Metastability

Lectures given at the 5th Prague Summer School on Mathematical Statistical Physics, 2006

Anton Bovier

Weierstraß-Institut für Angewandte Analysis und Stochastik
Mohrenstraße 39
10117 Berlin, Germany

Institut für Mathematik
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin, Germany

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Introduction.

In these lectures we will discuss Markov processes with a particular interest for a phenomenon called *metastability*. Basically this refers to the existence of two or more time-scales over which the system shows very different behaviour: on the short time scale, the systems reaches quickly a "pseudo-equilibrium" and remains effectively in a restricted subset of the available phase space; the particular pseudo-equilibrium that is reached will depend on the initial conditions. However, when observed on the longer time scale, one will occasionally observe *transitions* from one such pseudo-equilibrium to another one. In many cases (as we will see) there exists one particular time scale for each such pseudo-equilibrium; in other cases of interest, several, or even many, such distinct pseudo-equilibria exist having the same time scale of exit. Mathematically speaking, our interest is to derive the (statistical) properties of the process on these long time scales from the given description of the process on the microscopic time scale. In principle, our aim should be an effective model for the motion at the long time scale on a coarse grained state space; in fact, disregarding fast motion leads us naturally to consider a reduced state space that may be labelled in some way by the quasi equilibria.

The type of situation we sketched above occurs in many situations in nature. The classical example is of course the phenomenon of metastability in *phase transitions*: if a (sufficiently pure) container of water is cooled below freezing temperature, it may remain in the liquid state for a rather long period of time, but at some moment the entire container freezes extremely rapidly. In reality, this moment is of course mostly triggered by some slight external perturbation. Another example of the same phenomenon occurs in the dynamics of large bio-molecules, such as proteins. Such molecules frequently have several possible spatial *conformations*, transitions between which occur sporadically on often very long time scales. Another classical example is metastability in chemical reactions. Here reactants oscillate between several possible chemical compositions, sometimes nicely distin-

guished by different colours. This example was instrumental in the development of stochastic models for metastability by Eyring, Kramers and others [17, 26]. Today, metastable effects are invoked to explain a variety of diverse phenomena such as changes in global climate systems both on earth (ice-ages) and on Mars (liquid water presence), structural transitions on eco- and oeco systems, to name just a few examples.

Most modelling approaches attribute metastability to the presence of some sort of randomness in the underlying dynamics. Indeed, in the context of purely deterministic systems, once several equilibrium positions for the dynamics exist, transitions between such equilibria are impossible. It is then thought that metastable effects occur due to the presence of (small) random perturbations that should reflect the influence of unresolved degrees of freedom on very fast scales.

Mathematically, metastability is studied in a number of contexts of which we mention the following:

(i) **Small random perturbations of dynamical systems.** Here one considers a classical dynamical system in $\mathbb{R}^d$ with some added small stochastic noise term. This leads to a stochastic differential equation of the type

$$dx_\epsilon(t) = f_\epsilon(x_\epsilon(t))dt + \sqrt{e}g_\epsilon(x_\epsilon(t))dW(t) \tag{1.1}$$

Such systems have been extensively investigated e.g. in the work of Freidlin and Wentzell [19] and Kifer [24]. They have their origin in the work of Kramers [26].

(ii) **Markov chains with exponentially small transition rates.** Here we are dealing with Markov chains with discrete state space that are almost deterministic in the sense that the transition probabilities are either exponentially close to one or exponentially close to zero, in some small parameter ϵ. Such systems emerge in the analysis of Wentzell and Freidlin and are studied there. They found renewed interest in the context of low temperature dynamics for lattice models in statistical mechanics [31, 32, 1] and also in the analysis of stochastic algorithms for the solution of optimisation problems ("simulated annealing") [11, 10]. Recent result using the methods outlined here can be found in [6, 3].

(iii) **Glauber dynamics of mean field [9, 28, 18, 4] or lattice [33] spin systems**. Metastability in stochastic dynamics of spin systems is not restricted to the zero temperature limit, but happens whenever there is a first order phases transition. At finite temperature, this is much harder to analyse in general. The reason is that it is no longer true that the process on the micro-scale is close to deterministic, but that such a statement may at best be meaningful on a coarse grained scale. Mean field models lend themselves to such a course graining in a particularly nice way, and in many cases it is possible to construct an effective coarse grained Markovian dynamics that then is in some sense similar to the problems mentioned in (i).

