LECTURE 6

Proof of the universal theorems

§ CAPACITIES AND HARMONIC FUNCTIONS

Here is a reminder of some key formulas in Lectures 2–3.

1. The key object in our approach to metastability is the Dirichlet form

$$\mathcal{E}_\beta(h,h) = \frac{1}{2} \sum_{\xi,\xi' \in S} \mu_\beta(\xi) c_\beta(\xi,\xi')[h(\xi) - h(\xi')]^2, \; h\colon\; S \to [0,1],$$

where μ_β is the Gibbs measure and c_β is the kernel of transition rates. For Metropolis dynamics

$$Z_\beta \mu_\beta(\xi) c_\beta(\xi,\xi') = \mathrm{e}^{-\beta[H(\xi) \vee H(\xi')]}.$$

Given any pair of non-empty disjoint sets $A, B \subseteq S$, the capacity of the pair A, B is

$$\mathrm{cap}_\beta(A,B) = \min_{\substack{h\colon\; S \to [0,1] \\ h|_A \equiv 1, h|_B \equiv 0}} \mathcal{E}_\beta(h,h).$$

2. The unique minimizer $h_{A,B}$ of the Dirichlet form is called the equilibrium potential of the pair A, B, and is the solution of the equation

$$\begin{aligned} (-\mathcal{L}_\beta h)(\xi) &= 0, && \xi \in S\backslash(A \cup B), \\ h(\xi) &= 1, && \xi \in A, \\ h(\xi) &= 0, && \xi \in B, \end{aligned}$$

which is given by

$$\begin{aligned} h_{A,B}(\xi) &= \mathbb{P}_\xi(\tau_A < \tau_B), && \xi \in S\backslash(A \cup B), \\ h_{A,B}(\xi) &= 1, && \xi \in A, \\ h_{A,B}(\xi) &= 0, && \xi \in B. \end{aligned}$$

§ A PRIORI ESTIMATES ON CAPACITY

LEMMA 6.1 A priori estimates

For every pair of non-empty disjoint sets $A, B \subseteq S$ *there exist constants* $0 < C_1 \leq C_2 < \infty$ *(depending on* A, B*) such that*

$$C_1 \leq \mathrm{e}^{\beta\Phi(A,B)}\, Z_\beta \,\mathrm{cap}_\beta(A, B) \leq C_2 \qquad \forall\, \beta \in (0, \infty).$$

PROOF:

The proof is long. However, as we will explain later, the lemma is important because it yields the exponential term in the Arrhenius formula, and also provides bounds on the prefactor.

- Upper bound:

> The following argument suggested by Yoan Tardy and Tristan Pham-Mariotti improves the argument given in Chapter 16 of Bovier, den Hollander 2015.

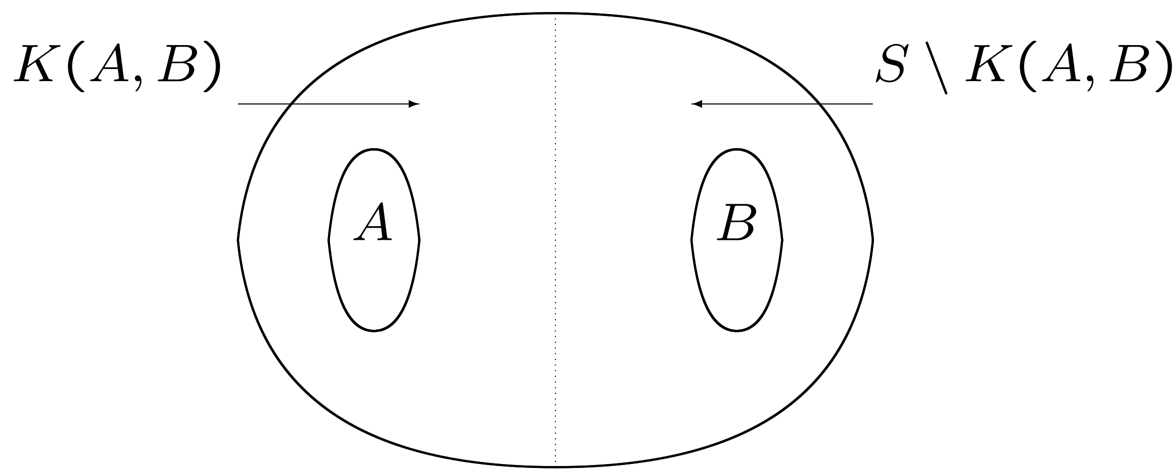
1. Pick as test function $h = 1_\Delta$ with $\Delta = K(A,B)\backslash B$ and

$$K(A,B) = \{\xi \in S\colon\ \Phi(\xi,A) \leq \Phi(\xi,B)\}.$$

Via the Dirichlet principle we get

$$\mathrm{cap}_\beta(A,B) \leq \mathcal{E}_\beta(1_\Delta, 1_\Delta),$$

where we note that $A \subset \Delta$, $B \subset S\backslash\Delta$, so that the boundary conditions on A and B are met.



A partition of S into sets of configurations from which the dynamics is more likely to hit A rather than B or the other way around.

While $A \subset K(A,B)$, possibly $B \cap K(A,B) \neq \emptyset$.

