LECTURE 5

Hypotheses and universal theorems

§ TARGETS

In Lectures 5–6 we describe the metastable behaviour of discrete systems with finite volume at low temperature that are subjected to a Metropolis dynamics. We derive three theorems under two hypotheses on the Hamiltonian.

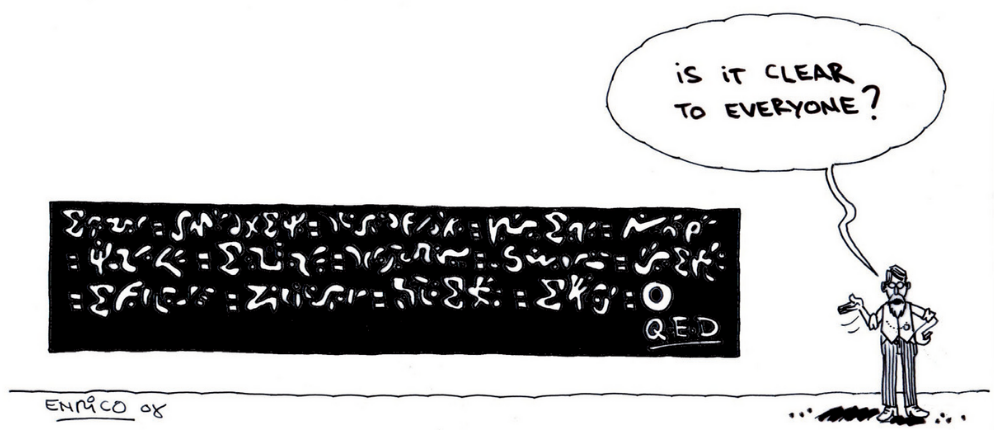
> The theorems are model-independent, and therefore underline the universal nature of metastability. However, they involve a number of key quantities that are model-dependent.

In Lectures 7–8 the hypotheses will be checked for Glauber dynamics and Kawasaki dynamics. The identification of the key quantities will be carried out there as well.

The axiomatic approach in Lectures 5–6 was developed in a succession of papers by

A. Bovier, E. Cirillo, F. den Hollander, F. Manzo, F.R. Nardi, A. Troiani, E. Scoppola, E. Olivieri

aiming at simplifying and generalising results that were obtained in specific examples.



§ METROPOLIS DYNAMICS AND GEOMETRIC DEFINITIONS

1. Let Λ be a finite set of elements referred to as vertices. With each vertex $x \in \Lambda$ we associate a variable $\xi(x) \in \Upsilon$, where Υ is a finite set of spin-values. A spin configuration $\xi = \{\xi(x)\colon\, x \in \Lambda\}$ is an element of $S = \Upsilon^\Lambda$.

2. To each configuration ξ we associate an energy given by a Hamiltonian $H\colon\, S \to \mathbb{R}$, which in general depends on one or more parameters. The Gibbs measure associated with H is

$$\mu_\beta(\xi) = \frac{1}{Z_\beta}\,\mathrm{e}^{-\beta H(\xi)}, \qquad \xi \in S,$$

where $\beta \in (0, \infty)$ is the inverse temperature, and Z_β is the normalising partition sum.

3. Equip S with a set of undirected edges E, connecting pairs of elements of S, such that (S, E) is a connected graph. Write $\xi \sim \xi'$ when $(\xi, \xi') \in E$.

4. For the dynamics we take the continuous-time Markov process $(\xi_t)_{t \geq 0}$ with state space S whose transition rates are given by

$$c_\beta(\xi, \xi') = \begin{cases} \mathrm{e}^{-\beta[H(\xi') - H(\xi)]_+}, & \xi \sim \xi', \\ 0, & \text{otherwise}, \end{cases}$$

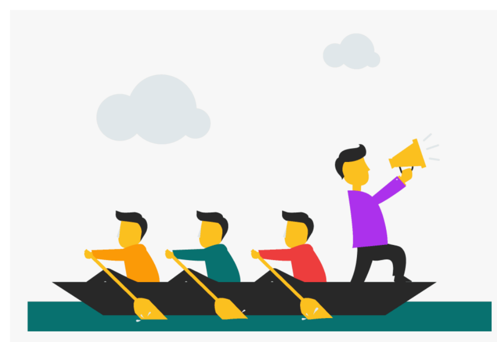
i.e., transitions occur along edges only. Thus, the edges represent the allowed moves.