The traditional methods to analyse such systems are

(a) **Large deviations.** Wentzell and Freidlin introduced the method of large deviations on path space in order to obtain a rigorous analysis of the probability for the deviations of solutions of the stochastic differential equations (1.1) from the solutions of the deterministic limiting equations. This method has proven very robust and has been adapted to all of the other contexts. The price to pay for generality is limited precision. In general, only the exponential rates of probabilities can be computed precisely. Frequently this is good enough in applications, but sometimes more precise results are desirable. In certain cases, refined estimates could, however, be obtained [16].

(b) **Asymptotic perturbation theory.** As we will see in detail in the course of these lectures, many key quantities of interest concerning Markov processes can be characterized as solutions of certain systems of linear equations, that are or are structurally similar to boundary value problems in partial differential equations. In particular cases of stochastic differential equations with small noise, or discrete versions whereof, one may use methods from perturbation theory of linear differential operators with the variance of the noise playing the rôle of a small parameter. This has been used widely in the physics literature on the subject (see e.g. the book by Kolokoltsov [25] for detailed discussions and further reference), however, due to certain analytic difficulties, with the exception of some very particular cases, a rigorous justification of these methods was not given. A further shortcoming of the method is that it depends heavily on the particular types of Markov processes studied and does not seem to be universally applicable. Very recently, Helffer, Nier and Klein have been able to develop a new analytic approach that allows to develop rigorous asymptotic expansion for the small eigenvalues for diffusion processes [22, 21, 30].

(c) **Spectral and variational methods.** Very early on it was noted that there should be a clear signature of metastability in the nature of the generator (or transition matrix) of the Markov process considered. To see this, note that if the Markov process was effectively reducible, i.e. had in stead of quasi invariant sets there were truly invariant sets, then the generator would have a degenerate eigenvalue zero with multiplicity equal to the number of invariant sets. Moreover, the eigenfunctions could be chosen as the indicator functions of these sets. It is natural to believe that a perturbed version of this picture remains true in the metastable setting. The computation of small eigenvalues and "spectral gaps" has thus be a frequent theme in the subject. Computations of eigenvalues can be done using variational representations of eigenvalues, and a number of rather precise results could be achieved in this way, e.g. in the work of Mathieu [27] and Miclo [29].

In these lectures I will explain an approach to metastability that is in some sense mixing ideas from (ii) and (iii) and that proves to be applicable in a wide variety of situations. One of its goals is to obtain a precise characterization of metastability in terms of spectral characteristics, and in particular a quantitatively precise relation between eigenvalues and physical quantities such as exit times from metastable domains. The main novel idea in this approach, that was developed in collaboration with M. Eckhoff, V. Gayrard, and M. Klein over the last years, is the systematic use of the so called "Newtonian capacity", a fundamental object in potential theory, and its variational representation. This will allow us to get in a rigorous way results that are almost as precise as those obtained from perturbation theory in a rather general context. In particular, we will see that certain structural relations between capacities, exit times and spectral characteristics hold without further model assumptions under some reasonable assumptions on what is to be understood by the notion of metastability.

2

Basic notions from the theory of Markov processes

A stochastic process $\{X_t\}_{t\in I}$, $X_t \in \Gamma$ is called a Markov process with *index set* I and *state space* Γ, if, for any collection $t_1 < \cdots < t_n < t \in I$,

$$\mathbb{P}\left[X_t \in \mathcal{A} | X_{t_n} = x_n, \ldots, X_{t_1} = x_1\right] = \mathbb{P}\left[X_t \in \mathcal{A} | X_{t_n} = x_n\right] \tag{2.1}$$

for any Borel set $\mathcal{A} \in \mathcal{B}(\Gamma)$. Here I is always an ordered set, in fact either $\mathbb{N}$ or $\mathbb{R}$. In the former case we call call the process a discrete time Markov chain, the second case is referred to as a continuous time Markov process. A further distinction concerns the nature of the state space Γ. This may be finite, countable, or uncountable ('continuous') .

