{P}(\tilde{\mathrm{X}}_{u_s}\in\Gamma)\, e^{-\sigma_3/\hat{\mathrm{T}}_k} \geqq \frac{1}{2}(\rho_{u_s}(\Gamma) + \mathrm{P}(\mathrm{X}_{u_s}\in\Gamma))\, e^{-\sigma_3/\hat{\mathrm{T}}_k}, \quad (323)$$

hence for $\hat{\mathrm{T}}_k$ large enough

$$-\rho_{u_s}(\Gamma) \geqq \frac{3}{8}\mathrm{P}(\mathrm{X}_{u_s}\in\Gamma)\, e^{-\sigma_3/\hat{\mathrm{T}}_k}, \quad (324)$$

hence coming back to equation (322)

$$-\rho_{u_m}(\Gamma) \geqq -\rho_{u_s}(\Gamma)\left(1-\frac{8}{9}\right), \quad (325)$$

hence

$$-\rho_{u_s}(\Gamma) \leqq -9\,\rho_{u_m}(\Gamma). \quad (326)$$

Moreover

LEMMA 4.10. – *There is some positive constant* α_{10} *such that for any positive* $s>1$ *such that* $s\,\mathrm{K}_1\, e^{-\alpha_7/\hat{\mathrm{T}}_k} \leqq \frac{1}{3} e^{-\sigma_3/\hat{\mathrm{T}}_k}$.

$$\mathrm{P}(\mathrm{X}_{u_s}\in \mathrm{E}-(\mathrm{G}_1\cup\Gamma)) \leqq e^{-\alpha_{10}/\hat{\mathrm{T}}_k}\, \mathrm{P}(\mathrm{X}_{u_s}\in\Gamma). \quad (327)$$

Proof of lemma 4.10. – We have

$$\begin{aligned} \mathrm{P}(\mathrm{X}_{u_s}\in \mathrm{E}-(\mathrm{G}_1\cup\Gamma)) &\leqq \mathrm{P}(\tau(\mathrm{E}^{**}, k)>u_s) \\ &+ \sum_{k\leqq m<l\leqq u_s}\ \sum_{j\in \mathrm{E}-(\mathrm{G}_1\cup\Gamma)} \mathrm{P}(\mathrm{X}_m=f)\, \mathrm{M}(\mathrm{E}^{**}, \mathrm{E}-(\mathrm{G}_1\cup\Gamma))_{f,m}^{j,l} \\ &\qquad \times \mathrm{P}(\tau(\mathrm{E}-(\mathrm{G}_1\cup\Gamma), l)>u_s \mid \mathrm{X}_l=j) \\ &\qquad + \mathrm{P}(\mathrm{X}_m=g)\, \mathrm{M}(\mathrm{E}^{**}, \mathrm{E}-(\mathrm{G}_1\cup\Gamma))_{g,m}^{j,l} \\ &\qquad\qquad \times \mathrm{P}(\tau(\mathrm{E}-(\Gamma\cup \mathrm{G}_1), l)>u_s \mid \mathrm{X}_l=j), \end{aligned} \quad (328)$$

where g is some given point of $\mathrm{F}(\Gamma)$. Thus equation (328) takes the form

$$\mathrm{P}(\mathrm{X}_{u_s}\in \mathrm{E}-(\mathrm{G}_1\cup\Gamma)) \leqq \mathrm{R}_1+\mathrm{R}_2+\mathrm{R}_3 \quad (329)$$

with, for some constants a, b

$$R_1 \leqq (1+b)\exp\left(-a \sum_{l=k+1}^{u_s} e^{-S(E)/T_l}\right)$$
$$\leqq (1+b)\exp\left(-a\, e^{(H(\Gamma)-S(E)-\sigma_2)/\hat{T}_k}\right) \quad (330)$$

and it is clear from the proof of lemma 4.9 that we can assume that $\sigma_2 < H(\Gamma) - S(E)$, hence, assuming that K is large enough we have for any $k \geqq K$

$$R_1 \leqq (1+b)\, e^{-(H(\Gamma)+U(\Gamma))/\hat{T}_k}. \quad (331)$$

There is a positive constant K_4 such that

$$R_2 \leqq K_4\, e^{-(H(G_1)-S(E))/\hat{T}_k} \quad (332)$$

[recall that $H(G_1) = H(\Gamma) + U(\Gamma)$] and

$$R_3 \leqq P(X_k \in \Gamma)\, K_4\, e^{-(H(\Gamma)-S(E))/\hat{T}_k}. \quad (333)$$

(These estimations of R_1, R_2 and R_3 are a consequence of propsition I.4.5 and the composition lemmas of the appendix.) Comparing these inequalities with equation (284) gives

$$P(X_{u_s} \in E - (G_1 \cup \Gamma)) \leqq e^{-\alpha_{10}/\hat{T}_k} P(X_k \in \Gamma)$$
$$\leqq e^{-\alpha_{10}/\hat{T}_k} P(X_{u_s} \in \Gamma)(1 + e^{-\sigma_3/\hat{T}_k}). \quad (334)$$

End of the proof of lemma 4.10.