2. We will show that

$$(*) \qquad \forall\, \zeta \in \Delta,\, \zeta' \notin \Delta,\, \zeta \sim \zeta' \colon\ H(\zeta) \vee H(\zeta') \geq \Phi(A,B).$$

This will imply that

$$Z_\beta \mathcal{E}_\beta(1_\Delta, 1_\Delta) = \sum_{\substack{\zeta \in \Delta, \zeta' \notin \Delta \\ \zeta \sim \zeta'}} \mathrm{e}^{-\beta[H(\zeta) \vee H(\zeta')]} \leq C_2\, \mathrm{e}^{-\beta \Phi(A,B)}$$

with $C_2 = |\{(\zeta,\zeta')\colon\ \zeta \in \Delta, \zeta' \notin \Delta, \zeta \sim \zeta'\}|$.

3. In the proof of $(*)$ we distinguish between the cases $\zeta' \notin K(A,B)$ and $\zeta' \in K(A,B) \cap B$.

- $\zeta' \notin K(A,B)$

Estimate in steps

$$\begin{aligned}\Phi(\zeta',A) &\le H(\zeta') \vee \Phi(\zeta,A) \le H(\zeta') \vee \Phi(\zeta,B)\\ &\le H(\zeta') \vee H(\zeta) \vee \Phi(\zeta',B) \le H(\zeta) \vee \Phi(\zeta,' B)\\ &= H(\zeta).\end{aligned}$$

The first and third use $\zeta \sim \zeta'$, the second $\zeta \in K(A,B)$, the fourth $H(\zeta') \le \Phi(\zeta',B)$ and the fifth $\zeta' \notin K(A,B)$. Since $\Phi(\zeta',B) < \Phi(\zeta',A) \le H(\zeta)$, it follows that $\Phi(\zeta',B) \le H(\zeta)$. Hence

$$\Phi(A,B) \le \Phi(\zeta',A) \vee \Phi(\zeta',B) \le H(\zeta).$$

- $\zeta' \in K(A,B) \cap B$

Because $\zeta' \in B$, it follows that

$$\Phi(\zeta', B) = H(\zeta'),$$

while $\zeta' \in K(A,B)$ implies that

$$\Phi(\zeta' A) \leq \Phi(\zeta', B) = H(\zeta').$$

Hence

$$\Phi(A,B) \leq \phi(\zeta', A) \vee \Phi(\zeta', B) \leq H(\zeta').$$

4. Combine the two cases to get $(*)$.

- Lower bound: The lower bound is obtained by picking any self-avoiding path

$$\gamma = (\gamma_0, \gamma_1, \dots, \gamma_L)$$

that realises the minimax in $\Phi(A,B)$ and ignoring all the transitions that are not in this path, i.e.,

$$\mathrm{cap}_\beta(A,B) \geq \min_{\substack{h\colon \gamma \to [0,1] \\ h(\gamma_0)=1,\, h(\gamma_L)=0}} \mathcal{E}^\gamma_\beta(h,h),$$

where the Dirichlet form $\mathcal{E}^\gamma_\beta$ is defined as $\mathcal{E}_\beta$ but with S replaced by γ. Due to the one-dimensional nature of the set γ, the variational problem in the right-hand side can be solved explicitly by elementary computations, as explained in Lecture 2.

The minimum equals

$$M = \left[\sum_{l=0}^{L-1} \frac{1}{\mu_\beta(\gamma_l) c_\beta(\gamma_l, \gamma_{l+1})} \right]^{-1}.$$

The minimum is uniquely attained at h given by

$$h(\gamma_l) = M \sum_{k=0}^{l-1} \frac{1}{\mu_\beta(\gamma_k) c_\beta(\gamma_k, \gamma_{k+1})}, \qquad l = 0, 1, \dots, L.$$

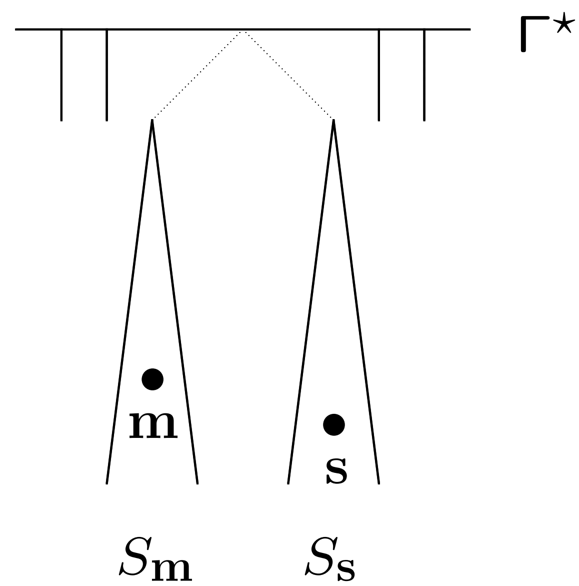
We thus have

$$\begin{aligned} Z_\beta \mathrm{cap}_\beta(A, B) &\geq Z_\beta M \\ &\geq \frac{1}{L} \min_{l=0,1,\dots,L-1} \mathrm{e}^{-\beta[H(\gamma_l) \vee H(\gamma_{l+1})]} = C_1 \, \mathrm{e}^{-\beta \Phi(A,B)} \end{aligned}$$

with $C_1 = 1/L$. □

§ GRAPH STRUCTURE OF ENERGY LANDSCAPE

We take a closer look at the geometric structure of the set S.



Schematic picture of $S^\star$ (on or below the top line), $S^{\star\star}$ (below the top line), and the connected components $S_{\mathbf{m}}$ and $S_{\mathbf{s}}$. The four vertical lines represent dead-ends.