The above dynamics is called the Metropolis dynamics with respect to H at inverse temperature β. It is ergodic and reversible with respect to μ_β:

$$\mu_\beta(\xi)c_\beta(\xi,\xi') = \mu_\beta(\xi')c_\beta(\xi',\xi) \qquad \forall\, \xi,\xi' \in S,$$

Choosing a particular model amounts to choosing Λ, Υ, E H and β. The generator $\mathcal{L}_\beta$ of the dynamics is

$$(\mathcal{L}_\beta f)(\xi) = \sum_{\xi' \sim \xi} c_\beta(\xi,\xi')[f(\xi') - f(\xi)], \qquad f\colon\, S \to \mathbb{R}.$$



§ DEFINITIONS

In order to formulate our metastability theorems, we need some general definitions.

DEFINITION 5.1 Energy landscape

(a) $\Phi(\xi,\xi')$ is the communication height between $\xi,\xi' \in S$ defined by

$$\Phi(\xi,\xi') = \min_{\gamma\colon\, \xi\to\xi'} \max_{\sigma\in\gamma} H(\sigma),$$

where $\gamma\colon\, \xi \to \xi'$ is any path of allowed moves from ξ to ξ'. For non-empty sets $A, B \subseteq S$ put

$$\Phi(A,B) = \min_{\xi\in A,\xi'\in B} \Phi(\xi,\xi').$$

(b) $\mathcal{S}(\xi,\xi')$ is the communication level set between $\xi,\xi' \in S$ defined by

$$\mathcal{S}(\xi,\xi') = \Big\{\zeta \in S\colon\ \exists\,\gamma\colon\ \xi \to \xi',\ \gamma \ni \zeta\colon \max_{\eta\in\gamma} H(\eta) = H(\zeta) = \Phi(\xi,\xi')\Big\}.$$

(c) V_ξ is the stability level of $\xi \in S$ defined by

$$V_\xi = \Phi(\xi, I_\xi) - H(\xi),$$

where

$$I_\xi = \{\zeta \in S\colon\ H(\zeta) < H(\xi)\}$$

is the set of configurations with energy lower than ξ.

(d) S_{stab} is the set of configurations with minimal energy, called stable configurations, defined by

$$S_{\text{stab}} = \Big\{\xi \in S\colon\ H(\xi) = \min_{\zeta \in S} H(\zeta)\Big\}.$$

(e) S_{meta} is the set of non-minimal configurations with maximal stability, called metastable configurations, defined by

$$S_{\text{meta}} = \Big\{\xi \in S\colon\ V_\xi = \max_{\zeta \in S\setminus S_{\text{stab}}} V_\zeta\Big\}.$$

DEFINITION 5.2 Paths, gates and dead-ends

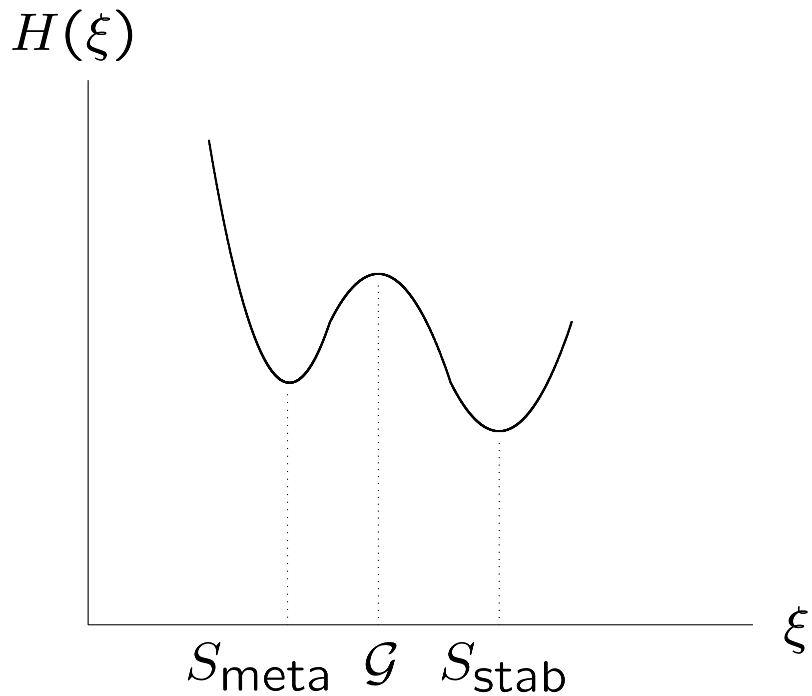
(a) $(\xi \to \xi')_{\text{opt}}$ is the set of paths realising the minimax in $\Phi(\xi,\xi')$.

