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Markov Chains with Exponentially Small Transition Probabilities: First Exit Problem from a General Domain. I. The Reversible Case

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We consider general ergodic aperiodic Markov chains with finite state space whose transition probabilities between pairs of different communicating states are exponentially small in a large parameter β. We extend previous results by M. I. Freidlin and A. D. Wentzell (FW) on the first exit problem from a general domain Q. In the present paper we analyze the case of *reversible* Markov chains. The general case will be studied in a forthcoming paper. We prove, in a purely probabilistic way and without using the FW graphical technique, some results on the first exit problem from a general domain Q containing many attractors. In particular we analyze the properties of special domains called *cycles* and, by using the new concept of *temporal entropy*, we obtain new results leading to a complete description of the typical tube of trajectories during the first excursion outside Q.

KEY WORDS: Markov chains; first exit problem; large deviations; reversibility.

1. INTRODUCTION

In this paper we consider ergodic, aperiodic Markov chains with finite state space S and with transition probabilities $P(x, y)$ satisfying the following:

Property $\mathscr{P}$. If x and y are communicating states, i.e., $x \neq y$ and $P(x, y) > 0$, then

$$\exp(-\Delta(x, y)\beta - \gamma\beta) \leqslant P(x, y) \leqslant \exp(-\Delta(x, y)\beta + \gamma\beta) \tag{1.1}$$

Dedicated to the memory of Claude Kipnis.

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where $\Delta(\cdot, \cdot)$ is a nonnegative function on the set of pairs of communicating states and $\gamma \to 0$ as $\beta \to \infty$.

Freidlin and Wentzell introduced this kind of Markov chain as an auxiliary structure in their study of the asymptotic properties of diffusion processes describing small random perturbations of dynamical systems.

Another very interesting application, which actually is our main motivation, comes from nonequilibrium statistical mechanics: stochastic dynamics for interacting particle systems at very low temperature, like Glauber dynamics for Ising-like models, in a finite volume, satisfy Property $\mathscr{P}$ (in this case β is the inverse temperature). (see, e.g., refs. 8, 9, 7, 11, 5, 6, and 3.)

We will mainly study the problem of the first exit from a domain $Q \subset S$ containing many attracting equilibrium states for the dynamics at $\beta = \infty$. Many results on this subject are already known: in particular, Freidlin and Wentzell proved estimates for the average exit time and the typical point, on the boundary of Q, reached during the first excursion outside Q. They also describe the tube of typical trajectories exiting from Q when this set contains a unique attracting state.

The study of the typical exiting trajectories is of fundamental importance and, in a certain sense, it is the central problem in the description of nucleation phenomena in the framework of general stochastic Ising models.[11,5,6] In that case we are interested in the analysis of a typical sequence of growing droplets and in particular in their shapes. Indeed the growth of the so-called critical nucleus can be seen as a particular case of the first exit from a noncompletely attracted domain.

It turns out, by looking at several particular models, that a crucial ingredient in the description of the growth is given by the *resistance times* inside some subsets of Q. These can be considered as a sort of *temporal entropy* related to fluctuations taking place during suitable random times which grow exponentially fast in β. This temporal entropy turns out to be necessary to give rise to an efficient escape mechanism. Neglecting these random fluctuations during the escape would lead to a mechanism extremely depressed in probability. Apparently the importance of these time fluctuations escaped many previous researchers on the subject.

We can say that the last escape from Q occurs in a very different way in the two cases of one or several attracting points in Q. In the completely attracted case, the typical trajectories during the first excursion outside Q spend a finite time independent of β to bring the process out of Q without any "hesitation." In the general case the last escape takes place by visiting a suitable sequence of more or less stable attractors $z_1,..., z_n$ and spending some suitable random times inside certain domains $A_1,..., A_n$ which can be considered as sort of generalized basins of attraction of $z_1,..., z_n$, respectively.

We can say that the formulation of the problem of the characterization of the tube of typical exiting trajectories in the general case requires new concepts with respect to what has been done in the completely attracted case.

On one hand, our work can be considered as a completion and a generalization of the results contained in Chap. 6 of Freidlin and Wentzell's book;[4] on the other hand, we formulate a general setup useful to treat, in a unified way, a large class of stochastic dynamics.

Our results are general and we are able to reduce the solution of the above-mentioned typical large-deviation problem connected to the escape from a general domain, to the solution of a well-defined sequence of variational problems. These variational problems constitute the model-dependent work to be done. In other words, we state the results concerning the general behavior of the class of Markov chains satisfying property $\mathscr{P}$ by specifying their common features and by reducing the model-dependent work to the solution of some well-specified problems whose formulation can be given in general.

In the present paper we concentrate on the *reversible* case (see Hypothesis M in Sec. 3) where the unique invariant measure μ of the chain has the Gibbsian form $\mu = \exp(-\beta H)/Z$ with a given energy function H on S.

For the general case we just give here the formulation of the problem, the complete treatment being the object of a forthcoming paper.

The discussion of the general case will require some generalization of the graphical technique introduced by Freidlin and Wentzel (see ref. 4, p. 177) and, more important, the use of the approach introduced by one of the authors.[12] This approach is based on the notion of *renormalized chains*, obtained by a time rescaling related to the degree of stability of different attracting equilibrium states.

The reversible case is much easier. The crucial point of our approach to that case is to base our discussion on the analysis of the "energy landscape."

We will provide new probabilistic proofs of results obtained by Freidlin and Wentzell with their graphical technique. Moreover, we will prove new results on the characterization of the tube of typical exiting trajectories.

The paper is organized as follows: In Section 2 we first discuss the case of a completely attracted domain and we outline the differences and the difficulties arising in the general, not completely attracted case. Then we recall some notions relative to the renormalized chains; finally we state the problem for the general case and we sketch the strategy for its solution.

The rest of the paper is devoted to the reversible case.

In Section 3 we first give definitions and properties concerning the so-called *cycles*; then we provide alternative and explicit proofs of known results about the asymptotics of first exit times and first exit points from a class of not completely attracted domains.

In Section 4 we state and prove our new results concerning the typical tube of trajectories during the first descent to the bottom of a domain (Theorem 1) or during the first escape (Theorem 2).

2. THE EXIT PROBLEM AND THE RENORMALIZATION PROCEDURE

Let X_t be a Markov chain satisfying Property $\mathscr{P}$ above; given any set of states $Q \subset S$, we will denote by τ_Q the first hitting time to Q:

$$\tau_Q \equiv \min\{t > 0;\ X_t \in Q\}$$

We define the (outer) boundary ∂Q of Q as the set

$$\partial Q = \{x \notin Q : \exists x' \in Q : P(x', x) > 0\}$$

A first description of the exit of the chain X_t from the set Q can be given by means of the following two quantities: the expectation of the first exit time from Q,

$$E_x \tau_{\partial Q} \tag{2.1}$$

and the spatial distribution of the first exit,

$$P_x(X_{\tau_{\partial Q}} = y) \tag{2.2}$$

with $x \in Q$, $y \in \partial Q$ (we denote by P_x the probability distribution on the process starting from x at $t = 0$; E_x denotes the corresponding expectation).

Estimates of the quantities (2.1) and (2.2), from above and from below, are given by Freidlin and Wentzell.[4] In fact they study diffusion process, describing small random perturbations of dynamical systems with the help of discrete Markov chains satisfying property $\mathscr{P}$. They show that the quantities (2.1) and (2.2) can be expressed in terms of sums of products of transition probabilities of the chain, and these products can be defined by means of graphs of arrows. Then their estimates can be reduced to a problem of minimization of a suitbale cost function associated with each graph (see ref. 4, Chapter 6, Section 3, p. 176).

Similar to what was done by Freidlin and Wentzel in the continuous case, we can develop for our Markov chains the usual theory of large deviations. To each path, i.e., to each function ϕ: $\mathbf{N} \to S$, $\phi = \{\phi_t\}_{t \in \mathbf{N}}$, we can associate a functional

$$I_{[0,t]}(\phi) \equiv \sum_{i=0}^{t-1} \Delta(\phi_i, \phi_{i+1}) \tag{2.3}$$

where the function $\Delta(x, y)$ is defined in (1.1) and we set $\Delta(x, x) = 0$ for each $x \in S$ and $\Delta(x, y) = \infty$ if $P(x, y) = 0$. This functional can be interpreted as the cost function of each path ϕ, and the corresponding large-deviation estimates can be easily proved.[12]

Lemma 2.1. Let ϕ e a fixed function starting from x at time 0; then:

(i) We have

$$P_x(X_s = \phi_s, \forall s \in [0, t]) \leqslant e^{-I_{[0,t]}(\phi)\beta + \gamma t\beta}$$

(ii) If ϕ is such that $\phi_s \neq \phi_{s+1}$ for any $s \in [0, t]$, then we have also a lower bound:

$$P_x(X_s = \phi_s, \forall s \in [0, t]) \geqslant e^{-I_{[0,t]}(\phi)\beta - \gamma t\beta}$$

(iii) For any constant $I_0 > 0$, for any sufficiently small $\alpha > 0$ [α strictly less than the minimal positive value of the function $\Delta(\cdot, \cdot)$], for any $t < e^{\alpha\beta}$, and for any sufficiently large β

$$\sup_x P_x(I_{[0,t]}(X_s) \geqslant I_0) \leqslant e^{-I_0\beta + \varepsilon\beta}$$

where $\varepsilon \to 0$ as $\beta \to \infty$.

An equivalence relation in the state space S can be defined by means of the functional $I_{[0,t]}(\phi)$: for each pair of states x, y we define

$$V(x, y) \equiv \inf_{t, \phi: \phi_0 = x, \phi_t = y} I_{[0,t]}(\phi) \tag{2.4}$$

and we set

$$\begin{aligned} &x \sim y \qquad \text{iff} \quad V(x, y) = V(y, x) = 0 \\ &(x)_\sim \equiv \{y \in S; y \sim x\} \end{aligned} \tag{2.5}$$

We say that x is a stable state if and only if

$$\text{for any} \quad y \not\to x, \qquad V(x, y) > 0 \tag{2.6}$$

i.e., if each path leaving from x has a positive cost.

We will denote by M the set of stable states.

It is immediate to see that if the set M contains a state x, then it contains the whole equivalence class of x, namely $M \supset (x)_{\sim}$.

An immediate consequence of Lemma 2.1 is the following Lemma 2.2, whose proof can be found in ref. 12.

Lemma 2.2. There exist constants $T_0 \in [0, |S|]$ and β_0 such that for any $\beta > \beta_0$:

(i) For any $t > T_0$:

$$\sup_{x \in S} P_x(\tau_M > t) \leqslant a^{[t/T_0]}$$

with $a = 1 - C^{T_0}$ for some constant $0 < C < 1$ and where $[\cdot]$ denotes the integer part.