THEOREM 6.2 Graph structure of the energy landscape

View S as a graph whose vertices are the configurations and whose edges connect pairs ofconfigurations that can be obtained from each other via an allowed move, i.e., (ξ, ξ') is an edge if and only if $\xi \sim \xi'$. Define

- *$S^\star$ is the subgraph of S obtained by removing all the vertices ξ with $H(\xi) > \Gamma^\star$ and all the edges incident to these vertices;*
- *$S^{\star\star}$ is the subgraph of $S^\star$ obtained by removing all the vertices ξ with $H(\xi) = \Gamma^\star$ and all the edges incident to these vertices:*
- *$S_{\mathbf{m}}$ and $S_{\mathbf{s}}$ are the connected components of $S^{\star\star}$ that contain $\mathbf{m}$ and $\mathbf{s}$, respectively.*

Then

$$S_{\mathbf{m}} = \{\xi \in S \colon\ \Phi(\xi, \mathbf{m}) < \Phi(\xi, \mathbf{s}) = \Gamma^\star\},$$
$$S_{\mathbf{s}} = \{\xi \in S \colon\ \Phi(\xi, \mathbf{s}) < \Phi(\xi, \mathbf{m}) = \Gamma^\star\}.$$

Moreover, $S_{\mathbf{m}}$ *and* $S_{\mathbf{s}}$ *are disconnected in* $S^{\star\star}$*, and*

$$\mathcal{P}^* \subseteq S_{\mathbf{m}}, \qquad \mathcal{C}^* \subseteq S^\star \backslash S_{\mathbf{m}},$$
$$\forall\, \xi \in \mathcal{C}^*\ \exists\, \gamma \colon\ \xi \to S_{\mathbf{s}} \text{ such that } \gamma \backslash \xi \subseteq S^\star \backslash S_{\mathbf{m}}.$$

PROOF: All paths connecting $\mathbf{m}$ and $\mathbf{s}$ reach energy level $\geq \Gamma^\star$ (recall that $H(\mathbf{m}) = 0$). Therefore $S_{\mathbf{m}}$ and $S_{\mathbf{s}}$ are disconnected in $S^{\star\star}$ (because $S^{\star\star}$ does not contain any vertices with energy $\geq \Gamma^\star$). The claims are immediate from the definition of $S_{\mathbf{m}}$ and $S_{\mathbf{s}}$, and from the earlier definitions.

□

§ METASTABLE PAIR

An important consequence of (H1) and LEMMA 6.1 is:

LEMMA 6.3 Metastable pair

The pair $\{\mathbf{m},\mathbf{s}\}$ *is a metastable set:*

$$\lim_{\beta\to\infty} \frac{\max_{\xi\notin\{\mathbf{m},\mathbf{s}\}} \mu_\beta(\xi)/\mathrm{cap}_\beta(\xi,\{\mathbf{m},\mathbf{s}\})}{\min_{\xi\in\{\mathbf{m},\mathbf{s}\}} \mu_\beta(\xi)/\mathrm{cap}_\beta(\xi,\{\mathbf{m},\mathbf{s}\}\backslash\xi)} = 0.$$

PROOF: Note that the no-deep-well property in LEMMA 5.9 and the lower bound in LEMMA 6.1 give that the numerator is bounded from above by $e^{\beta(V^\star - H(\mathbf{m}))}/C_1 = e^{\beta(\Gamma^\star-\delta)}/C_1$ for some $\delta > 0$, while the definition of $\mu_\beta, \Gamma^\star$ and the upper bound in LEMMA 6.1 give that the denominator is bounded from below by $e^{\Gamma^\star\beta}/C_2$ (the minimum being attained at $\mathbf{m}$). □

LEMMA 6.3 has an important consequence.

LEMMA 6.4 Link average crossover time and capacity
$\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = \frac{1}{Z_\beta \text{cap}_\beta(\mathbf{m},\mathbf{s})}\,[1+o(1)]$ *as* $\beta \to \infty$.

PROOF: As seen in Lecture 2,

$$\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = \frac{\mu_\beta(A(\mathbf{m}))}{\text{cap}_\beta(\mathbf{m},\mathbf{s})}\,[1+o(1)], \qquad \beta \to \infty,$$

where

$$\begin{aligned} A(\mathbf{m}) &= \Big\{\xi \in S\colon\ \mathbb{P}_\xi(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \geq \mathbb{P}_\xi(\tau_{\mathbf{s}} < \tau_{\mathbf{m}})\Big\} \\ &= \Big\{\xi \in S\colon\ h_{\mathbf{m},\mathbf{s}}(\xi) \geq \tfrac{1}{2}\Big\}, \end{aligned}$$

and the reduction $\sum_{\xi\in S} \mu_\beta(\xi) h_{\mathbf{m},\mathbf{s}}(\xi) = [1+o(1)]\mu_\beta(A(\mathbf{m}))$ comes from estimates on $h_{\mathbf{m},\mathbf{s}}$ via capacities.

It follows from LEMMA 6.5 below that

$$\lim_{\beta\to\infty} \min_{\xi\in S_{\mathbf{m}}} h_{\mathbf{m},\mathbf{s}}(\xi) = 1, \qquad \lim_{\beta\to\infty} \max_{\xi\in S_{\mathbf{s}}} h_{\mathbf{m},\mathbf{s}}(\xi) = 0.$$

Hence, for large enough β,

$$S_{\mathbf{m}} \subseteq A(\mathbf{m}) \subseteq S\backslash S_{\mathbf{s}}.$$

By LEMMA 5.8, $H(\xi) > 0 = H(\mathbf{m})$ for all $\xi \neq \mathbf{m}$ such that $\Phi(\xi,\mathbf{m}) \leq \Phi(\xi,\mathbf{s})$. Therefore, by the second inclusion,

$$\min_{\xi\in A(\mathbf{m})\backslash\mathbf{m}} H(\xi) > 0.$$

The latter in turn implies that $\mu_\beta(A(\mathbf{m}))/\mu_\beta(\mathbf{m}) = 1+o(1)$. Since $\mu_\beta(\mathbf{m}) = 1/Z_\beta$, we get the claim. $\square$

What LEMMA 6.4 shows is that the proof of THEOREM 5.5 revolves around getting sharp bounds on $Z_\beta \text{cap}_\beta(\mathbf{m},\mathbf{s})$.