(b) A set $\mathcal{W} \subseteq S$ is called a gate for $\xi \to \xi'$ if $\mathcal{W} \subseteq \mathcal{S}(\xi,\xi')$ and $\gamma \cap \mathcal{W} \neq \emptyset$ for all $\gamma \in (\xi \to \xi')_{\text{opt}}$.

(c) A set $\mathcal{W} \subseteq S$ is called a minimal gate for $\xi \to \xi'$ if it is a gate for $\xi \to \xi'$ and for any $\mathcal{W}' \subsetneq \mathcal{W}$ there exists a $\gamma' \in (\xi \to \xi')_{\text{opt}}$ such that $\gamma' \cap \mathcal{W}' = \emptyset$.

(d) A priori there may be several (not necessarily disjoint) minimal gates. Their union is denoted by $\mathcal{G}(\xi,\xi')$ and is called the essential gate for $(\xi \to \xi')_{\text{opt}}$.

(e) The configurations in $\mathcal{S}(\xi,\xi')\backslash\mathcal{G}(\xi,\xi')$ are called dead-ends for $(\xi \to \xi')_{\text{opt}}$.



Schematic picture of H, S_{meta}, S_{stab} and $\mathcal{G}$.

§ METASTABILITY THEOREMS AND HYPOTHESES

Theorems 5.4–5.6 below involve a pair of configurations

$$(\mathbf{m},\mathbf{s}) \in S_{\text{meta}} \times S_{\text{stab}}$$

that will be referred to as the metastable configuration and the stable configuration, respectively

Associated with $(\mathbf{m},\mathbf{s})$ is a pair of sets

$$(\mathcal{P}^*(\mathbf{m},\mathbf{s}), \mathcal{C}^*(\mathbf{m},\mathbf{s})),$$

which will be referred to as the protocritical set and the critical set, respectively, defined as follows.

DEFINITION 5.3 Protocritical set and critical set

Let

$$\Gamma^\star = \Phi(\mathbf{m},\mathbf{s}) - H(\mathbf{m}).$$

Then $(\mathcal{P}^*(\mathbf{m},\mathbf{s}),\mathcal{C}^*(\mathbf{m},\mathbf{s}))$ is the maximal subset of $S \times S$ such that:

(1) $\forall\,\xi \in \mathcal{P}^*(\mathbf{m},\mathbf{s})\ \exists\,\xi' \in \mathcal{C}^*(\mathbf{m},\mathbf{s})\colon\ \xi \sim \xi'.$

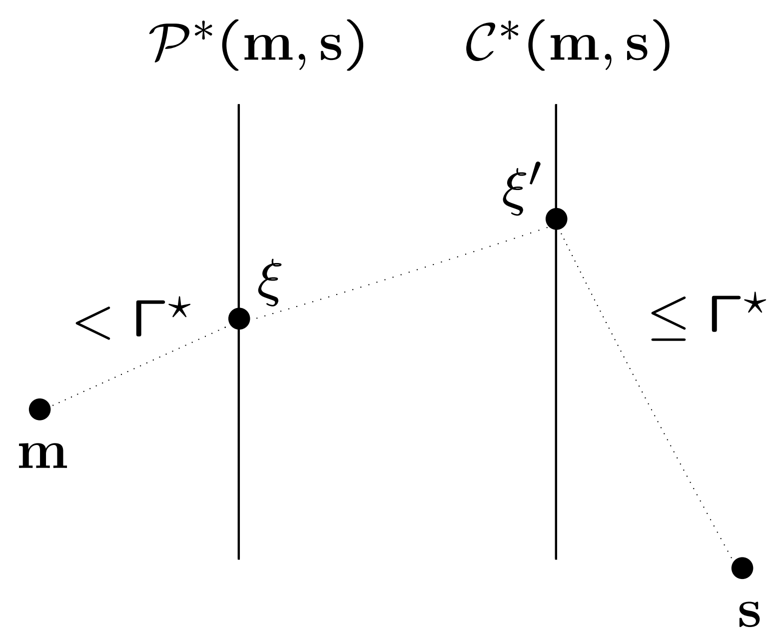
$\forall\,\xi' \in \mathcal{C}^*(\mathbf{m},\mathbf{s})\ \exists\,\xi \in \mathcal{P}^*(\mathbf{m},\mathbf{s})\colon\ \xi' \sim \xi.$