A key quantity in all cases is the family of probability measures, $p(s,t,x,\cdot)$, on $(\Gamma, \mathcal{B}(\Gamma))$,

$$p(s,t,x,\mathcal{A}) \equiv \mathbb{P}\left(X_t \in \mathcal{A} | X_s = x\right), \tag{2.2}$$

for any Borel set $\mathcal{A} \in \mathcal{B}(\Gamma)$. By (2.1), $p(t,s,,x,y)$ determines uniquely the law of the Markov process. In fact, any family of probability measures $p(s,t,x,dy)$ satisfying

$$p(s,s,x,\cdot) = \delta_x(\cdot) \tag{2.3}$$

and the relation for $s < t' < t$,

$$p(s,t,x,\cdot) = \int p(s,t',x,dz) p(t',t,z,\cdot) \tag{2.4}$$

defines a Markov process. If $p(s,t,dx,y)$ is a function of $t-s$ only, we call the Markov process *time-homogeneous* and set

$$p(s,t,x,\cdot) \equiv p_{t-s}(x,\cdot) \tag{2.5}$$

We will only be concerned with time-homogeneous Markov processes henceforth. In the case of discrete time the transition kernel is fully determined by the one-step transition probabilities, called transition matrix in the discrete space case,

$$p(x,\cdot) \equiv p_1(x,\cdot) \tag{2.6}$$

If space is discrete, we can of course simply specify the atoms, $p(x, y)$, of this measure; this object is then called the *transition matrix*.

Property (2.4) is often called the *semi-group* property and the transition kernel $p_t(x, \cdot)$ is called a *Markov semi-group*. In continuous time, one defines the *generator* (of the semi-group)[1]

$$L \equiv \lim_{t \downarrow 0} t^{-1}(1 - p_t) \tag{2.7}$$

It then follows that conversely

$$p_t = e^{-tL} \tag{2.8}$$

We will find it sometimes convenient to define a "generator" also in the discrete time case by setting

$$L \equiv 1 - p_1 \tag{2.9}$$

We will frequently think of p_t and L as operators acting on functions f on Γ as

$$p_t f(x) \equiv \int_\Gamma p_t(x, dy) f(y) \tag{2.10}$$

respectively on measures ρ on Γ, via

$$\rho p_t(\cdot) \equiv \int_\Gamma \rho(dx) p_t(x, \cdot) \tag{2.11}$$

If $\rho_0(\cdot) = \mathbb{P}(X_0 \in \cdot)$, then

$$\rho_0 p_t(\cdot) \equiv \rho_t(\cdot) = \mathbb{P}(X_t \in \cdot) \tag{2.12}$$

ρ_t is called the law of the process at time t started in ρ at time 0. It is easy to see from the semi-group property that ρ_t satisfies the equation

$$\frac{\partial}{\partial t} \rho_t(x, \cdot) = -\rho_t L(x, \cdot) \tag{2.13}$$

resp., in the discrete time case

$$\rho_{t+1}(x, \cdot) = -\rho_t L(x, \cdot) \tag{2.14}$$

This equation is called the *Focker-Planck* equation. A probability measure μ on Γ is called an *invariant measure* for the Markov process X_t if it is a stationary solution of (2.13), i.e. if

$$\mu p_t = \mu \tag{2.15}$$

for all $t \in I$. Note that (2.15) is equivalent to demanding that

$$\mu L = 0 \tag{2.16}$$

A priori the natural function space for the action of our operators is $L_\infty(\Gamma)$ for the action from the left, and locally finite measures for the action on the right.

[1] In the literature, one often defines the generator with an extra minus sign. I prefer to work with positive operators.

Given an invariant measure μ, there is, however, also a natural extension to the space $L_2(\Gamma, \mu)$. In fact, p_t is a *contraction* on this space, and L is a positive operator. To see this, just use the Schwartz inequality to show that

$$\int \mu(dx) \left(\int p_t(x, dy) f(y) \right)^2 \leq \mu(dx) \int p_t(x, dy) f(y)^2 = \int \mu(dy) f(y)^2 \tag{2.17}$$

L is in general not a bounded operator in L_2, and its domain is sometimes just a dense subspaces.