(ii) For any $\eta > 0$, for any $t \geqslant e^{\eta\beta}$ and β sufficiently large we have

$$\sup_{x \in S} P_x(\tau_M > t) \leqslant \exp\{-e^{\eta\beta/2}\}$$

Let us now come back to the problem of the exit of our chain X_t from a domain Q and let us suppose that this set contains a unique stable state x_0 which is a global attractor for Q in the sense that for each $y \in Q$ there exists a path $y_0 = y, y_1, \dots, y_n = x_0$ such that $\Delta(y_i, y_{i+1}) = 0$ $\forall i < n$, whereas for each $y \in Q$, $z \in \partial Q$, we have $\Delta(y, z) > 0$. In this case Freidlin and Wentzell can describe in complete detail the exit from Q.

We give their result in the discrete case of Markov chains (see ref. 4, Chapter 4, Theorem 2.3 for the continuous version of this result).

We want to notice here that in the continuous case of diffusion processes discussed in ref. 4, the dynamics corresponding to zero random noise was given by a dynamical system: the unperturbed system was completely deterministic and then for each starting point there was a unique deterministic path emerging from it. The tube of typical exiting trajectories was given in that case as a neighborhood in the uniform topology of such a deterministic path.

Here, in the discrete case of Markov chains the situation is different and even for $\beta = \infty$ the system can still be random. This means that there is not a unique deterministic path, but, in general, several possible paths emerging from the same starting point. Moreover, we do not have to consider a neighborhood, since the space is discrete. So the typical exiting tube in this case is a finite set of individual paths.

Proposition 2.1. Let Q be a set of states containing a unique stable state x_0 and for each α and β define

$$\Phi_{\alpha,\beta} \equiv \{\{\phi_s\}_{s\in\mathbb{N}};\ \phi_0 = x_0,\ \phi_{T_\phi} \in \partial Q,\ \phi_s \in Q,\ \forall s < T_\phi, \text{ with } T_\phi < e^{\alpha\beta}\} \tag{2.7}$$

and

$$\bar{\Phi}_{\alpha,\beta} \equiv \{\phi_s \in \Phi_{\alpha,\beta};\ I_{[0,T_\phi]}(\phi) = \min_{y\in\partial Q} V(x_0, y)\} \tag{2.8}$$

For any given sufficiently small α (see Lemma 2.1) we have

$$\lim_{\beta\to\infty} P_x(X_{\theta_{x_0}+t} = \phi_t,\ \forall t = 0,\ldots, \tau_{\partial Q} - \theta_{x_0}, \text{ for some } \phi \in \bar{\Phi}_{\alpha,\beta}) = 1 \tag{2.9}$$

where $\theta_{x_0} \equiv \max\{t < \tau_{\partial Q};\ X_t = x_0\}$.

A proof of this proposition can be easily obtained by applying Lemmas 2.1 and 2.2. Indeed, by Lemma 2.2 we are able to exclude that $\tau_{\partial Q} - \theta_{x_0}$ is exponentially too large in β, and then we can apply the large-deviation estimates. More precisely, the probability of the complementary event can be estimated from above as follows:

$$\begin{aligned}
&P_x(\{X_{\theta_{x_0}+t}\}_{t=0}^{\tau_{\partial Q}-\theta_{x_0}} \notin \bar{\Phi}_{\alpha,\beta})\\
&\quad = \sum_{s=0}^{\infty} P_x([\{X_{s+t}\}_{t=0}^{\tau_{\partial Q}-s} \notin \bar{\Phi}_{\alpha,\beta}] \cap [\theta_{x_0} = s])\\
&\quad = \sum_{s=0}^{\infty} P_x([\{X_{s+t}\}_{t=0}^{\tau_{\partial Q}-s} \notin \bar{\Phi}_{\alpha,\beta}] \cap [X_{s'} \in Q, \forall s' < s, X_s = x_0, X_{s+1} \neq x_0]\\
&\qquad \cap [X_{\tau^{(>s)}_{x_0\cup\partial Q}} \in \partial Q])
\end{aligned} \tag{2.10}$$

where

$$\tau^{(>s)}_{x_0\cup\partial Q} \equiv \min\{t > s;\ X_t \in \{x_0 \cup \partial Q\}\}$$

The r.h.s. of (2.10) can be estimated, by using the Markov property, as follows:

$$\begin{aligned}
&\leqslant \sum_{s=0}^{\infty} P_x(\tau_{\partial Q} > s)\, P_{x_0}([\{X_t\}_{t=0}^{\tau_{\partial Q}} \notin \bar{\Phi}_{\alpha,\beta}] \cap [X_1 \neq x_0, X_{\tau_{x_0}\cap\partial Q} \in \partial Q])\\
&\leqslant E_x\tau_{\partial Q} \cdot \{P_{x_0}([\{X_t\}_{t=0}^{\tau_{\partial Q}} \notin \Phi_{\alpha,\beta}] \cap [X_1 \neq x_0, X_{\tau_{x_0}\cap\partial Q} \in \partial Q])\\
&\qquad + P_{x_0}(\{X_t\}_{t=0}^{\tau_{\partial Q}} \in \Phi_{\alpha,\beta}\backslash\bar{\Phi}_{\alpha,\beta})\}
\end{aligned}$$

$$\leqslant \{\exp[\min_{y \in \partial Q} V(x_0, y)\beta + \delta\beta]\}$$

$$\times \{\exp(-e^{\alpha\beta/2}) + P(I_{[0,e^{\alpha\beta}]}(X_s(x_0)) \geqslant \min_{y \in \partial Q} V(x_0, y) + d)\}$$

for some positive constant d. The theorem follows by applying Lemma 2.1 and by using the fact that δ goes to 0 as $\beta \to \infty$ while d is fixed.

We remark that in this proposition the hypothesis of the uniqueness of the stable state in Q is crucial; in fact the large-deviation estimate can be applied, here as in the continuous case, only on intervals of time which do not grow too fast in β (they have to be bounded by $e^{\alpha\beta}$ with α sufficiently small). However, if the set Q contains several stable states, then the functions in $\bar{\Phi}_{\alpha,\beta}$ can (and we will see that they do) visit, before leaving Q, other stable states where the process is likely to spend exponentially long times. This means that in this case, due to the above-mentioned resistance times, the time $\tau_{\partial Q} - \theta_{x_0}$ is exponentially large with large probability. Thus an extension of Proposition 2.1 to a general domain Q would require a control on large-deviation estimates over exponentially long intervals of time. This is the crucial point to be solved. New ideas and techniques are necessary; new concepts will be needed to define the tube.

To solve this problem we will use a renormalization procedure for Markov chains satisfying Property $\mathscr{P}$, representing a completely different approach to the study of the long-time behavior of Markov chains.[12]

The main idea of this renormalization procedure can be summarized as follows.

The behavior of the chain X_t involves a sequence of different time scales T_1, T_2, T_3,..., exponentially large in β, related to the stability of the different states. Corresponding to any time scale T_i it is possible to define a renormalized chain $X_t^{(i)}$ by means of a pathwise construction. $X_t^{(i)}$ describes, on its times of order one, the behavior of the original chain X_t on times of order T_i. Indeed, $X_t^{(i)}$ is a coarse-grained version of the chain X_t in the sense that it gives a less detailed description of the process, but the loss of information concerns only events which occur in a typical time less than or equal to T_i.

The state spaces $S^{(i)}$, $i = 1, 2,...$, of the renormalized chains $X_t^{(i)}$, $i = 1, 2,...$, are smaller and smaller and they contain states that are more and more stable. The sequence of chains $X_t^{(i)}$ is constructed iteratively, and the transition probabilities $P^{(i)}(x, y)$ still satisfy Property $\mathscr{P}$ with suitable functions $\Delta^{(i)}(x, y)$. At each step of the iteration the equivalence classes of stable states of the chain $X_t^{(i)}$ constitute the states of the new chain $X_t^{(i+1)}$.

This sequence of renormalized chains has been used in refs. 12–14; it constitutes a possible alternative approach (w.r.t. the one due to Freidlin and Wentzell) to get control of quantities like (2.1), (2.2), and the invariant measure.

Here we propose a new application of this renormalization procedure: we use the renormalized chains $X_t^{(i)}$ to control the large-deviation phenomena for the Markov chain X_t taking place during exponentially long times T_i.

This renormalization procedure is then the new ingredient necessary for the construction of the exiting tube from a general domain Q containing several stable states.

A complete development of this idea will be given in ref. 10. Here we only give an outline of the basic strategy and some simple preliminary results.

In order to simpify the description of the first exit from the domain Q of a Markov chain X_t we can consider a new auxiliary chain X_t^Q on the state space $Q \cup \partial Q$ which is equivalent to X_t up to its first exit from Q, but with almost absorbing states in ∂Q. More precisely, we define the following transition probabilities:

$$P^Q(x, y) = P(x, y) \qquad \text{for any} \quad x \in Q \tag{2.11}$$

$$P^Q(x, y) = e^{-\beta \Delta(\partial Q)} P(x, y) \qquad \text{for} \quad x \in \partial Q, \quad y \neq x \tag{2.12}$$

where $\Delta(\partial Q) > \sum_{y,z \in Q} \Delta(y, z)$.

It is to this chain that we apply the renormalization procedure by introducing the sequence of renormalized chains $X_t^{(1)},..., X_t^{(i)},...$ and the corresponding sequence of state spaces $S^{(1)},..., S^{(i)},...$. We warn the reader of an abuse of notation: we will omit, for the rest of this section, the superscript Q.

Since $\Delta(\partial Q) > \sum_{y,z \in Q} \Delta(y, z)$, it is immediate to show that there exists a step N of the iteration such that in Q there are only unstable states. More precisely, let $N = N(Q) = \inf\{n;\, S^{(n+1)} \subset \partial Q\}$; then $X^{(N)}$ has stable states only on the boundary of Q and all the states in ∂Q are stable. Thus the description of the exit from Q for the chain $X_t^{(N)}$ is an easy task, since it is a downhill exiting. This means that for each $x \in S^{(N)} \cap Q$ there exists at least a time k and a sequence $x_0^{(N)},..., x_k^{(N)}$ of states in $S^{(N)}$ such that $x_0^{(N)} = x$, $x_i^{(N)} \in Q$ $\forall i < k$, $x_k^{(N)} \in \partial Q$, and $\Delta^{(N)}(x_i^{(N)}, x_{i+1}^{(N)}) = 0$ for each $i < k$. The sequence $x_0^{(N)},..., x_k^{(N)}$ is not necessarily unique and it represents a typical exit path from Q for the chain $X^{(N)}$.

Let us first suppose that this exiting path is unique. We can then give a first approximation of the tube of trajectories that the stochastic process follows with probability almost one when exiting from the domain Q starting from $x \in S^{(N)} \cap Q$. Indeed, let

$$\Phi(S) = \{\{\phi_i\}_{i \in \mathbf{N}}, \phi \in S\} \tag{2.13}$$

be the space of all the trajectories of the Markov chain X_t.

Since the renormalized chains are constructed path by path, to each path $\phi \in \Phi(S)$ we can associate a renormalized path $\phi^{(1)} \in \Phi(S^{(1)})$.

In this way we can define, for every $\phi \in \Phi(S)$, a sequence of trajectories $\{\phi_i^{(n)}\}_{i \in \mathbf{N}}$ in the spaces $\Phi(S^{(n)})$ with $n = 2, 3, \ldots$.