(2) $\forall\,\xi \in \mathcal{P}^*(\mathbf{m},\mathbf{s})\colon\ \Phi(\xi,\mathbf{m}) < \Phi(\xi,\mathbf{s}).$

(3) $\forall\,\xi' \in \mathcal{C}^*(\mathbf{m},\mathbf{s})\ \exists\,\gamma\colon$

$\xi' \to \mathbf{s}\colon\ \max_{\zeta\in\gamma} H(\zeta) - H(\mathbf{m}) \le \Gamma^\star,$

$\gamma \cap \{\zeta \in S\colon\ \Phi(\zeta,\mathbf{m}) < \Phi(\zeta,\mathbf{s})\} = \emptyset.$



Schematic picture of the protocritical set and the critical set.

- Think of $\mathcal{P}^*(\mathbf{m},\mathbf{s})$ as the set of configurations where the dynamics starting from $\mathbf{m}$ is almost on top of the hill.

- Think of $\mathcal{C}^*(\mathbf{m},\mathbf{s})$ as the set of configurations where the dynamics is on top of the hill and is capable of crossing over to $\mathbf{s}$ without returning to the valley around $\mathbf{m}$.

The latter restriction is put in to remove the dead-ends. Note that

$$H(\xi) - H(\mathbf{m}) = \Gamma^\star \qquad \forall\, \xi \in \mathcal{C}^*(\mathbf{m},\mathbf{s}).$$

Also note that

$$\mathcal{C}^*(\mathbf{m},\mathbf{s}) \left\{ \begin{array}{c} = \\ \supsetneq \\ \subsetneq \end{array} \right\} \mathcal{G}(\mathbf{m},\mathbf{s})$$

are all three possible. In Lectures 7–8 we will encounter examples.

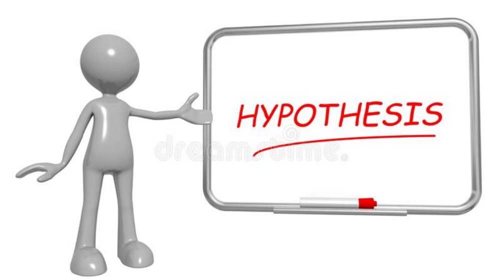
§ HYPOTHESES

Theorems 5.4–5.6 below will be proved subject to two key hypotheses:

(H1) $S_{\text{meta}} = \{\mathbf{m}\}$, $S_{\text{stab}} = \{\mathbf{s}\}$.

(H2) $\xi' \mapsto |\{\xi \in \mathcal{P}^*(\mathbf{m},\mathbf{s})\colon\ \xi \sim \xi'\}|$ is constant on $\mathcal{C}^*(\mathbf{m},\mathbf{s})$.

(H1) says that S_{meta} and S_{stab} are singletons, (H2) says that all configurations in $\mathcal{C}^*(\mathbf{m},\mathbf{s})$ have the same number of configurations in $\mathcal{P}^*(\mathbf{m},\mathbf{s})$ from which they can be reached via an allowed move.