The a priori estimates serve as a jump board, because together with LEMMA 6.4 they already yield the estimate

$$\frac{1}{C_2} \leq \mathrm{e}^{-\beta\Gamma^\star}\,\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) \leq C_1.$$

Thus, our task is to narrow down the constants leading to the identification of the prefactor K. The strategy to do so is the following.

STRATEGY

- Note that all the terms in the Dirichlet form involving configurations ξ with $H(\xi) > \Gamma^\star$, i.e., $\xi \in S\backslash S^\star$, at most contribute $C\mathrm{e}^{-\beta(\Gamma^\star+\delta)}$ for some $\delta > 0$ and can be neglected. Thus, effectively we can replace S by $S^\star$.

- Show that $h_{\mathbf{m},\mathbf{s}} = 1 - O(\mathrm{e}^{-\beta\delta})$ on $S_\mathbf{m}$ and $h_{\mathbf{m},\mathbf{s}} = O(\mathrm{e}^{-\beta\delta})$ on $S_\mathbf{s}$ for some $\delta > 0$. Thus, effectively we can replace $h_{\mathbf{m},\mathbf{s}}$ by 1 on $S_\mathbf{m}$ and by 0 on $S_\mathbf{s}$.

- Derive sharp estimates for $h_{\mathbf{m},\mathbf{s}}$ on $S^\star\backslash(S_\mathbf{m} \cup S_\mathbf{s})$ in terms of a variational formula involving the vertices and the edges that are on or incident to $S^\star\backslash(S_\mathbf{m} \cup S_\mathbf{s})$. Use this variational formula to identify K.

§ PROOF OF THE METASTABILITY THEOREMS

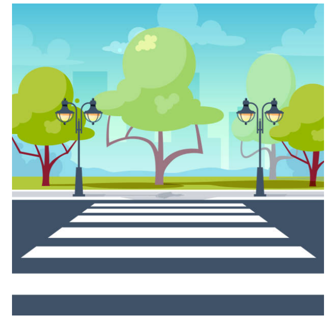
▶ Exponential distribution of the crossover time

PROOF:

Each time the dynamics reaches $\mathcal{C}^*(\mathbf{m},\mathbf{s})$, fails to enter $S_{\mathbf{s}}$ and falls back into $S_{\mathbf{m}}$, it has a probability exponentially close to 1 to return to $\mathbf{m}$, because $\mathbf{m}$ lies at the bottom of $S_{\mathbf{m}}$. Each time the dynamics returns to $\mathbf{m}$, it starts from scratch.

The dynamics manages to grow a critical droplet and go over the hill only after a large number of attempts that tends to infinity as $\beta \to \infty$, each having a small success probability that tends to zero as $\beta \to \infty$. Consequently, the time to go over the hill is exponentially distributed on the scale of its average. $\square$

▶ Average crossover time



PROOF:

Our task is to show that

$$Z_\beta \mathrm{cap}_\beta(\mathbf{m},\mathbf{s}) = \frac{1}{2} \sum_{\xi,\xi' \in S} Z_\beta \mu_\beta(\xi) c_\beta(\xi,\xi') \, [h_{\mathbf{m},\mathbf{s}}(\xi) - h_{\mathbf{m},\mathbf{s}}(\xi')]^2$$
$$= [1+o(1)] \, \Theta \, \mathrm{e}^{-\beta\Gamma^\star}, \qquad \beta \to \infty,$$

and to identify the constant $\Theta = 1/K$. This is done in three steps. In the first two steps we derive sharp estimates on $h_{\mathbf{m},\mathbf{s}}$. In the third step we use these estimates to derive a variational formula for Θ.

Recall that

$$Z_\beta \mu_\beta(\xi) c_\beta(\xi,\xi') = \mathrm{e}^{-\beta[H(\xi) \vee H(\xi')]}.$$

I. For all $\xi \in S \backslash S^\star$ we have $H(\xi) > \Gamma^\star$, and so there exists a $\delta > 0$ such that $Z_\beta \mu_\beta(\xi) \leq \mathrm{e}^{-\beta(\Gamma^\star+\delta)}$. Since $c_\beta(\xi,\xi') \leq 1$ for all $\xi,\xi' \in S$, we can therefore replace S by $S^\star$ in the sum in the Dirichlet form, at the cost of a prefactor $1 + O(\mathrm{e}^{-\beta\delta})$.