Conversely, for any given sequence of states in $S^{(n)}: x_1^{(n)}, x_2^{(n)}, \ldots, x_k^{(n)}$, we can define a tube of trajectories in $\Phi(S)$ as

$$\Theta(n, \{x_1^{(n)}, x_2^{(n)}, \ldots, x_k^{(n)}\}) = \{\phi \in \Phi(S); \phi_i^{(n)} = x_i^{(n)} \quad \forall i \leqslant k\} \tag{2.14}$$

In the case of uniqueness of the exiting path for the chain $X_t^{(N)}$ we can conclude that

$$P_x(X_t) \in \Theta(N, \{x_0^{(N)}, \ldots, x_k^{(N)}\}) \tag{2.15}$$

tends to one as $\beta \to \infty$.

Indeed

$$\{X_t \in \Theta(N, \{x_0^{(N)}, \ldots, x_k^{(N)}\})\} = \{X_i^{(N)} = x_i^{(N)}, \forall i = 0, \ldots, k\} \tag{2.16}$$

and the probability of the second event tends to one as $\beta \to \infty$ if $\{x_0^{(N)}, \ldots, x_k^{(N)}\}$ is the unique deterministic path exiting from $Q \cap S^{(N)}$ for the chain $X_t^{(N)}$.

In the case in which there are several exiting paths for the process $X_t^{(N)}$ we have to consider the union of these tubes.

We can easily find, using the above construction, the results on the mean exit time and on the best exit point from Q previously obtained by Freidlin and Wentzell, without using the graph techniques. Indeed, by the results proved in ref. 12 it is sufficient to evaluate the quantities $E\sigma_Q$ and $P(X_{\sigma_Q} = y)$ for the renormalized chain $X_t^{(N)}$.

In view of the determination of the minimal tube of trajectories that the stochastic process follows with high probability, we have to define a tube of exiting trajectories smaller than $\Theta(N, \{x_0^{(N)}, \ldots, x_k^{(N)}\})$. To this end we will need a complete description of the behavior of the original chain X_t in the interval of time corresponding to the transition $x_i^{(N)} \to x_{i+1}^{(N)}$ of the renormalized chain $X_t^{(N)}$.

As we will see in the second paper of this series, we can complete this program by introducing particular sets of states in S called *cycles*; to each renormalized state $x_i^{(n)}$ in $S^{(n)}$ one can associated a suitable cycle C_i in S.

These cycles C_i represent the subset of S containing the stable state in S associated to the renormalized state $x_i^{(n)}$ where the process X_t typically spends its time before the renormalized process $X_t^{(n)}$ performs a single jump.

In the rest of this paper we will consider the exit problem for reversible chains. We will not follow the strategy proposed in this section, but instead we will use the energy function H in order to give an explicit construction of the exiting tube.

In the reversible case the whole analysis becomes simpler and more intuitive.

The definition of cycles, the derivation of their properties, the determination of best exit point from a domain Q, and the other interesting properties and propositions do not require the introduction of the Freidlin–Wentzell graphical method. A straightforward analysis of the energy landscape will suffice to get the desired results.

Moreover, using reversibility, one can see a typical tube of trajectories during the first exit from a domain Q as the time reverse of a typical tube of descent from the boundary ∂Q of Q to the "bottom" of Q.

3. THE CYCLES AND THEIR PROPERTIES

We start our analysis of the reversible case. We consider an ergodic aperiodic Markov chain with a finite space state S and with transition probabilities $P(x, y)$ satisfying the following assumption:

Hypothesis M. There exists a function $H: S \to \mathbf{R}^+$ such that

$$P(x, y) = q(x, y) \exp(-\beta[H(y) - H(x)]_+) \tag{3.1}$$

where $q(x, y) = q(y, x)$ and $(a)_+$ is the positive part $(:= a \vee 0)$ of the real number a.

The above choice corresponds to a *Metropolis Markov chain* which is *reversible* in the sense that

$$\forall x, x' \in S : \mu(x)\, P(x, x') = \mu(x')\, P(x', x) \tag{3.2}$$

with

$$\mu(x) \propto \exp[-\beta H(x)] \tag{3.3}$$

Since the symmetric matrix q is independent of β we immediately get, from (3.2), that Property $\mathscr{P}$ is satisified.

We will use the above hypothesis (Metropolis form for P) in order to simplify the exposition. More general reversible Markov chains can be considered. Moreover, many propositions stated in the present paper can be extended even to the case of almost reversible Markov chains.[14]

From (3.3) one immediately deduces that μ is the unique invariant measure of the chain.

A *path* ω is a sequence $\omega := x_1, ..., x_N$, $N \in \mathbb{N}$, with x_j, x_{j+1}, $j = 1, ..., N-1$, communicating states [i.e., $P(x_j, x_{j+1}) > 0$]. We often write $\omega: x \to y$ to denote a path joining x to y.

We say that a state x is *downhill connected* to a state y if there exists a path $\omega = (x_0 = x, x_1, ..., x_k = y)$ with $H(x_{i+1}) \leqslant H(x_i)$, $i = 0, ..., k-1$.

A set $Q \subset S$ is *connected* if $\forall x, x' \in Q$ there exists a path $\omega: x \to x'$ all contained in Q.

Given $Q \subset S$, we denote by $U = U(Q)$ the set of all the minima of the energy on the boundary ∂Q of Q:

$$U(Q) = \{z \in \partial Q : \min_{x \in \partial Q} H(x) = H(z)\} \tag{3.4}$$

Given $Q \subset S$, we denote by $F = F(Q)$ the set of all the minima of the energy on Q:

$$F(Q) = \{y \in Q : \min_{x \in Q} H(x) = H(y)\} \tag{3.5}$$

A connected set of equal-energy states is called a *plateau*. It is easy to convince oneself that, in the framework of our asymptotic estimates which are exponential in the parameter β, we can identify these plateaux with single points. In other words, states which are equivalent with respect to the relation (2.5) of the previous section can be identified.

It is immediate to verify that in the reversible case a state x is stable, in the sense of definition (2.6), if either it is a local minimum of the function H or it belongs to a plateau equivalent to a local minimum.

For every $z \in S$ we denote by $\bar{P}(z)$ the plateau containing z.

Given a set Q on which H is constant, $H(x) = \bar{H}$, $\forall x \in Q$, we define, by abuse of notation, $H(Q) = \bar{H}$

Definition 3.1. A connected set A which satisfies

$$\max_{x \in A} H(x) = \bar{H} < \min_{z \in \partial A} H(z) = H(U(A))$$

is called a cycle.

It is easy to see that, under the reversibility hypothesis for our Markov chain, the above definition is strictly related to the one given by Freidlin and Wentzell (see ref. 4, p. 198).

In the following we will give some propositions (besides other definitions). Most of them are intended to clarify the structural properties of the cycles. For some of them the proof is immediate and we omit it. The most important statement is contained in Proposition 3.7, for which we provide a proof.

Proposition 3.1. Given a state $\bar{x} \in S$ and a real number c, the set of all x's connected to $\bar{x}$ by paths with energy always below c either coincides with S or it is a cycle A with

$$H(U(A)) \geqslant c$$

Proposition 3.2. Given two cycles A_1, A_2, either (1) $A_1 \cap A_2 = \emptyset$ or (2) $A_1 \subset A_2$ or, vice versa, $A_2 \subset A_1$.

Proof. Let $A_1 \cap A_2 \neq \emptyset$. It is immediate to see that one cannot have that, at the same time,

$$\exists x_1 \in \partial A_1 \cap A_2, \qquad \exists x_2 \in \partial A_2 \cap A_1$$

Otherwise one would have, at the same time,

$$H(x_1) < H(x_2)$$

and

$$H(x_2) < H(x_1)$$

Thus, either $A_1 \subset A_2$ or $A_2 \subset A_1$.

Definition 3.2. A cycle A such that $\forall z \in U(A)$ the set of all x's communicating with z for which

$$H(x) < H(z)$$

belong to A is called a stable or attractive cycle.

Definition 3.3. A cycle A for which there exists $y^* \in U(A)$ downhill connected to some point x in A^c is called transient; given a transient cycle A, the points y^* downhill connected to A^c are called minimal saddles. The set of all the minimal saddles of a transient cycle A is denoted by $\mathscr{S}(A)$.

A definition similar to $\mathscr{S}(A)$ can be given also for a general set which is not necessarily a cycle.

Definition 3.4. A transient cycle A such that $\exists \bar{x} \notin A$ with $H(\bar{x}) < H(F(A))$ there exists $y^* \in \mathscr{S}(A)$ and a path $\omega: y^* \to \bar{x}$ below y^* [namely $\forall x \in \omega : H(x) < H(y^*)$] is called metastable.

Definition 3.5. For each pair of states $x, y \in S$ we define their minimal saddle $\mathscr{S}(x, y)$ as the set of states corresponding to the solution of the following minimax problem:

Let, for any path ω

$$\hat{H}(\omega) = \max_{z \in \omega} H(z)$$

and

$$\bar{H}_{x,y} := \min_{\omega: x \to y} \hat{H}(\omega)$$

Find

$$\mathscr{S}(x, y) = \{z : H(z) = \bar{H}_{x,y}; \exists \omega: x \to y, \omega \ni z : \hat{H}(\omega) = \bar{H}_{x,y}\} \tag{3.6}$$

From our assumptions on the chain it immediately follows that $\mathscr{S}(x, y) = \mathscr{S}(y, x)$ $\forall x, y \in S$.

We write $\forall x \in S$, $Q \subset S$, $x \notin Q$

$$\mathscr{S}(x, Q) = \{z \in \mathscr{S}(x, w) \text{ for some } w \in Q : \min_{w \in Q} H(\mathscr{S}(x, w)) = H(z)\} \tag{3.7}$$

A saddle $\mathscr{S}(x, y)$ such that $\mathscr{S}(x, y) \ni x$ or $\mathscr{S}(x, y) \ni y$ is called *trivial.* We notice that saddles between stable states, not equivalent with respect to the relation $\sim$ introduced in (2.5), are not trivial. The saddles between non-equivalent stable states ($\in M$) will be called *natural saddles.*

Notice that the previously defined set $\mathscr{S}(A)$ only contains natural saddles.

Given a set Q, we denote by $C(Q)$ the (possibly empty) set of its internal natural saddles; namely

$$C(Q) = \{y \in Q : \exists x, x' \in M, x \nsim x' : y \in \mathscr{S}(x, x')\} \tag{3.8}$$

Proposition 3.3. If A is a cycle, then:

(i) For each x, y, $z \in A$ and $w \notin A$

$$H(\mathscr{S}(x, y)) < H(\mathscr{S}(z, w))$$

(ii) For any $x \in A$ the set $\mathscr{S}(x, A^c)$ does not depend on x and coincides with $U(A)$.

Proof. By definition of cycle, for any x, $y \in A$ there exists a path ω: $x \to y$ contained in A such that for any $x_i \in \omega$ one has $H(x_i) < H(U(A))$. On the other hand, any path going from $z \in A$ to $w \in \partial A$ maximizes H in ∂A.