Any pair of configurations $(\mathbf{m},\mathbf{s})$ satisfying (H1) is referred to as a metastable pair. Without loss of generality we may assume that

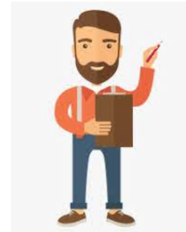
$$H(\mathbf{m}) = 0.$$

We write $\mathbb{P}_\xi$ to denote the law of $(\xi_t)_{t\geq 0}$ given $\xi_0 = \xi \in S$, and write

$$\tau_A = \inf\{t \geq 0\colon\ \xi_t \in A,\ \exists\, 0 < s < t\colon\ \xi_s \neq \xi_0\}$$

to denote the first hitting time of $A \subseteq S$ after the starting configuration has been left. In what follows we abbreviate $\mathcal{P}^* = \mathcal{P}^*(\mathbf{m},\mathbf{s})$ and $\mathcal{C}^* = \mathcal{C}^*(\mathbf{m},\mathbf{s})$.

§ UNIVERSAL THEOREMS



THEOREM 5.4 Critical gate and uniform entrance distribution

(a) $\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{m}}(\tau_{\mathcal{C}^*} < \tau_{\mathbf{s}} \mid \tau_{\mathbf{s}} < \tau_{\mathbf{m}}) = 1$.

(b) $\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{m}}(\xi_{\tau_{\mathcal{C}^*}} = \chi) = 1/|\mathcal{C}^*|$ *for all* $\chi \in \mathcal{C}^*$.

THEOREM 5.5 Mean crossover time

There exists a constant $K \in (0,\infty)$ *such that*

$$\lim_{\beta\to\infty} \mathrm{e}^{-\beta\Gamma^\star} \mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = K.$$

THEOREM 5.6 Spectrum and exponential law of crossover time

(a) $\lim_{\beta\to\infty} \lambda_\beta \mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = 1$, *with* λ_β *the second eigenvalue of* $-\mathcal{L}_\beta$, *with* $\mathcal{L}_\beta$ *the generator of the Metropolis dynamics.*

(b) $\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{m}}(\tau_{\mathbf{s}}/\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) > t) = \mathrm{e}^{-t}$ *for all* $t \geq 0$.

While (H1) plays a central role in the derivation of Theorems 5.4–5.6, (H2) is needed for Theorem 5.4(b) only.

It turns out that typically $\Gamma^\star$ is independent of Λ (provided Λ is large enough) and is relatively robust against variations of the dynamics, while K depends on Λ and is rather sensitive to the details of the dynamics.

In Lecture 6 we will see that K is given by a non-trivial variational formula involving the set of all configurations where the dynamics can enter and exit $\mathcal{C}^*$. This set includes the border of the valleys around $\mathbf{m}$ and $\mathbf{s}$, and possibly the border of wells in $\mathcal{S}(\mathbf{m},\mathbf{s})$, i.e., configurations with energy $< \Gamma^\star$ but communication height $\Gamma^\star$ towards both $\mathbf{m}$ and $\mathbf{s}$.

We will see in Lecture 7 that for Glauber dynamics there are no wells and K can be computed explicitly. We will see in Lecture 8 that for Kawasaki dynamics there are wells, but they are sometimes harmless, e.g. when Λ is a large box in $\mathbb{Z}^2$ whose size tends to infinity (after the limit $\beta \to \infty$ has been taken).

§ REMARKS

1. Theorem 5.4(a) says that $\mathcal{C}^*$ is a gate for the crossover, i.e., on its way from $\mathbf{m}$ to $\mathbf{s}$ the dynamics passes through $\mathcal{C}^*$ with probability tending to 1 in the limit as $\beta \to \infty$.

Theorem 5.4(b) says that all configurations in $\mathcal{C}^*$ are equally likely to be seen upon first entrance in $\mathcal{C}^*$.

Theorem 5.5 states that the average crossover time from $\mathbf{m}$ to $\mathbf{s}$ is asymptotic to $K\mathrm{e}^{\Gamma^\star\beta}$, which is the Arrhenius law.

Theorem 5.6(a) says that the spectral gap of $-\mathcal{L}_\beta$ scales like the inverse of the average crossover time.

Theorem 5.6(b) says that asymptotically the crossover time is exponentially distributed on the scale of its average.

2. Theorems 5.4–5.6 are model-independent, i.e., they hold in the same form for all finite systems subject to Metropolis dynamics in the limit of low temperature, and for any pair $(\mathbf{m}, \mathbf{s})$ satisfying hypotheses (H1–H2).

We will see that (H1–H2) are essentially the minimal assumptions needed to prove Theorems 5.4–5.6.