LEMMA 6.5 Bounds on harmonic function

There exist $C < \infty$ and $\delta > 0$ such that

$$\min_{\xi \in S_{\mathbf{m}}} h_{\mathbf{m},\mathbf{s}}(\xi) \geq 1 - C\mathrm{e}^{-\beta\delta}, \qquad \max_{\xi \in S_{\mathbf{s}}} h_{\mathbf{m},\mathbf{s}}(\xi) \leq C\mathrm{e}^{-\beta\delta},$$

$$\forall\, \beta \in (0,\infty).$$

Proof: Combine LEMMA 3.4 and LEMMA 6.1. □

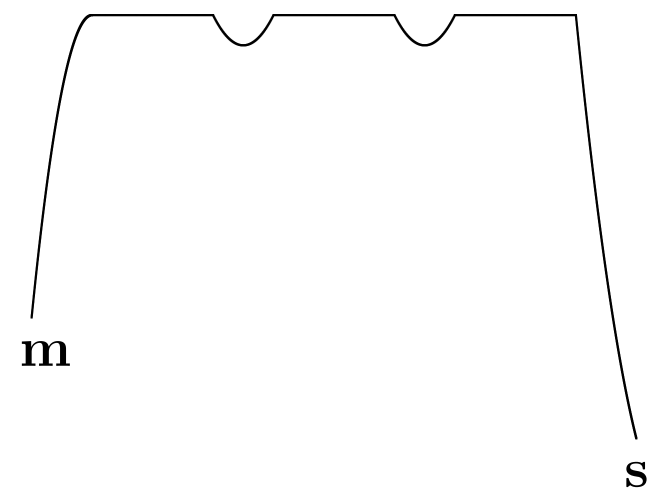
II. Because of Lemma 6.5, on the set $S_{\mathbf{m}} \cup S_{\mathbf{s}}$, $h_{\mathbf{m},\mathbf{s}}$ is trivial and its contribution to the sum in the Dirichlet form can be put into the prefactor $1 + o(1)$. Consequently, all that is needed is to understand what $h_{\mathbf{m},\mathbf{s}}$ looks like on the set

$$S^\star \backslash (S_{\mathbf{m}} \cup S_{\mathbf{s}}) = \{\xi \in S^\star \colon\ \Phi(\xi, \mathbf{m}) = \Phi(\xi, \mathbf{s}) = \Gamma^\star\}.$$

Lemma 6.6 below shows that $h_{\mathbf{m},\mathbf{s}}$ is also trivial on the set

$$S^{\star\star} \backslash (S_{\mathbf{m}} \cup S_{\mathbf{s}}) = \bigcup_{i=1}^{I} S_i,$$

which is a union of wells S_i, $i = 1, \ldots, I$, in $\mathcal{S}(\mathbf{m}, \mathbf{s})$ for some $I \in \mathbb{N}$. Each S_i is a minimal set of communicating configurations with energy $< \Gamma^\star$ and with communication height $\Gamma^\star$ towards both $\mathbf{m}$ and $\mathbf{s}$.



Schematic picture of the wells S_i, $i = 1, \ldots, I$.

LEMMA 6.6 Harmonic function flat in dead-ends

There exist $C < \infty$ *and* $\delta > 0$ *such that*

$$\max_{\xi,\xi' \in S_i} |h_{\mathbf{m},\mathbf{s}}(\xi) - h_{\mathbf{m},\mathbf{s}}(\xi')| \leq C\mathrm{e}^{-\beta\delta},$$

$$\forall\, i = 1, \ldots, I,\ \beta \in (0, \infty).$$

PROOF: Fix $i \in \{1, \ldots, I\}$ and $\xi, \xi' \in S_i$. Estimate

$$h_{\mathbf{m},\mathbf{s}}(\xi) = \mathbb{P}_\xi(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \leq \mathbb{P}_\xi(\tau_{\mathbf{m}} < \tau_{\xi'}) + \mathbb{P}_\xi(\tau_{\xi'} < \tau_{\mathbf{m}} < \tau_{\mathbf{s}}).$$

Combining Lemma 3.4 and LEMMA 6.1, we have

$$\mathbb{P}_\xi(\tau_{\mathbf{m}} < \tau_{\xi'}) \leq \frac{\mathrm{cap}_\beta(\xi, \mathbf{m})}{\mathrm{cap}_\beta(\xi, \xi')} \leq C\,\mathrm{e}^{-\beta[\Phi(\xi,\mathbf{m}) - \Phi(\xi,\xi')]} \leq C\,\mathrm{e}^{-\beta\delta},$$

where we use that $\Phi(\xi, \mathbf{m}) = \Gamma^\star$ and $\Phi(\xi, \xi') < \Gamma^\star$.

But

$$\mathbb{P}_\xi(\tau_{\xi'} < \tau_{\mathbf{m}} < \tau_{\mathbf{s}}) = \mathbb{P}_\xi(\tau_{\xi'} < \tau_{\mathbf{m}\cup\mathbf{s}})\,\mathbb{P}_{\xi'}(\tau_{\mathbf{m}} < \tau_{\mathbf{s}})$$
$$\leq \mathbb{P}_{\xi'}(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) = h_{\mathbf{m},\mathbf{s}}(\xi').$$

Combining the above estimates we get

$$h_{\mathbf{m},\mathbf{s}}(\xi) \leq C\,\mathrm{e}^{-\beta\delta} + h_{\mathbf{m},\mathbf{s}}(\xi').$$

Interchange ξ and ξ' to get the claim. □

Lemma 6.6 shows that the contribution to the Dirichlet form of the transitions inside a well can also be put into the prefactor $1 + o(1)$. Thus, only the transitions in and out of wells contribute.

III. In view of the above observations, the estimation of $Z_\beta \mathrm{cap}_\beta(\mathbf{m},\mathbf{s})$ reduces to the study of a simpler variational problem.