Thus we have

$$\min_{w \in \partial A} H(\mathscr{S}(x, w)) = H(U(A))$$

Definition 3.6. Given a stable state $x \in M$, i.e., a local minimum for the energy, we define the following basins for x:

(i) the wide basin of attraction of x:

$$\hat{B}(x) = \{z : \exists \text{ downhill path } \omega: z \to x\} \tag{3.9}$$

(ii) The basin of attraction of x given by

$$\bar{B}(x) = \{z : \text{every downhill path starting from } z \text{ ends in } x\} \tag{3.10}$$

(iii) The strict basin or attraction of x, $B(x)$, given by

$$B(x) = \bar{B}(x) = S$$

if the whole state space S coincides with $\bar{B}(x)$. Otherwise

$$B(x) = \{z \in \bar{B}(x) : H(z) < H(U(\bar{B}(x)))\} \tag{3.11}$$

Remarks. (1) $\hat{B}(x)$ is necessarily nonempty, whereas $\bar{B}(x)$ could be empty. $\bar{B}(x)$ can be seen as the usual basin of attraction of x with respect to the $\beta = \infty$ dynamics.

(2) Every local minimum for the energy is (a trivial) cycle.

(3) The above definitions of different basins of attraction can immediately be extended to the case in which, in place of a local minimum x, there is a generic cycle A. In this way one gets $\hat{B}(A)$, $\bar{B}(A)$, $B(A)$. Of course one can even consider the basins of attraction of more general sets (not necessarily cycles).

(4) The case of a Markov chain for which the state space S reduces itself to the basin of attraction of the absolute minimum $\bar{x}$ for the energy H is, in a sense, almost trivial; we shall refer to this case as to the *one-well* case.

Proposition 3.4. Suppose that S is not one-well. Let G be a subset of S and suppose that there exist $x \in G$, $x' \notin G$ with the following properties:

(i) G is connected

(ii) There exists a path ω contained in G, $\omega: x \to y^*$ for some $y^* \in U(G)$, with

$$H(z) < H(y^*) \qquad \forall z \in \omega, \quad z \neq y$$

(iii) There exists a path ω outside G, $\omega: y^* \to x'$ with

$$H(z) < H(y^*) \qquad \forall z \in \omega, \quad z \neq y$$

[obviously one has to have $H(x') < H(y^*)$].

Then if $A = \{z : \exists \omega: z \to x;\ \forall y \in \omega,\ H(y) < H(y^*)\} \equiv$ maximal connected set containing x with energy less than $H(y^*)$:

(1) $A \subset G$.

(2) A is a cycle with $U(A) \ni y^*$.

(3) y^* is a minimax between x and x', namely $y^* \in \mathscr{S}(x, x')$.

The above proposition provides a constructive criterion to find the minimax between different points.

The notion of local minimum and of its basins of attraction will be useful to provide a decomposition of the cycles. More precisely, give a cycle A containing several local minima, we will consider some smaller cycles A_i contained in A, by looking at the sequence of internal saddles between minima in A. Let us start with a trivial corollary of Proposition 3.2:

Proposition 3.5. If a cycle A contains an internal natural saddle y, namely a nontrivial minimax between two stable states $z, z' \in A \cap M$ with energy $H(y) < H(U(A))$, then it contains all the cycles A_j such that $y \in U(A_j)$.

Proposition 3.6. Let A be a cycle and suppose that it is not a subset (proper or not) of a strict basin of attraction of some local minimum x [i.e., $C(A)$ is nonempty]. Let $y_1,..., y_m$ be the set of its internal natural saddles with maximal energy; namely, if

$$\max_{z \in C(A)} H(z) = H_0 \tag{3.12}$$

then

$$y_1,..., y_m = \{y \in C(A) : H(y) = H_0\}$$

The number m of internal saddles with maximal energy of a cycle A is denoted by $N(A)$. Then the following is true:

(i) The cycle A can be decomposed as

$$A = A_1 \cup \cdots \cup A_k \cup V \tag{3.13}$$

where $A_1,..., A_k$ are transient cycles with $H(U(A_i)) = H_0$, $i = 1,..., k$, and $\forall x_i \in A_i, x_j \in A_j : \mathscr{S}(x_i, x_j) \subset \{y_1,..., y_m\}$.

(ii) At least one of the A_j must contain points in $F(A)$, i.e., $F(A) \cap \{\bigcup_j A_j\} \neq \varnothing$.

(iii) We have

$$V = \{y_1\} \cup \cdots \cup \{y_m\} \cup \tilde{V} \tag{3.14}$$

where $\tilde{V}$, if it is nonempty, is made by points with energy greater than or equal to H_0 and it is completely attracted by the union

$$\tilde{A} = A_1 \cup \cdots \cup A_k \tag{3.15}$$

namely

$$\tilde{V} \cap M = \varnothing, \qquad \tilde{V} \subset \bar{B}(\tilde{A})$$

(iv) For all y_k there exists $\omega: y_k \to F(A)$:

$$H(x) \leqslant H_0 \qquad \forall x \in \omega$$

Remarks. (1) If we consider a cycle A being a subset of the basin of attraction $\bar{B}(x)$, for some x, then we have $N(A) = 0$, $\tilde{A} = x$, and $V \equiv \tilde{V} = A \setminus \{x\}$.

(2) The simplest nontrivial example is the one in which $k = 2$ and the number of internal saddles of maximal energy is one:

$$A = A_1 \cup A_2 \cup V$$
$$V = \tilde{V} \cup \{y_1\}$$

and

$$|F(A)| = 1: \qquad F(A) \equiv \{x\}$$

Proof. Since A is a cycle, then $H(U(A)) > H_0$. By Propositions 3.1 and 3.5 the maximal connected components $A_1,..., A_k \subset A$ of states in A with energy strictly less than H_0 are cycles contained in A with $H(U(A_i)) = H_0$.

Given A_i, A_j, $\forall x_i \in A_i$, $x_j \in A_j$, by Proposition 3.3, $\mathscr{S}(x_i, x_j)$ takes the same value for every $x_i \in A_i$ and $x_j \in A_j$; moreover, $\forall x_i \in A_i$, $x_j \in A_j$: $\mathscr{S}(x_i, x_j) =: \mathscr{S}(F(A_i), F(A_j)) \subset \{y_1,..., y_m\}$.

From this, points (i)–(iii) immediately follow.

Point (iv) easily follows from the fact that

$$\forall x \in A \cap M, \qquad H(\mathcal{S}(x, F(A))) \leqslant H_0$$

since $\{y_1, ..., y_m\}$ are the internal natural saddles with maximal energy.

We recall now a simple but useful result based on reversibility providing a lower bound in probability to the first hitting time to a particular state.

Lemma 3.1. For every $\varepsilon > 0$ and any pair of states y, x such that $H(y) > H(x)$, one has

$$\lim_{\beta \to \infty} P_x(\tau_y < \exp\{\beta(H(y) - H(x) - \varepsilon)\}) = 0$$

Proof. The straightforward proof can be found in ref. 5 (cf. Lemma 1 therein).

The results contained in the following Proposition 3.7 are less immediate than the previous ones. As a matter of fact, they are already known even in a more general situation (see ref. 4 for a proof based on the FW graphical technique). We provide here, in the reversible case, a new, purely probabilistic proof which, in our opinion, is much more transparent. It is based on a simple intuitive argument involving the construction of suitable events taking place on suitable, exponentially large in β intervals of time. We see here (and we will see more explicitly in the next section) the appearance of what we have called the *resistance times* and why they play an important role in providing an efficient mechanism of escape.

Proposition 3.7. Suppose Hypothesis M is satisfied. Given a cycle A:

(i) For all $\varepsilon > 0$ there exist $\beta_0 > 0$ and $k > 0$ such that for any $\beta > \beta_0$ and $\forall x \in A$

$$P_x(\tau_{\partial A} < \exp(\{\beta[H(U(A)) - H(F(A)) + \varepsilon]\}) \geqslant 1 - e^{-k\beta}$$

(ii) There exist $\delta > 0$, $\beta_0 > 0$, and $k' > 0$ such that for all $\beta > \beta_0$ and $\forall x, x' \in A$

$$P_x(\tau_{x'} < \tau_{\partial A}; \tau_{x'} < \exp\{\beta[H(U(A)) - H(F(A)) - \delta]\}) \geqslant 1 - e^{-k'\beta}$$

(iii) $\forall x \in A$, $\forall \varepsilon > 0$, $\hat{y} \in \partial A$, and β sufficiently large

$$P_x(X_{\tau_{\partial A}} = \hat{y}) \geqslant \exp\{-\beta[H(\hat{y}) - H(U(A)) + \varepsilon]\}$$

Proof. The proof uses induction on the total number of the internal natural saddles $|C(A)|$. We first assume that properties (i)–(iii) are verified for all the cycles A with $|C(A)| \leqslant n$, for a given integer $n \geqslant 0$, and we prove them for all the cycles A with $|C(A)| = n+1$; then we verify (i)–(iii) for the case $n=0$, the basis of the induction. This case corresponds to A being the strict basin of attraction of a "plateau" $F(A)$ of communicating points having the same energy [in particular, $F(A)$ could be a single local minimum x].

Consider a generic cycle A with $|C(A)| = n+1$ and with a number of internal *maximal* saddles $N(A) = m$. We can use the decomposition given by Proposition 3.6, namely

$$A = \{y_1, ..., y_m\} \cup \tilde{V} \cup \tilde{A}$$

where $\tilde{A}$, defined in (3.15), is a union of cycles A_j which, beyond satisfying the properties specified in Proposition 3.6, have, $\forall j = 1, ..., m$, a number of internal saddles $|C(A_j)|$ less than or equal to n, and then satisfy the recursive hypotheses (i)–(iii).

Let us start by proving (i) for our cycle A. Given any sufficiently small $\varepsilon > 0$, let

$$T_1 = T_1(\varepsilon) := \exp\{\beta[H(y_j) - H(F(A)) + \varepsilon/2]\} \tag{3.16}$$

and

$$T_2 = T_2(\varepsilon) := \exp\{\beta[H[U(A)) - H(F(A)) + \varepsilon]\} \tag{3.17}$$

Then the argument goes as follows: we will construct, for every state $x \in A$, an event $\mathscr{E}_{x,T_1}$ containing trajectories starting from x at time $t=0$, taking place in the interval of time $[0, T_1]$, and satisfying the following conditions:

1. If $\mathscr{E}_{x,T_1}$ takes place, our Markov chain X_t hits ∂A before T_1.
2. We have

$$\inf_{x \in A} P(\mathscr{E}_{x,T_1}) \geqslant \alpha_{T_1} > 0 \qquad \text{with} \qquad \lim_{\beta \to \infty} (1 - \alpha_{T_1})^{T_2/T_1} = 0 \tag{3.18}$$

In particular, we will take

$$\alpha_{T_1} = \exp\{-\beta[H(U(A)) - H(y_j) + \varepsilon/4]\} \tag{3.19}$$

Let us now divide the interval $[0, T_2]$ into $q = [T_2/T_1]$ (here [ ] means integer part) intervals of length T_1; by properties 1 and 2 above of $\mathscr{E}_{x,T_1}$, we easily get the proof of Proposition 3.7. For, if $\tau_{\partial A} > T_2$, necessarily, by property 1, in none of the q intervals of length T_1 can the (translation of) event $\mathscr{E}_{x,T_1}$ have taken place; by property 2 and the strong Markov property, part (i) of our proposition directly follows. Then we are reduced to the construction of such an event $\mathscr{E}_{x,T_1}$.