Using lemma 4.10 we see that there are positive constants α_{11} and α_{12} such that

$$-\rho_{u_s}(V_2 - \Gamma) \leqq P(X_{u_s} \in E - (G_1 \cup \Gamma))$$
$$\leqq e^{-\alpha_{10}/\hat{T}_k} P(X_{u_s} \in \Gamma)$$
$$\leqq e^{-\alpha_{10}/\hat{T}_k}(-\rho_{u_s}(\Gamma))\frac{8}{3} e^{\sigma_3/\hat{T}_k}$$
$$\leqq e^{-\alpha_{11}/\hat{T}_k}(-\rho_{u_s}(\Gamma)) \leqq e^{-\alpha_{12}/\hat{T}_k}(-\rho_{u_s}(V_2)) \quad (335)$$

as soon as σ_3 has been chosen small enough. Hence we deduce from equation (326) that

$$-\rho_{u_s}(V_2) \leqq 10(-\rho_{u_m}(V_2)). \quad (336)$$

Coming back to equation (321) we have

$$\frac{1}{2}|\rho_{u_m}|(E) \leqq \frac{1}{2}|\rho_{u_0}|(E)\, e^{-m\alpha_7/\hat{T}_k} + \left(1 + 10\frac{e^{-\alpha_7/T_k}}{1 - e^{-\alpha_7/\hat{T}_k}}\right)(-\rho_{u_{m-1}}(V_2)). \quad (337)$$

We can take for m the integer part of $\frac{1}{3K_1} e^{(\alpha_7-\sigma_3)/\hat{T}_k}$ and we can choose $\sigma_3 < \frac{\alpha_7}{2}$, in this way we get

$$\frac{1}{2}|\rho_{u_m}|(E) \leqq \exp\left(-\frac{\alpha_7}{\hat{T}_k} e^{\alpha_7/(3\hat{T}_k)}\right) + (1+e^{-\alpha_{13}/\hat{T}_k})(-\rho_{u_m}(V_2)) \leqq (1+e^{-\alpha_{14}/\hat{T}_k})(-\rho_{u_m}(V_2)). \quad (338)$$

Hence we have

$$\rho_{u_{m+1}}(f) \geqq (1-e^{-\alpha_7/\hat{T}_k})\,\rho_{u_m}(V_1) \geqq (1-e^{-\alpha_{15}/\hat{T}_k})\frac{1}{2}|\rho_{u_m}|(E) \geqq (1-e^{-\alpha_{15}/\hat{T}_k})\,\rho^+_{u_{m+1}}(E), \quad (339)$$

and in the same way

$$\rho_{u_{m+1}}(g) \geqq \frac{1}{|F(\Gamma)|}(1-e^{-\alpha_7/\hat{T}_k})\,\rho_{u_m}(V_1) \geqq \frac{1}{|F(\Gamma)|}(1-e^{-\alpha_{15}/\hat{T}_k})\,\rho^+_{u_{m+1}}(E). \quad (340)$$

We conclude from (339), (340) and proposition 4.7 that the for any $n \geqq u_{m+1}$ we have $\rho_n(f) > 0$. Hence $(T_n)_{1 \leqq n \leqq N}$ cannot be optimal for $N \geqq u_{m+1}$.

End o the proof of theorem 4.1.

Proof of theorem 4.2. – Let T be in $\mathscr{T}(E, U, q, \mathscr{L}_0, T_0)$. For N large enough, let us put, with the notations of the remark following theorem 4.1

$$M = \sup\left\{k \,\middle|\, \sum_{l=k+1}^{n} e^{-H(\Gamma)/\tilde{T}^N_l} \geqq e^{-\alpha/\tilde{T}^N_k}\right\}. \quad (341)$$

Let $\hat{T}$ be the cooling schedule

$$1/\hat{T}_n = \frac{1}{H(\Gamma)} \ln\left(\frac{|F(\Gamma)|^\delta \tilde{q} n}{1+\delta^{-1}}\right), \qquad n \geqq 1. \quad (342)$$

Then we know that for some positive constants K and β, for N large enough and for any $k \in [K, M]$

$$1/\tilde{T}^N_k \leqq 1/\hat{T}_k + e^{-\beta/\hat{T}_k}. \quad (343)$$

Let us consider the time

$$J = \sup\{k \mid 1/\tilde{T}^N_k \leqq 1/\hat{T}_k\} \vee M \quad (344)$$

We will show that the triangular cooling schedule T defined by

$$\left.\begin{array}{ll} 1/T_k^N = 1/\hat{T}_k, & k \leqq J, \\ 1/T_k^N = 1/\tilde{T}_k^N, & k > J, \end{array}\right\} \tag{345}$$

has the properties stated in theorem 4.2.