Within this L_2-theory, it is natural to define the adjoint operators p_t^* and L^* via

$$\int \mu(dx) g(x) p_t^* f(x) \equiv \int \mu(dx) f(x) p_t^* g(x) \tag{2.18}$$

respectively

$$\int \mu(dx) g(x) L^* f(x) \equiv \int \mu(dx) f(x) L g(x) \tag{2.19}$$

for any pair of functions $f, g \in L_2(\Gamma, \mu)$. We leave it as an exercise to show that p_t^* and L^* are Markov semi-groups, resp. generators, whenever μ is an invariant measure. Thus they define an *adjoint* or reverse process. In the course of these lectures we will mainly be concerned with the situation where p_t and L are *self-adjoint*, i.e. when $p_t = p_t^*$ and $L = L^*$. This will entrain a number of substantial simplifications. Results on the general case can often be obtained by comparison with symmetrized processes, e.g. the process generated by $(L + L^*)/2$. Note that whenever a Markov generator is self-adjoint with respect to a measure μ, then this measure is invariant (Exercise!). We call Markov processes whose generator is self-adjoint with respect to some probability measure *reversible*. The invariant measure is then often called the *reversible measure* (although I find this expression abusive; symmetrizing measure would be more appropriate).

Working with reversible Markov chains brings the advantage to make full use of the theory of self-adjoint operators, which gives far richer results then in the general case. In many applications one can work by choice with reversible Markov processes, so that in practical terms this restriction is not too dramatic.

Hitting times Henceforth we denote by $\mathbb{P}_x$ the law of the process conditioned on $X_0 = x$. For any (measurable) set $D \subset \Gamma$ we define the hitting time τ_D as

$$\tau_D \equiv \inf (t > 0 : X_t \in D) \tag{2.20}$$

Note that τ_D is a *stopping time*, i.e. the random variable τ_D depends only on the behaviour of X_t for $t \leq \tau_D$. Denoting by $\mathcal{F}_t$ sigma-algebra generated by $\{X_s\}_{0 \leq s \leq t}$, we may say that the event $\{\tau_D \leq t\}$ is measurable with respect to $\mathcal{F}_t$.

3

Discrete space, discrete time Markov chains

We will now turn to our main tools for the analysis of metastable systems. To avoid technical complications and to focus on the key ideas, we will first consider only the case of discrete (or even finite) state space and discrete time (the latter is no restriction). We set $p_1(x, y) = p(x, y)$. We will also assume that our Markov chain is irreducible, i.e. that for any $x, y \in \Gamma$, there is $t \in \mathbb{N}$ such that $p_t(x, y) > 0$. If in addition Γ is finite, this implies the existence of a unique invariant (probability) measure μ. We will also assume the our Markov chain is reversible.

3.1 Equilibrium potential, equilibrium measure, and capacity

Given two disjoint subsets A, D, of Γ, and $x \in \Gamma$, we are interested in

$$\mathbb{P}_x[\tau_A < \tau_D] \tag{3.1}$$

One of our first, and as we will see main tasks is to compute such probabilities. We consider first the case of discrete time and space.

If $x \notin A \cup D$, we make the elementary observation that the first step away leads either to D, and the event $\{\tau_A < \tau_D\}$ fails to happen, or to A, in which case the event happens, or to another point $y \notin A \cup D$, in which case the event happens with probability $\mathbb{P}_y[\tau_A < \tau_D]$. Thus

$$\mathbb{P}_x[\tau_A < \tau_D] = \sum_{y \in A} p(x, y) + \sum_{y \notin A \cup D} p(x, y) \mathbb{P}_y[\tau_A < \tau_D] \tag{3.2}$$

We call an equation based on this reasoning a *forward* equation. Note that we can write this in a nicer form if we introduce the function

$$h_{A,D}(x) = \begin{cases} \mathbb{P}_x[\tau_A < \tau_D], & \text{if } x \notin A \cup D \\ 1, & \text{if } x \in A \\ 0, & \text{if } x \in D \end{cases} \tag{3.3}$$

Then (3.2) implies that for $x \notin A \cup D$,

$$h_{A,D}(x) = \sum_{y \in \Gamma} p(x,y) h_{A,D}(y) \tag{3.4}$$

In other words, the function $h_{A,D}$ solves the *boundary value problem*

$$\begin{aligned} Lh_{A,D}(x) &= 0, \quad x \in \Gamma \backslash (A \cup D), \\ h_{A,D}(x) &= 1, \quad x \in A, \\ h_{A,D}(x) &= 0, \quad x \in D. \end{aligned} \tag{3.5}$$

If we can show that the problem (3.4) has a *unique* solution, then we can be sure to have reduced the problem of computing probabilities $\mathbb{P}_x[\tau_A < \tau_D]$ to a problem of linear algebra.