Let us first give a rapid description, in words, of $\mathscr{E}_{x,T_1}$.

Let y^* be a state in $U(A)$; by definition there exists a downhill path from y^* to the set $\tilde{A}$:

$$\bar{x}_0 = y^*, \qquad \bar{x}_1, \bar{x}_2,..., \bar{x}_k \in \tilde{A}; \qquad \bar{x}_1,..., \bar{x}_{k-1} \in V$$

[with $H(\bar{x}_{i+1}) \leqslant H(\bar{x}_i)$]. We set $k=1$ if y^* is communicating with $\tilde{A}$. Let A_{j^*} be the particular component of $\tilde{A}$ hit by this path (i.e., $\bar{x}_k \in A_{j^*}$). The event $\mathscr{E}_{x,T_1}$ is then defined by requiring that the process hits the set A_{j^*} in a time much shorter than T_1, and then, after reaching the boundary ∂A_{j^*} of A_{j^*}, follows the path obtained by $\bar{x}_0,..., \bar{x}_k$ by time reversal.

More precisely, let $\varepsilon' < \varepsilon/2$ and let

$$\tau_{\partial A_{j^*}}^{(>\tau_{A_{j^*}})} := \min\{t > \tau_{A_{j^*}};\, X_t \notin A_{j^*}\}$$

where, as before, $\tau_{A_{j^*}}$ is the first hitting time to the set A_{j^*}. Then

$$\mathscr{E}_{x,T_1} := \{\tau_{A_{j^*}} < T_1 e^{-\varepsilon'\beta}\} \cap \{\tau_{\partial A_{j^*}}^{(>\tau_{A_{j^*}})} < T_1 e^{-\varepsilon'\beta}\} \cap \{X_{\tau_{\partial A_{j^*}}^{(>\tau_{A_{j^*}})}} = \bar{x}_{k-1}\}$$
$$\cap \left\{\bigcap X_{\tau_{\partial A_{j^*}}^{(>\tau_{A_{j^*}})}+s} = \bar{x}_{k-1-s},\ \forall s = 1,..., k-1\right\}$$

By using the strong Markov property we have

$$\begin{aligned} P(\mathscr{E}_{x,T_1}) = \sum_{y \in A_{j^*}} & P_x(\tau_{A_{j^*}} < T_1 e^{-\varepsilon'\beta};\, X_{\tau_{A_{j^*}}} = y) \\ & \cdot P_y(\{\tau_{\partial A_{j^*}} < T_1 e^{-\varepsilon'\beta}\} \cap \{X_{\tau_{\partial A_{j^*}}} = \bar{x}_{k-1}\}) \\ & \cdot P(\bar{x}_{k-1}, \bar{x}_{k-2}) \cdot P(\bar{x}_{k-2}, \bar{x}_{k-3}) \cdots P(\bar{x}_1, y^*) \end{aligned} \tag{3.20}$$

We start by estimating the first term in the r.h.s. of (3.20). For any path ω going from x to A_{j^*}, we define the following times, depending on ω:

$$s_0 = 0$$
$$t_k = \min\{t \geqslant s_{k-1};\, \omega_t \in \tilde{A}\}$$
$$s_k = \min\{t > t_k;\, \omega_t \notin A_{j_k}\}$$

where $j_k = j_k(\omega)$ is such that $\omega_{t_k} \in A_{j_k}$ and $k = 1,..., l(\omega)$, so that $j_{l(\omega)} = j^*$. Let

$$\bar{A} := \tilde{A} \cup \{x \in A : H(x) = H(y_i)\}$$

From Proposition 3.6 it is easy to see that there exists a set of paths $\bar{\Omega}$ going from x to A_{j^*} with the following characteristics:

Given any $\bar{\omega} \in \bar{\Omega}$, if $\bar{\omega}_1 = x$ with $x \notin \bar{A}$, $\bar{\omega}$ first enters $\bar{A}$, following a downhill sequence, and then it no longer leaves $\bar{A}$. In A, $\bar{\omega}$ follows a well-specified sequence of cycles $A_1,..., A_{j^*}$ and saddles $y_1,..., y_l$, spending a certain time in each A_j (typically of order of $\exp\{\beta[H(y_j) - H(F(A_j))]\}$), exiting from A_j through the saddles $y_j \in \partial A_j$. Moreover, the path $\bar{\omega}$ does not visit more than once the same saddle y_j and it is downhill for each $t \in (s_k, t_{k+1})$ for each $k = 1,..., l(\bar{\omega})$, $l(\bar{\omega}) \leqslant m$, and $H(\bar{\omega}_{s_k}) = H(\mathscr{S}(A_{j_k})) = H(y_i)$. The existence of such an $\bar{\Omega}$ suggests the way to estimate the first factor in the r.h.s. of (3.20). In order to simplify the notation we set

$$A_{j_1(\bar{\omega})},..., A_{j_{l(\bar{\omega})}} =: A_1,..., A_l$$

$$s_1(\bar{\omega}),..., s_{l(\bar{\omega})}(\bar{\omega}) =: s_1,..., s_l$$

We have

$$\begin{aligned} &P_x(\tau_{A_l} < T_1 e^{-\varepsilon'\beta}) \\ &\quad \geqslant P_x(X_t = \bar{\omega}_t, \forall t \leqslant t_1) \min_{x \in A_1} P_x\left(\left\{\tau_{\partial A_1} < \frac{T_1}{l(\bar{\omega})} e^{-\varepsilon'\beta}\right\} \cap \{X_{\tau_{\partial A_1}} = \bar{\omega}_{s_1}\}\right) \\ &\quad\quad \cdots \min_{x \in A_{l-1}} P_x\left(\left\{\tau_{\partial A_{l-1}} < \frac{T_1}{l(\bar{\omega})} e^{-\varepsilon'\beta}\right\} \cap \{X_{\tau_{\partial A_{l-1}}} = \bar{\omega}_{s_{l-1}}\}\right) \\ &\quad\quad \cdot P_{\bar{\omega}_{s_{l-1}}}(X_t = \bar{\omega}_{t+s_{l-1}}, \forall t \in (0, t_l - s_{l-1})) \end{aligned}$$

Now, since $\bar{\omega}$ is downhill for any $t \in (s_{k-1}, t_k)$, $\forall k = 1,..., l$, by using the obvious inequality

$$P_{\bar{\omega}_{s_n}}(X_t = \bar{\omega}_{t+s_n}, \forall t \in (0, t_{n+1} - s_n)) \geqslant e^{-\alpha'\beta}$$

for some $\alpha' \to 0$ as $\beta \to \infty$ and by using the iterative hypotheses, which imply

$$\max_{j=1,...,l} P\left(\left\{\tau_{\partial A_j} < \frac{T_1}{l(\bar{\omega})} e^{-\varepsilon'\beta}\right\} \cap \{X_{\tau_{\partial A_j}} = \bar{\omega}_{s_j}\}\right) > e^{-\alpha''\beta}$$

with $\alpha'' \to 0$ as $\beta \to \infty$, we have

$$P_x(\tau_{A_l} < T_1 e^{-\varepsilon'\beta}) \geqslant e^{-\alpha\beta}$$

with $\alpha \to 0$ as $\beta \to \infty$.

Notice that we have used $\bar{\omega}$ only to deduce from it a sequence $A_1,..., A_l$ of cycles and a sequence of downhill paths emerging from saddles.

Moreover, in the above argument it is essential to give the process the freedom to spend in each cycle A_j a suitable random time.

Again by the iterative hypotheses the second term in r.h.s. of (3.20), for $\varepsilon' < \varepsilon/2$ and β large, is estimated by

$$\begin{aligned} P_y(\{\tau_{\partial A_{j^*}} < T_1 \exp(-\varepsilon'\beta)\} \cap \{X_{\tau_{\partial A_{j^*}}} = \bar{x}_{k-1}\}) \\ \geqslant \exp(-\varepsilon\beta) \exp\{-\beta[H(\bar{X}_{k-1}) - H(U(A_{j^*}))]\} \end{aligned}$$

and in conclusion we obtain the following estimate:

$$\begin{aligned} P(\mathscr{E}_{x,T_1}) &\geqslant \exp(-\alpha'''\beta) \exp\{-\beta[H(y^*) - H(U(A_{j^*}))]\} \\ &= \exp(-\alpha'''\beta) \exp\{-\beta[H(U(A)) - H(y_i)]\} \end{aligned}$$

with $\alpha''' \to 0$ as $\beta \to \infty$.

This concludes the proof of property (i) for A.

Let us now go to the proof of (ii). We proceed similarly to what we did to prove (i), using recurrence in $\tilde{A}$ and the strong Markov property. We first prove that, for some positive δ,

$$\lim_{\beta \to \infty} P_x(\tau_{x'} < \exp\{\beta[H(U(A)) - H(F(A)) - \delta]\} = 1 \qquad (3.21)$$

Again for any pair x, $x' \in A$ appearing in (ii) we construct an event $\mathscr{E}'_{x,x',T_1}$ similar to $\mathscr{E}_{x,T_1}$; $\mathscr{E}'_{x,x',T_1}$ contains paths of our process starting from x and ending at x' during a time interval at most T_1. Notice that $T_1(\varepsilon)$, for ε sufficiently small, is of the form $\exp\{\beta[H(U(A)) - H(F(A)) - \delta]\}$ [appearing in (ii)] with, say, $\delta = [H(U(A) - H(y_j)]/2$.

We describe $\mathscr{E}'_{x,x',T_1}$ in words, leaving to the reader the easy task of a precise definition, along the same lines previously used for $\mathscr{E}_{x,T_1}$.

If $\mathscr{E}'_{x,x',T_1}$ takes place, then, starting from x, we first descend in a time much shorter than $T_1(\varepsilon)/3$ to $\tilde{A}$ (if we still were not there) and this happens with a probability almost one for β large; then in a time of order $T_1(\varepsilon)/3$, if ε is chosen sufficiently small: (1) we never get out of the set $\bar{A}$; this happens with probability approaching one for $\beta \to \infty$, as follows from Lemma 3.1, since, to get out of $\bar{A}$, it will typically take a time of order $\exp\{\beta[H(U(A) - H(F(A))]\}$, much larger than $T_1(\varepsilon)$ for ε sufficiently small, because, of course, $H(y_j) < H(U(A))$; (2) we enter the cycle A_j, say A', containing x'. It follows from the recursive hypothesis (ii) valid for A' that, $\forall \varepsilon > 0$ and β large, with probability almost one, before leaving A', and in a time typically much shorter that $T_1(\varepsilon)/3$, we touch x'. This concludes the proof of (3.21).