Let us define the temperature τ by

$$P(\tilde{X}_N^N \neq f) = e^{-U(\Gamma)/\tau}. \tag{346}$$

Let us put

$$R = \inf\left\{ k \,\middle|\, 1/\tilde{T}_k^N \geqq \frac{1}{2\tau} \right\}. \tag{347}$$

For N large enough (and hence τ small enough) we have

$$\begin{aligned} P(\tilde{X}_J^N \in \Gamma) &\geqq P(\tilde{X}_R^N \in \Gamma)\left(1 - 2q(\Gamma) \sum_{l=R+1}^{J} e^{-H(\Gamma)/\tilde{T}_l^N}\right) \\ &\geqq \frac{|F(\Gamma)|}{2} e^{-U(\Gamma)/(2\tau)}\left(1 - 2q(\Gamma) \sum_{l=R+1}^{J} e^{-H(\Gamma)/\tilde{T}_l^N}\right). \end{aligned} \tag{348}$$

On the other side, as $J \geqq M$,

$$P(\tilde{X}_J^N \in \Gamma) \leqq 2\, P(\tilde{X}_N^N \in \Gamma), \tag{349}$$

hence there are positive constants a and b such that

$$1 - a \sum_{l=R+1}^{J} e^{-H(\Gamma)/\tilde{T}_l^N} \leqq b\, P(\tilde{X}_N^N \neq f)^{1/2}. \tag{350}$$

Hence for N large enough

$$\sum_{l=R+1}^{N} e^{-H(\Gamma)/\tilde{T}_l^N} \geqq \frac{1}{2}, \tag{351}$$

and, applying proposition 4.5 we see that there exist positive constants β_1 and β_2 such that for any t such that

$$\sum_{l=t+1}^{N} e^{-H(\Gamma)/\tilde{T}_l^N} \leqq e^{-\alpha/(2\,\tilde{T}_M^N)}$$

we have

$$P(\tilde{X}_t^N \neq f) \leqq e^{-\beta_1/(2\tau)} + P(\tilde{X}_t^N \in \Gamma) \leqq P(\tilde{X}_N^N \neq f)^{\beta_2}. \tag{352}$$

Writing equation (227) for $\tilde{X}$, we deduce from equation (352) and from theorem 1.12 and lemma 2.6 that there exists a positive constant β_3 such that for N large enough

$$P(\hat{X}_J = i) \leqq (1 + P(\tilde{X}_N^N \neq f)^{\beta_3})\, P(\tilde{X}_J^N = i), \qquad i \in E. \tag{353}$$

Hence, as $X_J^N = \hat{X}_J$ and as the conditional probabilities $P(X_N^N | X_J^N)$ and $P(\tilde{X}_N^N | \tilde{X}_J^N)$ are the same, we have

$$P(X_N^N = i) \leqq (1 + P(\tilde{X}_N^N \neq f)^{\beta_3}) P(\tilde{X}_N^N = i), \qquad i \in E, \tag{354}$$

hence

$$P(X_N^N \neq f) - P(\tilde{X}_N^N \neq f) \leqq P(\tilde{X}_N^N \neq f)^{1+\beta_3}. \tag{355}$$

As it is easy to see that for N large enough

$$P(\tilde{X}_N^N \neq f) \leqq \frac{1}{N^d} \tag{356}$$

this ends the proof.

End of the proof of theorem 4.2.

CONCLUSION

Our aim in this second paper about sharp large deviations estimates was to give applications. These applications are linked to the central problem of quasi-equilibrium.

We would like to have convinced the reader that it is important to add a constant term to the "expansion" of $1/T_n$, writing $1/T_n = d^{-1} \ln n + B$.

Interestingly quasi-equilibrium is not strictly speaking maintained for those schedules, but the density of the law of the system with respect to the law at thermal equilibrium stays bounded if B is small enough.

We would like also to convince people that it is natural to consider simulated annealing algorithms up to a finite time N and to let the whole cooling schedule depend on N. The fact that the initial shape of the "best" triangular cooling schedules is $1/T_n = d^{-1} \ln + B + o(1)$ is a serious objection to the common belief that quasi-equilibrium should be maintained during the simulation.

Let us conclude by recalling that the precision of sharp estimates was fully needed to obtain this set of results.

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