The model-dependent ingredients of Theorems 5.4–5.6 are the pair $(\mathbf{m}, \mathbf{s})$ and the triple $(\Gamma^\star, \mathcal{C}^*, K)$. In Lectures 7–8 we will identify the latter for Glauber dynamics and Kawasaki dynamics, and prove (H1–H2).

§ CONSEQUENCES OF THE HYPOTHESES

Lemmas 5.7–5.10 below are immediate consequences of (H1) and will be needed in Lecture 6.

LEMMA 5.7 *(H1) implies that* $V_{\mathbf{m}} = \Gamma^\star$.

PROOF: By Definition 5.1(c-e), $\mathbf{s} \in I_{\mathbf{m}}$ and hence $V_{\mathbf{m}} \le \Gamma^\star$. We show that (H1) implies $V_{\mathbf{m}} = \Gamma^\star$. The proof is by contradiction.

Suppose that $V_{\mathbf{m}} < \Gamma^\star$. Then there exists a $\xi_0 \in I_{\mathbf{m}}$ such that

$$\Phi(\mathbf{m}, \xi_0) = \Phi(\mathbf{m}, \xi_0) - H(\mathbf{m}) \le V_{\mathbf{m}} < \Gamma^\star.$$

Since (H1) says that $\mathbf{m}$ has the largest stability level, we can proceed to reduce the energy further until we hit $\mathbf{s}$.

Indeed, the finiteness of S guarantees that there exists an $m \in \mathbb{N}_0$ and a sequence $\xi_1, \ldots, \xi_m \in S \backslash \mathbf{m}$ with $\xi_m = \mathbf{s}$ such that $\xi_{i+1} \in I_{\xi_i}$ and $\Phi(\xi_i, \xi_{i+1}) - H(\xi_i) < V_{\mathbf{m}}$ for $i = 0, \ldots, m-1$. Therefore we have

$$\Phi(\xi_0, \mathbf{s}) \le \max_{i=0,\ldots,m-1} \Phi(\xi_i, \xi_{i+1}) < \max_{i=0,\ldots,m-1} [H(\xi_i) + V_{\mathbf{m}}]$$
$$= H(\xi_0) + V_{\mathbf{m}} < H(\mathbf{m}) + \Gamma^\star = \Gamma^\star,$$

where in the first inequality we use the ultrametricity of the communication height,

$$\Phi(\xi, \chi) \le \max\{\Phi(\xi, \zeta), \Phi(\zeta, \chi)\} \qquad \forall\, \xi, \chi, \zeta \in S,$$

and in the last inequality we use that $H(\xi_0) < H(\mathbf{m})$ since $\xi_0 \in I_{\mathbf{m}}$. It follows that

$$\Gamma^\star = \Phi(\mathbf{m}, \mathbf{s}) \le \max\{\Phi(\mathbf{m}, \xi_0), \Phi(\xi_0, \mathbf{s})\} < \Gamma^\star,$$

which is a contradiction. $\square$

LEMMA 5.8 *(H1) implies that* $H(\xi) > 0$ *for all* $\xi \in S\backslash\mathbf{m}$ *with* $\Phi(\xi, \mathbf{m}) \leq \Phi(\xi, \mathbf{s})$.

PROOF: The proof is again by contradiction. Fix $\xi_0 \in S\backslash\mathbf{m}$ with $\Phi(\xi_0, \mathbf{m}) \leq \Phi(\xi_0, \mathbf{s})$ and suppose that $H(\xi_0) \leq 0$. Then $\mathbf{m} \notin I_{\xi_0}$. As in the proof of Lemma 5.7, there exist an $m \in \mathbb{N}_0$ and a sequence $\xi_0, \ldots, \xi_m \in S$ with $\xi_m = \mathbf{s}$ such that $\xi_{i+1} \in I_{\xi_i}$ and $\Phi(\xi_i, \xi_{i+1}) - H(\xi_i) < V_{\mathbf{m}} = \Gamma^\star$ for $i = 0, \ldots, m-1$. Therefore, we get $\Phi(\xi_0, \mathbf{s}) - H(\xi_0) < V_{\mathbf{m}} = \Gamma^\star$. Hence