By using again Lemma 3.1, we get the full condition (ii), since with probability tending to one as $\beta \to \infty$ for every $x \in A$, $\varepsilon > 0$ one has

$$\tau_{\partial A} > \exp\{\beta[H(U(A)) - H(F(A)) - \varepsilon\} \tag{3.22}$$

and choosing ε sufficiently small, we have

$$\exp\{\beta[H(U(A)) - H(F(A)) - \delta]\} < \exp\{\beta[H(U(A)) - H(F(A)) - \varepsilon\}$$

Let us now prove point (iii). Given $y \in F(A)$, we can estimate from below the probability $P_x(X_{\tau_{\partial A}} = \hat{y})$ by imposing that the process visits the state y before the exit time $\tau_{\partial A}$ as follows:

$$\begin{aligned} P_x(X_{\tau_{\partial A}} = \hat{y}) \geqslant & \sum_{z \in A} \sum_{s=0}^{\infty} P_x(X_{s'} \in A, \forall s' \leqslant s, X_s = z)\, P_z(\tau_y < \tau_{\partial A}) \\ & \times \sum_{t=1}^{\infty} \sum_{\bar{x}_1, \dots, \bar{x}_{t-1} \in A \backslash y} P_y(X_1 = \bar{x}_1, \dots, X_{t-1} = \bar{x}_{t-1}, X_t = \hat{y}) \end{aligned} \tag{3.23}$$

By using reversibility and the already proved point (ii), valid now for the whole cycle A, we can estimate the last term in the r.h.s. of (3.23) as follows:

$$\begin{aligned} &\sum_{t=1}^{\infty} \sum_{\bar{x}_1, \dots, \bar{x}_{t-1} \in A \backslash y} P_y(X_1 = \bar{x}_1, \dots, X_{t-1} = \bar{x}_{t-1}, X_t = \hat{y}) \\ &\quad = e^{-\beta[H(\hat{y}) - H(y)]} \sum_{t=1}^{\infty} \sum_{\bar{x}_1, \dots, \bar{x}_{t-1} \in A \backslash y} P_{\hat{y}}(X_1 = \bar{x}_{t-1}, \dots, X_{t-1} = \bar{x}_1, X_t = y) \\ &\quad e^{-\beta[H(\hat{y}) - H(y)]} \left[P(\hat{y}, y) + \sum_{t=2}^{\infty} \sum_{\bar{x}_{t-1} \in A \backslash y} P(\hat{y}, \bar{x}_{t-1}) \right. \\ &\qquad \left. \times \sum_{\bar{x}_1, \dots, \bar{x}_{t-2} \in A \backslash y} P_{\bar{x}_{t-1}}(X_1 = \bar{x}_{t-2}, \dots, X_{t-1} = y) \right] \\ &\quad \geqslant e^{-\beta[H(\hat{y}) - H(y) + \varepsilon']} \min_{z \in A \backslash y} P_z(\tau_y < \tau_{\partial A}) \end{aligned}$$

Putting this estimate in (3.23) and using again point (ii) to estimate from below the quantity $P_z(\tau_y < \tau_{\partial A})$, we obtain, for β large enough,

$$\begin{aligned} P_x(X_{\tau_{\partial A}} = \hat{y}) &\geqslant e^{-\beta[H(\hat{y}) - H(y) + 2\varepsilon']} \sum_{s=0}^{N} P_x(\tau_{\partial A} \geqslant s) \\ &\geqslant e^{-\beta[H(\hat{y}) - H(y) + 2\varepsilon']} N P_x(\tau_{\partial A} \geqslant N) \end{aligned}$$

It follows from the reversibility Lemma 3.1 that there exists ζ going to zero as $\beta \to \infty$ such that if we choose $N = \exp\{\beta[H(U(A)) - H(F(A)) - \zeta]\}$ we have $P_x(\tau_{\partial A} \geqslant N) > 1/2$.

This concludes the proof of (iii).

To conclude the proof of our proposition we have to show that properties (i)–(iii) are true for A such that the number $N(A)$ of internal natural saddles is zero, namely when A is part of (or coincides with) the strict basin of attraction of $F(A)$, $F(A)$ being a plateau in the previously specified sense.

Suppose such an A is given. Property (i) easily follows by the same argument used before: we construct, for any $x \in A$, $\varepsilon > 0$ an event $\mathscr{E}_{x,T}$ with $T = T(\varepsilon) = \exp(\beta\varepsilon/2)$ which consists in descending from x to $F(A)$ in a time at most $T/2$ following a downhill path ω from x to $F(A)$, then in following an uphill path ω' from $F(A)$ up to $U(A)$ in a time shorter that $T/2$. This path ω' is the time reverse of a path going downhill from $U(A)$ to $F(A)$. The paths ω and ω' certainly exist, as A is the strict basin of attraction of $F(A)$.

With T_2 given by (3.17) we easily verify, in the present case, (3.18) and (3.19) with $T_1 := T(\varepsilon)$, since (1) for every $\varepsilon > 0$ the descent to $F(A)$ along a downhill path takes place in a suitable finite time much smaller than $T(\varepsilon)$ with a probability approaching one as $\beta \to \infty$, and (2) the ascent from $F(A)$ to $U(A)$ along an uphill path in a suitable finite time much smaller than $T(\varepsilon)$, $\forall \varepsilon > 0$ and β sufficiently large, takes place with a probability larger than $\exp\{\beta[H(U(A)) - H(F(A)) + \varepsilon/4]\}$. Then property (i) easily follows.

Combining the methods that we used to prove (ii) and (iii) starting from the inductive hypothesis with the idea leading to the construction of the above event $\mathscr{E}_{x,T}$, we easily get, in our present case of $A = \bar{B}(F(A))$, (ii) and (iii) (we leave the details to the reader).

This concludes the proof of Proposition 3.7.

We will analyze now in more detail the first exit from a cycle A. In particular, following the ideas developed in the framework of the so-called "pathwise approach to metastability,"[1] we will prove asymptotic exponentiality of the properly renormalized first exit time from any cycle in the limit $\beta \to \infty$. Then we will deduce the asymptotic behavior of the expectation of this exit time; notice that the methods developed in the previous sections naturally lead only to estimates in probability of the exit times, but, as we will see, we can even get a good control on the tails of the distribution of these random variables and this will be important to get the asymptotics of the averages.

Let A be a given cycle. Given a point $x \in F(A)$, let the time $T_\beta = T_\beta(x)$ be defined by

$$P_x(\tau_{\partial A} > T_\beta(x)) = e^{-1} \tag{3.24}$$

The above definition is interesting since T_β does not depend on $x \in A$, in the sense of logarithmic equivalence; namely we have, $\forall x, y \in A$,

$$\lim_{\beta \to \infty} \frac{1}{\beta} \log \left[\frac{T_\beta(x)}{T_\beta(y)} \right] = 0, \qquad \lim_{\beta \to \infty} \frac{1}{\beta} \log[T_\beta(x)] = H(U(A)) - H(F(A)) \tag{3.25}$$

Moreover, the asymptotic distribution (in the sense of the most probable behavior) of the first exit time from A does not depend on $x \in A$ in the sense of logarithmic equivalence. Namely, $\forall x, y \in A$, $\varepsilon > 0$,

$$\lim_{\beta \to \infty} P_x(T_\beta(y)\, e^{-\varepsilon\beta} < \tau_{\partial A} < T_\beta(y)\, e^{+\varepsilon\beta}) = 1 \tag{3.26}$$

Indeed Proposition 3.7 (i) and Lemma 3.1 give, $\forall \varepsilon > 0$, $\forall x \in A$,

$$\begin{aligned} &\lim_{\beta \to \infty} P_x(\exp(\beta[H(U(A)) - H(F(A)) - \varepsilon]) \\ &\qquad < \tau_{\partial A} < \exp(\beta[H(U(A)) - H(F(A)) + \varepsilon]) = 1 \end{aligned} \tag{3.27}$$

From (3.24) and (3.27) it easily follows that, $\forall \varepsilon > 0$, $\forall x \in A$,

$$\begin{aligned} &\exp\{\beta[H(U(A)) - H(F(A)) - \varepsilon\} \\ &\qquad < T_\beta(x) < \exp\{\beta[H(U(A)) - H(F(A)) + \varepsilon]\} \end{aligned} \tag{3.28}$$

which implies, $\forall x, y \in A$, (3.25) and then (3.26).

Proposition 3.8. Let $T^*_\beta = T_\beta(x^*)$, where x^* is a particular point in A chosen once for all. Then $\forall x \in A$, $\forall s \in \mathbf{R}^+$,

$$\lim_{\beta \to \infty} P_x\left(\frac{\tau_{\partial A}}{T^*_\beta} > s \right) = e^{-s} \tag{3.29}$$

Proof. Given s, $t \in \mathbf{R}^+$, we write

$$\begin{aligned} &P_x(\tau_{\partial A} > (t+s)\, T_\beta(x)) \\ &\quad = \sum_{y \in A} P_x(\tau_{\partial A} > (t+s)\, T_\beta(x);\, X_{T_\beta(x)t} = y) \\ &\quad = \sum_{y \in A} P_x(\tau_{\partial A} > tT_\beta(x);\, X_{T_\beta(x)t} = y)\, P_y(\tau_{\partial A} > sT_\beta(x)) \end{aligned} \tag{3.30}$$

We can write, $\forall T < sT_\beta(x)$,

$$P_y(\tau_{\partial A} > sT_\beta(x)) = P_y(\tau_{\partial A} > sT_\beta(x);\ \tau_x < T) + P_y(\tau_{\partial A} > sT_\beta(x);\ \tau_x \geqslant T) \tag{3.31}$$

We have

$$P_y(\tau_{\partial A} > sT_\beta(x);\ \tau_x < T) = \sum_{t=1}^{T-1} P_x(\tau_{\partial A} > sT_\beta(x) - t)\ P_y(X_r \in A\backslash\{x\}, \forall r \in [1, t], X_t = x) \tag{3.22}$$

From Proposition 3.7(ii) we know that there exists a $\delta > 0$ such that if the time $\bar{T}_1$ is defined as

$$\bar{T}_1 = \exp\{\beta[H(U(A)) - H(F(A)) - \delta]\} \tag{3.33}$$

we have, using (3.32) and taking also into account that for β sufficiently large, $\bar{T}_1 < sT_\beta(x)$,

$$\begin{aligned} P_y(\tau_{\partial A} > sT_\beta(x)) - o(\beta) &\leqslant P_y(\tau_{\partial A} > sT_\beta(x);\ \tau_x < \bar{T}_1) \\ &\leqslant P_x(\tau_{\partial A} > s[T_\beta(x) - \bar{T}_1/s]) \end{aligned} \tag{3.34}$$

where $o(\beta)$ denotes an infinitesimal quantity as $\beta \to \infty$.