LEMMA 6.7 Variational formula for the prefactor

As $\beta \to \infty$,

$$Z_\beta \mathrm{cap}_\beta(\mathbf{m},\mathbf{s}) = [1+o(1)]\,\Theta\,\mathrm{e}^{-\beta\Gamma^\star}$$

with

$$\Theta = \min_{C_1\dots,C_I} \min_{\substack{h:\ S^\star\to[0,1] \\ h|_{S_\mathbf{m}}\equiv 1,\, h|_{S_\mathbf{s}}\equiv 0,\, h|_{S_i}\equiv C_i\,\forall\, i=1,\dots,I}} \frac{1}{2}\sum_{\xi,\xi'\in S^\star} 1_{\{\xi\sim\xi'\}}\,[h(\xi)-h(\xi')]^2.$$

PROOF:

Abbreviate

$$\mathcal{E}_{\beta,S}(h) = \frac{1}{2} \sum_{\xi,\xi' \in S} \mu_\beta(\xi) c_\beta(\xi,\xi') [h(\xi) - h(\xi')]^2.$$

1. Write

$$Z_\beta \, \mathrm{cap}_\beta(\mathbf{m},\mathbf{s}) = Z_\beta \min_{\substack{h:\ S \to [0,1] \\ h(\mathbf{m})=1,\, h(\mathbf{s})=0}} \mathcal{E}_{\beta,S}(h)$$

$$= O\left(\mathrm{e}^{-(\Gamma^\star+\delta)\beta}\right) + Z_\beta \min_{\substack{h:\ S^\star \to [0,1] \\ h(\mathbf{m})=1,\, h(\mathbf{s})=0}} \mathcal{E}_{\beta,S^\star}(h).$$

With the help of Lemmas 6.1, 6.3–6.5, we can write

$$
\begin{aligned}
&\min_{\substack{h:\ S^\star \to [0,1] \\ h(\mathbf{m})=1,\, h(\mathbf{s})=0}} \mathcal{E}_{\beta,S^\star}(h) \\
&= \min_{\substack{h:\ S^\star \to [0,1] \\ h=h_{\mathbf{m},\mathbf{s}} \text{ on } S_{\mathbf{m}}\cup S_{\mathbf{s}}\cup(S_1,\dots,S_I)}} \mathcal{E}_{\beta,S^\star}(h) \\
&= \min_{C_1,\dots,C_I} \\
&\qquad \min_{\substack{h:\ S^\star \to [0,1] \\ h|_{S_{\mathbf{m}}}=1-O(\mathrm{e}^{-\beta\delta}),\, h|_{S_{\mathbf{s}}}=O(\mathrm{e}^{-\beta\delta}),\, h|_{S_i}=C_i+O(\mathrm{e}^{-\beta\delta})\,\forall\, i=1,\dots,I}} \mathcal{E}_{\beta,S^\star}(h) \\
&= [1-O(\mathrm{e}^{-\delta\beta})] \min_{C_1,\dots,C_I} \\
&\qquad \min_{\substack{h:\ S^\star \to [0,1] \\ h|_{S_{\mathbf{m}}}\equiv 1,\, h|_{S_{\mathbf{s}}}\equiv 0,\, h|_{S_i}\equiv C_i\,\forall\, i=1,\dots,I}} \mathcal{E}_{\beta,S^\star}(h).
\end{aligned}
$$

where the error term $O(\mathrm{e}^{-\delta\beta})$ arises after we replace the approximate boundary conditions

$$h = \begin{cases} 1 - O(\mathrm{e}^{-\beta\delta}) & \text{on } S_{\mathbf{m}}, \\ O(\mathrm{e}^{-\beta\delta}) & \text{on } S_{\mathbf{s}}, \\ C_i + O(\mathrm{e}^{-\beta\delta}) & \text{on } S_i,\ i = 1, \ldots, I, \end{cases}$$

coming from Lemma 6.5 by the sharp boundary conditions

$$h = \begin{cases} 1 & \text{on } S_{\mathbf{m}}, \\ 0 & \text{on } S_{\mathbf{s}}, \\ C_i & \text{on } S_i,\ i = 1, \ldots, I. \end{cases}$$

2. The minimum with sharp boundary conditions serves as an upper bound for the minimum with approximate boundary conditions.

Conversely, removal from the minimum with approximate boundary conditions of all the transitions that stay inside $S_{\mathbf{m}}$, $S_{\mathbf{s}}$ or S_i for some $i = 1, \ldots, I$ yields a lower bound that is within a factor $1 - O(\mathrm{e}^{-\beta\delta})$ of the minimum with sharp boundary conditions.

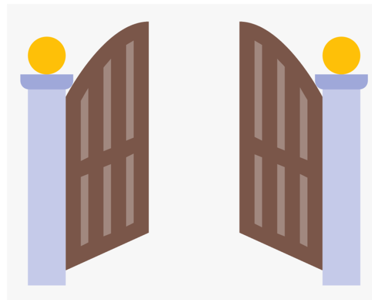
3. By the definition of $\mu_\beta(\xi)$ and $c_\beta(\xi,\xi')$, together with reversibility, we have

$$Z_\beta \mu_\beta(\xi) c_\beta(\xi,\xi') = \mathrm{e}^{-\beta[H(\xi) \vee H(\xi')]} = 1_{\{\xi \sim \xi'\}}\, \mathrm{e}^{-\beta \Gamma^\star}$$

for all $\xi,\xi' \in S^\star$ that are not both in $S_\mathbf{m}$ or both in $S_\mathbf{s}$ or both in S_i for some $i = 1,\ldots,I$. Indeed, by THEOREM 6.2 and the decomposition $S^{\star\star} \backslash (S_\mathbf{m} \cup S_\mathbf{s}) = \cup_{i=1}^I S_i$, in each of these cases either $H(\xi) = \Gamma^\star > H(\xi')$ or $H(\xi) < \Gamma^\star = H(\xi')$, because there are no allowed moves between $S_\mathbf{m}$, $S_\mathbf{s}$ and S_i, $i = 1,\ldots,I$. Combining the above observations, we arrive at the claim. □

The variational formula for $\Theta = 1/K$ is non-trivial because it depends on the wells S_i, $i = 1,\ldots,I$. In Lectures 7–8 we will see how to compute K for Glauber dynamics and Kawasaki dynamics.