$$\begin{aligned}\Gamma^\star = \Phi(\mathbf{m}, \mathbf{s}) &\leq \max\{\Phi(\mathbf{m}, \xi_0), \Phi(\xi_0, \mathbf{s})\} \\ &= \Phi(\xi_0, \mathbf{s}) \leq \Phi(\xi_0, \mathbf{s}) - H(\xi_0) < \Gamma^\star,\end{aligned}$$

which is a contradiction. □

LEMMA 5.9 *(H1) implies that there exists a* $V^\star < \Gamma^\star$ *such that* $\Phi(\xi, \{\mathbf{m}, \mathbf{s}\}) - H(\xi) \leq V^\star$ *for all* $\xi \in S \backslash \{\mathbf{m}, \mathbf{s}\}$.

PROOF: In the proof of Lemma 5.8 we have shown that $\Phi(\xi_0, \mathbf{s}) - H(\xi_0) < \Gamma^\star$ for all $\xi_0 \in S \backslash \mathbf{m}$. But

$$\Phi(\xi_0, \{\mathbf{m}, \mathbf{s}\}) = \min\{\Phi(\xi_0, \mathbf{m}), \Phi(\xi_0, \mathbf{s})\} \leq \Phi(\xi_0, \mathbf{s}),$$

while $\Phi(\mathbf{m}, \{\mathbf{m}, \mathbf{s}\}) - H(\mathbf{m}) = 0 < \Gamma^\star$, and so the claim actually holds for all $\xi \in S$. □

LEMMA 5.10 *Let*

$$\bar{\mathcal{C}}^* = \{\xi' \in S \setminus (\mathcal{P}^* \cup \mathcal{C}^*) \colon\ H(\xi') \le \Gamma^\star, \exists\, \xi \in \mathcal{C}^* \colon\ \xi \sim \xi'\}.$$

Then for every $\xi' \in \bar{\mathcal{C}}^*$ *every path in* $(\xi' \to \mathbf{m})_{\text{opt}}$ *passes through* $\mathcal{P}^*$*.*

PROOF: Pick any $\xi' \in \bar{\mathcal{C}}^*$, any $\gamma \in (\xi' \to \mathbf{m})_{\text{opt}}$ and any $\xi \in \mathcal{C}^*$ such that $\xi \sim \xi'$. We have $\max_{\zeta \in \gamma} H(\zeta) \le \Gamma^\star$, because $H(\xi') \le \Gamma^\star$ and $\Phi(\mathbf{m}, \xi) \le \Gamma^\star$ by Definition 5.3. The reverse of γ can be extended by the single move from ξ' to ξ to obtain a path $\gamma' \colon \mathbf{m} \to \xi$ such that $\max_{\zeta \in \gamma'} H(\zeta) \le \Gamma^\star$. By Definition 5.3(3), this path can be further extended by a path $\gamma'' \colon \xi \to \mathbf{s}$ such that $\max_{\zeta \in \gamma''} H(\zeta) \le \Gamma^\star$ and $\gamma'' \cap \mathcal{P}^* = \emptyset$.

The concatenation $\gamma' \cup \gamma''$ is an optimal path, i.e., $\gamma' \cup \gamma'' \in (\mathbf{m} \to \mathbf{s})_{\text{opt}}$. However, by the maximality in Definition 5.3, *any* path in $(\mathbf{m} \to \mathbf{s})_{\text{opt}}$ must hit $\mathcal{P}^*$. Since γ'' does not hit $\mathcal{P}^*$, it follows that γ' hits $\mathcal{P}^*$. But $\xi \in \mathcal{C}^*$ and $\mathcal{P}^* \cap \mathcal{C}^* = \emptyset$, and hence the piece of γ' between $\mathbf{m}$ and ξ' hits $\mathcal{P}^*$. □

§ REMARKS

Lemmas 5.7–5.8 say that $\mathbf{m}$ lies at the bottom of a valley of depth $\Gamma^\star$ and no other configuration does.

Lemma 5.9 says that there are no deeper valleys anywhere else.

Lemma 5.10 says that once an optimal path from $\mathbf{m}$ to $\mathbf{s}$ is over the hill it cannot go back to $\mathbf{m}$ without passing through the protocritical set.

LITERATURE:

Chapter 16 in Bovier and den Hollander 2015, and references therein.