Similarly we get from (3.32) and from Proposition 3.7

$$P_x(\tau_{\partial A} > sT_\beta(x))[1 - o(\beta)] \leqslant P_y(\tau_{\partial A} > sT_\beta(x);\ \tau_x < \bar{T}_1) \leqslant P_y(\tau_{\partial A} > sT_\beta(x)) \tag{3.35}$$

From (3.24), (3.30), (3.34), and (3.35), since from (3.33) we know that $\lim_{\beta \to \infty} \bar{T}_1/T_\beta(x) = 0$, we get

$$\lim_{\beta \to \infty} P_x\left(\frac{\tau_{\partial A}}{T_\beta(x)} > s\right) = e^{-s} \tag{3.36}$$

On the other hand, from (3.34) and (3.35) we get that $\forall x, y \in A$, $s \in \mathbf{R}^+$,

$$\lim_{\beta \to \infty} \left[P_x\left(\frac{\tau_{\partial A}}{T_\beta(x)} > s\right) - P_y\left(\frac{\tau_{\partial A}}{T_\beta(x)} > s\right)\right] = 0 \tag{3.37}$$

and this concludes the proof of the proposition.

Proposition 3.9. For every $x \in A$ and $\varepsilon > 0$, if $\mathbf{E}_x$ denotes the average over the trajectories of the process starting, at $t = 0$, from x, we have

$$\begin{aligned} &\exp\{\beta[H(U(A)) - H(F(A)) - \varepsilon]\} \\ &\qquad < \mathbf{E}_x(\tau_{\partial A}) < \exp\{\beta[H(U(A)) - H(F(A)) + \varepsilon]\} \end{aligned} \tag{3.38}$$

Proof. For every integer-valued random variable ξ we have

$$\mathbf{E}(\xi) = \sum_{m=1}^{\infty} \mathbf{P}(\xi \geqslant m) \tag{3.39}$$

Now, following the argument of the proof of Proposition 3.7(i), based on the introduction of the set $\mathscr{E}_{x, T_1}$, using the estimate (3.17) with nT_2 in place of $T_2 = T_2(\varepsilon)$ and the strong Markov property, it is easy to get the following estimate:

$$P_x(\tau_{\partial A} > nT_2) < \exp(-nc) \tag{3.40}$$

valid for every $x \in A$, $\varepsilon > 0$, for a suitable positive constant c independent of β; we recall that

$$T_2 = T_2(\varepsilon) := \exp\{\beta[H(U(A)) - H(F(A)) + \varepsilon]\}$$

Applying formula (3.39), we get

$$\mathbf{E}_x^{(\beta)}(\tau_{\partial A}) = \sum_{m=1}^{\infty} P_x^{(\beta)}(\tau_{\partial A} \geqslant m) \tag{3.41}$$

where we have put in evidence with a superscript the dependence on β of the distribution of our process.

Now the result of Proposition 3.9 follows, via (3.40), from standard arguments (see, for instance, ref. 1).

4. THE EXIT TUBE

This section is devoted to the study of the typical trajectories of the first excursion outside a cycle A.

We first consider the first descent from any point y_0 in A to $F(A)$. Then we will analyze the problem of a typical tube of trajectories during the first excursion outside a cycle A. As already observed by Schonmann[11] for the case of stochastic Ising models, it will turn out, using reversibility, that this tube is simply related, via a time reversal transformation, to the typical tube followed by the process during the first descent to the bottom $F(A)$ of A.

In order to define the tube of typical trajectories of this first descent, the basic objects will be what we call *standard cascades* emerging from y_0. They specify the geometric characteristics of the tube; roughly speaking, these cascades will consist of sequences of minimaxes $y_1,..., y_n$ toward $F(A)$, decreasing in energy, intercalated by sequences of downhill paths $\omega_1,..., \omega_n$ and sets $Q_1,..., Q_n$ which are a sort of generalized cycle.

We will prove that our system, during its first descent to $F(A)$, with high probability will follow one of the possible standard cascades; moreover, we will also give information about the temporal law of the descent by specifying the typical values of the random times spent inside each one of the sets Q_i (see Theorem 1 below).

Given any point y_0 in A and a downhill path ω_1 starting from y_0, we will define a set $Q_1 = Q_1(y_0, \omega_1)$. This set Q_1 is a union of cycles having common minimal saddles of the same height. Q_1 will represent the first set where our process, during its first excursion to $F(A)$, is captured if it follows the path ω_1; after entering into Q_1 it will spend some time inside it before leaving it to enter, after another downhill path ω_2, into another similar set Q_2 and so on until it enters a cycle containing part of $F(A)$.

The Construction of Q_1

Given y_0, let us consider a downhill path ω_1 starting from y_0. We stress once more that this path is not in general unique. This means that the whole construction we are defining must be repeated for each path.

Let x_1 be the first stable state in ω_1 (see Fig. 1 as an example). If such a point x_1 is in $F(A)$, then y_0 belongs to the wide basin of attraction of a connected component $G = G(A, y_0, \omega_1)$ of $F(A)$, i.e., $y_0 \in \hat{B}(G)$.

In this degenerate case we set $Q_1 := G(A, y_0, \omega_1)$ and the *cascade of saddles* $y_0, y_1, \dots, y_n$ reduces to y_0.

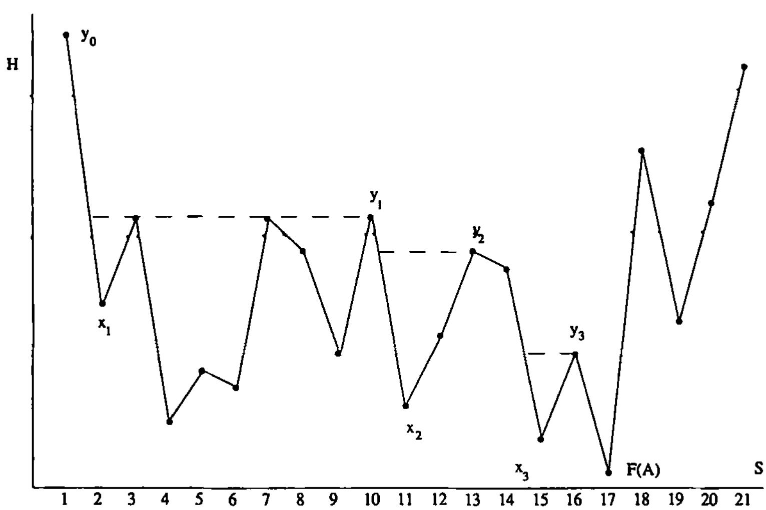

Fig. 1. $P(x, y) = 0$ if $|x - y| > 1$. $A = \{1, 2, \dots, 21\}$, $A^{(1)} = \{2\}$, $A_1^{(2)} = \{4, 5, 6\}$, $A_1^{(3)} = \{8, 9\}$; $N = 3$; $Q_1 = \{2, \dots, 10\}$, $Q_2 = \{11, 12, 13\}$, $Q_3 = \{15, 16\}$.

Let us now suppose that $x_1 \notin F(A)$. Let H_1 be the energy of the saddle (not necessarily unique) between x_1 and $F(A)$:

$$H(\mathscr{S}(x_1, F(A))) = H_1$$

We denote by $A^{(1)}$ the cycle containing x_1 with energy less than H_1. By definition of H_1 we have that $A^{(1)} \cap F(A) = \varnothing$. We define

$$\mathscr{S}^{(1)} := \mathscr{S}(A^{(1)})$$

and

$$\bar{\mathscr{S}}^{(1)} := \bigcup_{z \in \mathscr{S}^{(1)}} \bar{P}(z)$$

Remark. Notice that, by definition (see Definition 3.3) the set $\mathscr{S}(A^{(1)})$ is contained in $\partial A^{(1)}$. Its extension $\bar{\mathscr{S}}^{(1)}$ (containing all the plateaus connected to $\mathscr{S}^{(1)}$) coincides with $\mathscr{S}(x_1, (A^{(1)})^c)$ [see (3.8)].

Let us now consider the cycles $A_1^{(2)},..., A_{k_2}^{(2)}$ with energy less than H_1 not coinciding with $A^{(1)}$ and with which $\bar{\mathscr{S}}^{(1)}$ is downhill communicating and such that $A_j^{(2)} \cap F(A) = \varnothing$, $\forall j = 1,..., k_2$. If there are no such cycles, we define $N = 1$; otherwise we continue, by iteration, the construction as follows.

We call $A^{(2)}$ the union of all the cycles $A_j^{(2)}$ [which do not contain points in $F(A)$],

$$A^{(2)} = \bigcup_j A_j^{(2)}$$

and $\bar{\mathscr{S}}^{(2)}$ the union of all the plateaus containing minimal saddles of the $A_j^{(2)}$ which are not contained in $\bar{\mathscr{S}}^{(1)}$. Now consider, similar to before, the cycles $A_1^{(3)},..., A_{k_3}^{(3)}$ with energy less than H_1, not coinciding with any of the previous $A_j^{(2)}$, with which $\bar{\mathscr{S}}^{(2)}$ is downhill communicating and such that $A_j^{(3)} \cap F(A) = \varnothing$, $\forall j = 1,..., k_3$.

If there are no such cycles, we define $N = 2$; otherwise we iterate the construction.

This procedure stops at a given finite index $N = N(x_1, A)$.

It easy to convince oneself that

$$\forall j = 2,..., N: \qquad A^{(j)} \cap A^{(l)} = \varnothing \qquad \forall l = 1,..., j-1$$

and

$$\forall j = 2,..., N-1: \qquad \mathscr{S}^{(j)} \cap \mathscr{S}^{(l)} = \varnothing \qquad \forall l = 1,..., j-1$$

We set

$$Q_1 = Q_1(y_0, \omega_1) := \left(\bigcup_{j=1}^{N} A^{(j)} \right) \cup \left(\bigcup_{j=1}^{N} \bigcup_{z \in U(A^{(j)})} \bar{P}(z) \right)$$

It is easily seen that Q_1 is the maximal connected set, containing x_1, of points x such that

$$H(\mathscr{S}(x, F(A))) = H_1$$

The boundary of Q_1 is given by

$$\partial Q_1 = \partial^u Q_1 \cup \partial^d Q_1, \qquad \partial^u Q_1 \cap \partial^d Q_1 = \varnothing$$

where $\partial^u Q_1$ is made of points z with energy larger than H_1 and so, trivially, with

$$H(\mathscr{S}(z, F(A))) > H_1$$

whereas $\partial^d Q_1$ is made of points z with energy smaller than H_1, belonging to some cycle containing points of $F(A)$ and then such that

$$H(\mathscr{S}(z, F(A))) < H_1$$

Let us call $\bar{\mathscr{S}}_1$ the subset of $\bar{\mathscr{S}}^{(1)} \cup \cdots \cup \bar{\mathscr{S}}^{(N-1)}$ which is downhill communicating with $\partial^d Q_1$. Choose a point y_1 in $\bar{\mathscr{S}}_1$ and a downhill path ω_2 starting from y_1 not belonging to Q_1. Start again from y_1, ω_2 a hierarchical construction totally analogous to the previous one. Denote by x_2 the first stable state in ω_2 and by H_2 the energy of the saddle between x_2 and $F(A)$. By definition $H_2 < H_1$. As before, we construct new sets Q_2 (depending on the choice of y_1 in $\bar{\mathscr{S}}_1$ and of the path ω_2 starting from y_1).