▶ Gate for the crossover and uniform entrance distribution



PROOF:

(a) We will show that there exist $\delta > 0$ and $C < \infty$ such that for all β,

$$\mathbb{P}_{\mathbf{m}}\left(\tau_{\mathcal{C}^*} < \tau_{\mathbf{s}} \mid \tau_{\mathbf{s}} < \tau_{\mathbf{m}}\right) \geq 1 - C\mathrm{e}^{-\beta\delta},$$

which implies the claim. Abbreviate $c_\beta(\xi) = \sum_{\xi' \in S} c_\beta(\xi, \xi')$.

1. We have $\mathrm{cap}_\beta(\mathbf{m}, \mathbf{s}) = \mu_\beta(\mathbf{m})\, c_\beta(\mathbf{m}) \mathbb{P}_{\mathbf{m}}(\tau_{\mathbf{s}} < \tau_{\mathbf{m}})$ with $\mu_\beta(\mathbf{m}) = 1/Z_\beta$. From the lower bound in LEMMA 6.1 it therefore follows that

$$\mathbb{P}_{\mathbf{m}}(\tau_{\mathbf{s}} < \tau_{\mathbf{m}}) \geq C_1\, \mathrm{e}^{-\beta\Gamma^\star} \frac{1}{c_\beta(\mathbf{m})}.$$

We will show that

$$\mathbb{P}_{\mathbf{m}}\left(\{\tau_{\mathcal{C}^*} < \tau_{\mathbf{s}}\}^c,\, \tau_{\mathbf{s}} < \tau_{\mathbf{m}}\right) \le C_2\, \mathrm{e}^{-\beta(\Gamma^\star+\delta)}\, \frac{1}{c_\beta(\mathbf{m})}.$$

Combining, we get the claim with $C = C_2/C_1$.

2. Any path from $\mathbf{m}$ to $\mathbf{s}$ that does not pass through $\mathcal{C}^*$ must hit a configuration ξ with $H(\xi) > \Gamma^\star$. Therefore there exists a set U, with $H(\xi) \ge \Gamma^\star + \delta$ for all $\xi \in U$ and some $\delta > 0$, such that

$$\mathbb{P}_{\mathbf{m}}\left(\{\tau_{\mathcal{C}^*} < \tau_{\mathbf{s}}\}^c,\, \tau_{\mathbf{s}} < \tau_{\mathbf{m}}\right) \le \mathbb{P}_{\mathbf{m}}\left(\tau_U < \tau_{\mathbf{m}}\right).$$

Now estimate, with the help of reversibility,

$$
\begin{aligned}
\mathbb{P}_{\mathbf{m}}\left(\tau_U < \tau_{\mathbf{m}}\right) &\leq \sum_{\xi \in U} \mathbb{P}_{\mathbf{m}}\left(\tau_\xi < \tau_{\mathbf{m}}\right) \\
&= \sum_{\xi \in U} \frac{\mu_\beta(\xi) c_\beta(\xi)}{\mu_\beta(\mathbf{m}) c_\beta(\mathbf{m})} \mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_\xi\right) \\
&\leq \frac{1}{c_\beta(\mathbf{m})} \sum_{\xi \in U} |\{\xi' \in S \backslash \xi \colon\ \xi \sim \xi'\}| \, \mathrm{e}^{-\beta H(\xi)} \\
&\leq \frac{1}{c_\beta(\mathbf{m})} C_2 \, \mathrm{e}^{-\beta(\Gamma^\star + \delta)}
\end{aligned}
$$

with $C_2 = |\{(\xi, \xi') \in U \times S \backslash \xi \colon\ \xi \sim \xi'\}|$, where we use that $H(\mathbf{m}) = 0$ and $c_\beta(\xi, \xi') \leq 1$. Combine to get the claim.

(b) For $\xi \in \mathcal{C}^*$, write

$$\mathbb{P}_{\mathbf{m}}\left(\xi_{\tau_{\mathcal{C}^*}} = \xi \mid \tau_{\mathcal{C}^*} < \tau_{\mathbf{m}}\right) = \frac{\mathbb{P}_{\mathbf{m}}(\xi_{\tau_{\mathcal{C}^*}} = \xi,\, \tau_{\mathcal{C}^*} < \tau_{\mathbf{m}})}{\mathbb{P}_{\mathbf{m}}(\tau_{\mathcal{C}^*} < \tau_{\mathbf{m}})}.$$

1. By reversibility,

$$\begin{aligned}\mathbb{P}_{\mathbf{m}}\left(\xi_{\tau_{\mathcal{C}^*}} = \xi,\, \tau_{\mathcal{C}^*} < \tau_{\mathbf{m}}\right) &= \frac{\mu_\beta(\xi)c_\beta(\xi)}{\mu_\beta(\mathbf{m})c_\beta(\mathbf{m})}\,\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right)\\ &= \mathrm{e}^{-\Gamma^\star\beta}\,\frac{c_\beta(\xi)}{c_\beta(\mathbf{m})}\,\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right).\end{aligned}$$

Moreover,

$$\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right) = \sum_{\substack{\xi' \in S\setminus\mathcal{C}^* \\ \xi \sim \xi'}} \frac{c_\beta(\xi,\xi')}{c_\beta(\xi)}\, h_{\mathbf{m},\mathcal{C}^*}(\xi'),$$

where

$$h_{\mathbf{m},\mathcal{C}^*}(\xi') = \begin{cases} 0 & \text{if } \xi' \in \mathcal{C}^*,\\ 1 & \text{if } \xi' = \mathbf{m},\\ \mathbb{P}_{\xi'}(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}) & \text{otherwise.}\end{cases}$$