Proposition 3.1.1 *If Γ is a finite set, and A, D are not empty. Assume that for any $x, y \in \Gamma$, there exists $n < \infty$ such that $p_n(x,y) > 0$. then the problem (3.4) has a unique solution.*

The function $h_{A,D}$ is called the *equilibrium potential* of the *capacitor* A, B. The fact that

$$\mathbb{P}_x[\tau_A < \tau_D] = h_{A,D}(x) \tag{3.6}$$

for $x \in \Gamma \backslash (A \cup D)$ is the first fundamental relation between the theory of Markov chains and *potential theory*.

The next question is what happens for $x \in D$? Naturally, using the same reasoning as the one leading to (3.2), we obtain that

$$\mathbb{P}_x[\tau_A < \tau_D] = \sum_{y \in A} p(x,y) + \sum_{y \in \Gamma \backslash (A \cup D)} p(x,y) \mathbb{P}_y[\tau_A < \tau_D] = \sum_{y \in \Gamma} p(x,y) h_{A,D}(y) \tag{3.7}$$

It will be even more convenient to define, for all $x \in \Gamma$

$$e_{A,D}(x) \equiv -(Lh_{A,D})(x) \tag{3.8}$$

Then

$$\mathbb{P}_x[\tau_A < \tau_D] = \begin{cases} h_{A,D}(x), & \text{if } x \in \Gamma \backslash (A \cup D) \\ e_{A,D}(x), & \text{if } x \in D \\ 1 - e_{D,A}(x) & \text{if } x \in A \end{cases} \tag{3.9}$$

Let us now define the *capacity* of the capacitor A, D as

$$\mathrm{cap}(A, D) \equiv \sum_{x \in D} \mu(x) e_{A,D}(x) \tag{3.10}$$

By the properties of $h_{A,D}$ it is easy to see that we can write

$$\sum_{x\in D}\mu(x)e_{A,D}(x) = \sum_{x\in\Gamma}\mu(x)(1-h_{A,D}(x))(-Lh_{A,,D})(x) \tag{3.11}$$
$$= \sum_{x\in\Gamma}\mu(x)h_{A,D}(x)(Lh_{A,,D})(x) - \sum_{x\in\Gamma}\mu(x)Lh_{A,,D})(x)$$

Since $\mu(x)L = 0$, we get that

$$\mathrm{cap}(A,D) = \sum_{x\in\Gamma}\mu(x)h_{A,D}(x)(Lh_{A,,D})(x) \equiv \Phi(h_{A,D}) \tag{3.12}$$

where

$$\Phi(h) \equiv \sum_{x\in\Gamma}\mu(x)h(x)Lh(x) = \frac{1}{2}\sum_{x,y}\mu(x)p(x,y)\left(h(x)-h(y)\right)^2 \tag{3.13}$$

is called the *Dirichlet form* associated to the Markov process with generator L. In fact, we will sometimes think of the Dirichlet form as the quadratic form associated to the generator and write

$$\Phi(f,g) \equiv (f,Lg)_\mu = \frac{1}{2}\sum_{x,y}\mu(x)p(x,y)\left(f(x)-f(y)\right)\left(g(x)-g(y)\right). \tag{3.14}$$

The representation of the capacity in terms of the Dirichlet form will turn out to be of fundamental importance. The reason for this is the ensuing variational representation, known as the *Dirichlet principle:*

Theorem 3.1.2 *Let $\mathcal{H}_D^A$ denote the space of functions*

$$\mathcal{H}_D^A \equiv (h:\Gamma\to[0,1], h(x)=1, x\in A, h(x)=0, x\in D) \tag{3.15}$$

Then

$$\mathrm{cap}(A,D) = \inf_{h\in\mathcal{H}_D^A}\Phi(h) \tag{3.16}$$

Moreover, the variational problem (3.15) has a unique minimizer that is given by the equilibrium potential $h_{A,D}$.