If we continue in this way and recursively construct a sequence of the form y_2, ω_3, $Q_3\, y_3$,..., we necessarily end up with a y_{M-1}, ω_M for some finite M, with x_M belonging to a connected component G^* (plateau) of $F(A)$.

We set $Q_M := G^*$.

Suppose first that a particular choice is made of y_0, ω_1, y_1, ω_2,..., y_{M-1}, ω_M, compatible with the above construction.

Then, automatically, x_2,..., x_{M-1}, x_M, Q_1,..., Q_{M-1}, Q_M are given.

Let

$$\mathscr{T}(y_0, \omega_1, y_1, \omega_2, \ldots, y_{N-1}, \omega_M) = y_0 \cup \omega_1 \cup Q_1 \cup \omega_2, \ldots, Q_{N-1} \cup \omega_M \cup Q_M \tag{4.1}$$

Any sequence like $\mathscr{T}(y_0, \omega_1, y_1, \omega_2, \ldots, y_{N-1}, \omega_M)$ obtained via the above construction will be called a *standard cascade*; it can be visualized as a sequence of falls and communicating lakes.

Notice that, by construction,

$$H(y_{j-1}) < H(y_j), \qquad \max_{F(Q_j)} H < H(y_{j-1}), \qquad j = 1, \ldots, M$$

and $F(Q_1), \ldots, F(Q_{M-1})$ are strictly higher, in energy, than $F(A)$.

A particularly simple case is when each Q_j is reduced to a single cycle A_j^*.

Now we can state our main result.

Theorem 1. Given a cycle A, for every $y_0 \in A$:

(i) We have

$$\exists \delta > 0 \qquad \text{such that} \quad \lim_{\beta \to \infty} P_{y_0}(\tau_{F(A)} < \exp\{\beta[H(y_1) - H(F(A)) - \delta]\} = 1$$

(ii) We have

$$\lim_{\beta \to \infty} P_{y_0}(\forall t \leqslant \tau_{F(A)} : x_t \in \mathscr{T}(y_0, \omega_1, y_1, \omega_2, \ldots, y_{M-1}, \omega_M)$$

$$\text{for some} \quad y_0, \omega_1, y_1, \omega_2, \ldots, y_{M-1}, \omega_M) = 1$$

(iii) Moreover, with probability $\to 1$ as $\beta \to \infty$, there exists a sequence $y_0, \omega_1, y_1, \omega_2, \ldots, y_{M-1}, \omega_M$ such that our process starting at $t = 0$ from y_0, between $t = 0$ and $t = \tau_{F(A)}$, after having followed the initial downhill path ω_1, visits sequentially the sets $Q_1, Q_2, \ldots, Q_{M-1}$ exiting from Q_j through y_j and then follows the path ω_{j+1} before entering Q_{j+1}.

For every $\varepsilon > 0$ with a probability tending to one as $\beta \to \infty$ the process spends inside each Q_j a time less than $\exp\{\beta[H(y_j) - H(F(Q_j)) + \varepsilon]\}$.

Finally: before exiting from Q_j it can perform an arbitrary sequence of passages through the cycles $A^{(j)}$ belonging to Q_j. Each passage is made through a minimal saddle z_j in the boundary of $A^{(j)}$; for every $\varepsilon > 0$ with a probability tending to one as $\beta \to \infty$, once the system enters into a particular $A^{(j)}$, it spends there a time T:

$$\exp\{\beta[H(z_j) - H(F(A^{(j)})) - \varepsilon]\} < T < \exp\{\beta[H(z_j) - H(F(A^{(j)})) + \varepsilon]\}$$

Proof. By construction, using Proposition 3.7 applied either directly to our original cycle A if $y_0 \in \bar{B}(F(A))$ or to the cycles in Q_1 otherwise. The rest of the theorem also easily follows from Proposition 3.7 applied to the cycles contained in the Q_j. We leave the details to the reader.

Now, given any cycle A, we want to describe, in the maximal possible detail, the first excursion from $F(A)$ to ∂A.

Following Schonmann,[11] we first give some simple general definitions.

Given $x, y \in S$, we denote by $\Omega^*(x, y)$ the set of all paths ω starting in x, visiting y at some finite time t, and never visiting x and y in between:

$$\Omega^*(x, y) := \{\omega = x_1,..., x_t \text{ for some } t\text{: } x_1 = x, x_t = y; x_2,..., x_{t-1} \neq x, y\} \quad (4.2)$$

We denote by R the time reversal operator defined on finite paths:

$$\forall \omega := (x_1,..., x_t) : R\omega := \bar{\omega} := (x_t,..., x_1) \quad (4.3)$$

We naturally define, for every set of paths Δ,

$$R\Delta = \{\bar{\omega} = R\omega; \omega \in \Delta\}$$

Let us call $\bar{\tau}_x$ the last time our process visits the state x before touching for the first time y, namely

$$\bar{\tau}_x := \max\{t < \tau_y : X_t = x\} \quad (4.4)$$

Given a finite path $\tilde{\omega} = \tilde{x}_1,..., \tilde{x}_t$, we say that our process $\{X_t\}_{t>0}$ *starts as* $\tilde{\omega}$ if $X_1 = \tilde{x}_1,...,X_t = \tilde{x}_t$.

For any $x, y \in S$ we define a measure ρ on the (infinite) paths $\omega = x_1,..., x_t,...$ starting at $x(x_1 := x)$ as follows:

- If $\omega \notin \Omega^*(x, y)$, then $\rho(\omega) = 0$.
- If $\omega \in \Omega^*(x, y)$, we set $\tilde{\omega}_i = \omega_i$ for all $i < \inf\{t > 0; \omega_t = y\}$, that is, $\tilde{\omega}$ is the finite path given by the first segment of ω before hitting y. Then

$$\rho(\omega) = P_x(\{X_t\}_{t \geqslant 0} \text{ starts as } \tilde{\omega} \mid \omega \in \Omega^*(x, y))$$

and by $\bar{\rho}(\omega)$ the measure on the paths $\omega = x_1,..., x_t,...$ given by

$$\bar{\rho}(\omega) = P_y(\{X_t\}_{t \geqslant 0} \text{ starts as } R\tilde{\omega} \mid \omega \in \Omega^*(y, x)) \qquad \text{if} \quad \omega \in \Omega^*(y, x)$$
$$\bar{\rho}(\omega) = 0 \qquad \text{otherwise}$$

In ref. 11 it is proven that, for every $x, y \in S$, every $\Lambda \in \Omega^*(x, y)$,

$$P_x(X_t \in \Lambda, \forall t \in [\bar{\tau}_x, \tau_y]) = \rho(\Lambda) = \bar{\rho}(R\Lambda) = P_y(X_t \in R\Lambda, \forall t \in [\bar{\tau}_y, \tau_x]) \quad (4.5)$$

Let us now denote by $\partial^- F(A)$ the set of all $\hat{x} \in F(A)$, uphill communicating with $A \backslash F(A)$. Given a point $\hat{x}$ in $\partial^- F(A)$, consider the set $V(\hat{x})$ of all the points $x \in A$ uphill communicating with some point $\hat{y} \in U(A)$ and such that there exists a standard cascade $\mathscr{T}(y_0=\hat{y}, \omega_1, y_1, \omega_2,..., y_{N-1}, \omega_M)$ starting from $\hat{y}$ and ending in $\hat{x}$: $\hat{x}$ will belong to some component G^* of $F(A)$; $G^* := Q_M$ and ω_M will end entering into Q_M at $\hat{x}$.

Now we are able to state our main result about the typical trajectories realizing the escape from a cycle A.

Theorem 2. Let

$$\bar{\tau}_{F(A)} = \max\{t < \tau_{S\setminus A} : X_t \in F(A)\}$$

Call $\bar{\partial}^- A$ the set of all the points $x \in A$ uphill connected to $U(A)$ and

$$\mathscr{T} = \bigcup_{y_0 \in \bar{\partial}^- A} \mathscr{T}_{y_0} \tag{4.6}$$

the set of all possible standard tubes starting from points in $\bar{\partial}^- A$ and ending in $F(A)$. Then:

(i)

$$P_{F(A)}(X_{\tau_{S\setminus A}} \in U(A); X_t \in R\mathscr{T}, \forall t \in [\bar{\tau}_{F(A)}, \tau_{S\setminus A} - 1]) \to 1 \qquad \text{as} \quad \beta \to \infty \tag{4.7}$$

(ii) Given $\hat{x} \in \partial^- F(A)$ and any $x \in A$,

$$P_x(\exists \hat{y} \in V(\hat{x}) : X_t \in R\mathscr{T}(y_0 = \hat{y}, \omega_1, y_1, \omega_2,..., y_{M-1}, \omega_M),$$
$$\forall t \in [\bar{\tau}_{\hat{x}}, \tau_{\hat{y}} - 1] \quad \text{for some } \hat{y}, \omega_1, y_1, \omega_2,..., y_{M-1}\omega_M \mid X_{\bar{\tau}_{F(A)}} = \hat{x}) \to 1$$
$$\text{as} \quad \beta \to \infty \tag{4.8}$$

(iii) During the first excursion from $F(A)$ to $S\setminus A$, conditioning to $X_{\bar{\tau}_{F(A)}} = \hat{x}$ [for some $\hat{x} \in \partial^- F(A)$], to $X_{\tau_{S\setminus A} - 1} = \hat{y}$ [for some $\hat{y} \in V(\hat{x})$], and following a particular "anticascade" $R\mathscr{T}(y_0 = \hat{y}, \omega_1, y_1, \omega_2,..., y_{N-1}, \omega_M)$ between $\bar{\tau}_{\hat{x}}$ and $\tau_{\hat{y}}$, all the "time reverses" of the properties specified in point (iv) of Theorem 1 hold true; namely $\forall \varepsilon > 0$, with probability tending to one as $\beta \to \infty$, our process, during the above-mentioned first excursion, visits the time reverse of the sequence specified in point (iv) of Theorem 1 spending in each set the same typical times given there.

Remark. • In the particular case (relevant for the applications to stochastic Ising models) where the sets Q_i always coincide with a single cycle A_i, it immediately follows from Theorem 2 that the typical tube of trajectories during the first excursion from $F(A)$ to $S\setminus A$ is an anticascade starting from $\hat{x} \in \partial^- F(A)$ and ending in some $y^* \in U(A)$ given by a sequence $\bar{A}_1, \bar{\omega}_1, \bar{y}_1, \bar{A}_2, \bar{\omega}_2, \bar{y}_2,..., \bar{A}_M, \bar{\omega}_M, y^*$ with the properties:

(i) $H(\bar{y}_i) < H(\bar{y}_{i+1})$, $1 = 1,\ldots, M-1$.

(ii) $\bar{y}_i \in S(\bar{A}_{i+1})$.

Some ω_i can be empty; in that case $\bar{y}_i$ is also a saddle point in $\partial \bar{A}_i$.

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After the completion of the present paper we became aware that concepts and arguments related to the ones developed in the present paper, have been considered by Catoni[2] in the framework of the theory of simulated annealing. We thank G. Ben Arous for pointing out to us this reference.

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