2. Because $\mathcal{P}^* \subseteq S_{\mathbf{m}}$, we have

$$\Phi(\xi', \mathcal{C}^*) - \Phi(\xi', \mathbf{m}) = \Gamma^\star - \Phi(\xi', \mathbf{m}) \geq \delta$$

for all $\xi' \in \mathcal{P}^*$ and some $\delta > 0$. Therefore, as in the proof of Lemma 3.4, it follows that

$$\min_{\xi' \in \mathcal{P}^*} h_{\mathbf{m},\mathcal{C}^*}(\xi') \geq 1 - C\mathrm{e}^{-\beta\delta}.$$

3. Let

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

By Lemma 5.10, any path from $\bar{\mathcal{C}}^*$ to $\mathbf{m}$ that avoids $\mathcal{C}^*$ must reach an energy level above $\Gamma^\star$, and so $h_{\mathbf{m},\mathcal{C}^*}(\xi') \leq h_{S\backslash S^\star,\mathcal{C}^*}(\xi')$ for all $\xi' \in \bar{\mathcal{C}}^*$. But $\Phi(\xi', S\backslash S^\star) - \Phi(\xi', \mathcal{C}^*) = \Phi(\xi', S\backslash S^\star) - \Gamma^\star \geq \delta$ for all $\xi' \in \bar{\mathcal{C}}^* \cap S^\star$ and some $\delta > 0$. Therefore, again as in the proof of LEMMA 3.4, it follows that

$$\max_{\xi' \in \bar{\mathcal{C}}^* \cap S^\star} h_{\mathbf{m},\mathcal{C}^*}(\xi') \leq C\mathrm{e}^{-\beta\delta}.$$

4. The above estimates can be used as follows. By restricting the sum over $\xi' \in S \backslash \mathcal{C}^*$ to $\xi' \in \mathcal{P}^*$ and using the lower boud in item 2, we get the lower bound

$$\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right) \geq \left(1 - C\mathrm{e}^{-\beta\delta}\right) \frac{c_\beta(\xi, \mathcal{P}^*)}{c_\beta(\xi)}, \qquad \xi \in \mathcal{C}^*.$$

On the other hand, by using the upper bound in item 3 in combination with the fact that $c_\beta(\xi, S\backslash(\mathcal{C}^* \cup \bar{\mathcal{C}}^*)) = c_\beta(\xi, \mathcal{P}^*)$ for all $\xi \in \mathcal{C}^*$, and $c_\beta(\xi, \xi') \leq \mathrm{e}^{-\beta\delta}$ for all $\xi \in \mathcal{C}^*$ and $\xi' \in S \backslash S^\star$, we get the upper bound

$$\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right) \leq \frac{c_\beta(\xi, \mathcal{P}^*)}{c_\beta(\xi)} + C\mathrm{e}^{-\beta\delta}|\bar{\mathcal{C}}^*| + \mathrm{e}^{-\beta\delta}|S \backslash S^\star|, \quad \xi \in \mathcal{C}^*.$$

5. Because $H(\xi') < H(\xi) = \Gamma^\star$ for all $\xi \in \mathcal{C}^*$ and $\xi' \in \mathcal{P}^*$,

$$c_\beta(\xi, \mathcal{P}^*) = \sum_{\xi' \in \mathcal{P}^*} c_\beta(\xi, \xi') = |\{\xi' \in \mathcal{P}^* \colon \xi \sim \xi'\}|, \qquad \xi \in \mathcal{C}^*,$$

and, since $c_\beta(\xi) \leq |S|$, it follows that $c_\beta(\xi, \mathcal{P}^*)/c_\beta(\xi) \geq C$ with $C > 0$. Combine this observation with the upper and lower bounds on $\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right)$ derived above, to get

$$\mathbb{P}_\xi\left(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*}\right) = \left[1 + O(\mathrm{e}^{-\beta\delta})\right] \frac{c_\beta(\xi, \mathcal{P}^*)}{c_\beta(\xi)}, \qquad \xi \in \mathcal{C}^*.$$

Combine this in turn with the formulas derived earlier for $\mathbb{P}_{\mathbf{m}}(\xi_{\tau_{\mathcal{C}^*}} = \xi \mid \tau_{\mathcal{C}^*} < \tau_{\mathbf{m}})$, to arrive at

$$\mathbb{P}_{\mathbf{m}}\left(\xi_{\tau_{\mathcal{C}^*}} = \xi \mid \tau_{\mathcal{C}^*} < \tau_{\mathbf{m}}\right) = \frac{c_\beta(\xi)\,\mathbb{P}_\xi(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*})}{\sum_{\xi' \in \mathcal{C}^*} c_\beta(\xi')\,\mathbb{P}_{\xi'}(\tau_{\mathbf{m}} < \tau_{\mathcal{C}^*})}$$

$$= \left[1 + O(\mathrm{e}^{-\beta\delta})\right] \frac{c_\beta(\xi, \mathcal{P}^*)}{\sum_{\xi' \in \mathcal{C}^*} c_\beta(\xi', \mathcal{P}^*)}, \ \xi \in \mathcal{C}^*.$$

6. Finally, by (H2) and the formula for $c_\beta(\xi, \mathcal{P}^*)$, $\xi \mapsto c_\beta(\xi, \mathcal{P}^*)$ is constant on $\mathcal{C}^*$. Together with the last display, this proves the claim about the gate. $\square$

LITERATURE:

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