Proof Differentiating $\Phi(h)$ with respect to $h(x)$ (for $x\in\Gamma\backslash(A\cup D)$) yields

$$\frac{\partial}{\partial h(x)}\Phi(h) = 2\mu(x)Lh(x) \tag{3.17}$$

Thus if h minimizes Φ, it must be true that $Lh(x)=0$. Since we have already seen that the Dirichlet problem (3.3) has a unique solution, the theorem is proven. □

While in general the capacity is a weighted sum over certain probabilities, if we choose for the set D just a point $x\in\Gamma$, we get that

$$\mathbb{P}_x[\tau_A<\tau_x] = \frac{1}{\mu(x)}\mathrm{cap}(A,x)$$

We will call these quantities sometimes *escape probabilities*. We see that they have, by virtue of Theorem 3.1.2 a direct variational representation. They play a crucial rôle in what will follow. Let us note the fact that $\mathrm{cap}(x,y) = \mathrm{cap}(y,x)$ implies that

$$\mu(x)\mathbb{P}_x[\tau_y < \tau_x] = \mu(y)\mathbb{P}_y[\tau_x < \tau_y] \tag{3.18}$$

which is sometimes helpful to get intuition. Note that this implies in particular that

$$\mathbb{P}_x[\tau_y < \tau_x] \leq \frac{\mu(y)}{\mu(x)}$$

which is quite often already a useful bound (provided of course $\mu(y) < \mu(x)$).

3.2 The one-dimensional chain

We will now consider the example of a one-dimensional nearest neighbor random walk (with inhomogeneous rates). For reasons that will become clear later, we introduce a parameter $\epsilon > 0$ and think of our state space as a one-dimensional "lattice" of spacing ϵ, that is we take $\Gamma \subset \epsilon\mathbb{Z}$, and transition probabilities

$$p(x,y) = \begin{cases} \sqrt{\frac{\mu(y)}{\mu(x)}}g(x,y), & \text{if } y = x \pm \epsilon, \\ 1 - p(x,x+\epsilon) - p(x,x-\epsilon), & \text{if } x = y, \\ 0, & \text{else} \end{cases} \tag{3.19}$$

where $\mu(x) > 0$, and g is such that $p(x,x) \geq 0$.

Equilibrium potential. Due to the one-dimensional nature of our process, we only equilibrium potentials we have to compute are of the form

$$h_{b,a}(x) = \mathbb{P}_x[\tau_b < \tau_a] \tag{3.20}$$

where $a < x < b$. The equations (3.5) then reduce to the one-dimensional discrete boundary value problem

$$\begin{aligned} p(x,x+\epsilon)(h(x+\epsilon) - h(x)) + p(x,x-\epsilon)(h(x-\epsilon) - h(x)) &= 0, \quad a < x < b \\ h(a) &= 0 \\ h(b) &= 1 \end{aligned} \tag{3.21}$$

We can solve this by recursion and get

$$h(x) = \frac{\sum_{y=a+\epsilon}^{x} \frac{1}{\mu(y)} \frac{1}{p(y,y-\epsilon)}}{\sum_{y=a+\epsilon}^{b} \frac{1}{\mu(y)} \frac{1}{p(y,y-\epsilon)}} \tag{3.22}$$

Capacities. Given the explicit formula for the equilibrium potential, we can readily compute capacities. Without going into the detailed computations, I just quote the result:

$$\mathrm{cap}(a,b) = \frac{1}{\sum_{y=a+\epsilon}^{b} \frac{1}{\mu(y)} \frac{1}{p(y,y-\epsilon)}} \tag{3.23}$$

Remark 3.2.1 Formula (3.23) suggests another common "electrostatic" interpretation of capacities, namely as "resistances". In fact, if we interpret $\mu(x)p(x,x-\epsilon) = \mu(x-\epsilon)p(x-\epsilon,x)$ as the conductance of the "link" (resistor) $(x-\epsilon,x)$, then by Ohm's law, formula (3.23) represents the conductance of the chain of resistors from a to b. This interpretation is not restricted to the one-dimensional chain, but holds in general for reversible Markov chains. The capacity of the capacitor (A,D) may then be seen as the conductance of the resistor network between the two sets. In this context, the monotonicity properties of the capacities obtain a very natural interpretation: removing a resistor or reducing its conductivity can only decrease the conductivity of the network. There is a very nice account on the resistor network interpretation of Markov chains and some of its applications in a book by Doyle and Snell

3.3 Mean hitting times

Our next task is to derive formulas for the mean values of hitting times τ_A. As in Section 3.1 we first derive a forward equation for $\mathbb{E}_x\tau_A$ by considering what can happen in the first step:

$$\mathbb{E}_x\tau_A = \sum_{y\in A} p(x,y) + \sum_{y\not\in A} p(x,y)(1+\mathbb{E}_y\tau_A) \tag{3.24}$$

if $x \notin A$. If we define a function

$$w_A(x) \equiv \begin{cases} \mathbb{E}_x\tau_A, & \text{if } x \in \Gamma\backslash A \\ 0, & \text{if } x \in A \end{cases} \tag{3.25}$$

we see that (3.24) can be written in the nicer form

$$w_A(x) = \sum_{y\in\Gamma} p(x,y) w_A(y) + 1 \tag{3.26}$$

for $x \notin A$; i.e. w_A solves the *inhomogeneous Dirichlet problem*

$$\begin{aligned} Lw_A(x) &= 1, \quad x \in G\backslash A \\ w_A(x) &= 0, \quad x \in A \end{aligned} \tag{3.27}$$

Note that for $x \in A$ we can compute $\mathbb{E}_x\tau_A$ by considering the first step:

$$\mathbb{E}_x\tau_A = \sum_{y\in A} p(x,y) + \sum_{y\not\in A} p(x,y)(1+\mathbb{E}_y\tau_A) \tag{3.28}$$

or in compact form

$$\mathbb{E}_x \tau_A = Pw_A(x) + 1 = -Lw_A(x) + 1 \tag{3.29}$$

Equations (3.27) is a special cases of the general Dirichlet problem

$$\begin{aligned} Lf(x) &= g(x), \quad x \in \Gamma \backslash B \\ f(x) &= 0 \end{aligned} \tag{3.30}$$

for some set B and some function f. We have seen in Proposition 3.1.1 that the homogeneous boundary value problem (i.e. if $g \equiv 0$) has the unique solution $f(x) \equiv 0$. This implies that the problem (3.30) has a unique solution that can (by linearity) be represented in the form

$$f(x) = \sum_{y \in \Gamma \backslash B} G_{\Gamma \backslash B}(x, y) g(y) \tag{3.31}$$

Of course, $G_{\Gamma \backslash B}$ is simply the matrix inverse of the matrix $L^{\Gamma \backslash B}$ whose elements are

$$\begin{aligned} L^{\Gamma \backslash B}(x, y) &= L(x, y), \quad x, y \in \Gamma \backslash B \\ L^{\Gamma \backslash B}(x, y) &= 0, \quad x \in B \vee y \in B \end{aligned} \tag{3.32}$$

We will call $L^{\Gamma \backslash B}$ the Dirichlet operator on $\Gamma \backslash B$. Note that while L is a positive operator, due to Proposition 3.1.1, $L^{\Gamma \backslash B}$ is *strictly positive* whenever $B \not\emptyset$. The inverse operator $G_{\Gamma \backslash B}(x, y)$ is usually called the *Green's function*.

We see that we would really like to compute this Green's function. What we will actually show now is that the Green's function can be computed in terms of equilibrium potentials and equilibrium measures. To see this, let us return to (3.8) and interpret this as an equation for $h_{D,A}$ where the boundary conditions are only prescribed on A but not on D: Note first that since $h_{A,D}(x) = 1 - h_{D,A}(x)$, (3.8) can also be written as

$$e_{A,D}(x) = Lh_{D,A}(x) \tag{3.33}$$

This can be rewritten as

$$\begin{aligned} Lh_{D,A}(x) &= 0, \quad x \in \Gamma \backslash (A \cup D) \\ Lh_{D,A}(x) &= e_{A,D}(x), \quad x \in D \\ h_{D,A}(x) &= 0, \quad x \in A \end{aligned} \tag{3.34}$$

Thus we can write

$$h_{D,A}(x) = \sum_{y \in D} G_{\Gamma \backslash A}(x, y) e_{A,D}(y) \tag{3.35}$$

Now consider a solution of the Dirichlet problem (3.30). Multiplying $f(x)$ by $\mu(x) e_{B,x}(x)$, for $x \in \Gamma \backslash B$, and then using the representation (3.31) we get

$$f(x)\mu(x)e_{B,x}(x) = \sum_{y\in\Gamma\setminus B} G_{\Gamma\setminus B}(x,y)g(y)\mu(x)e_{B,x}(x) \tag{3.36}$$

Now due to the symmetry of L,

$$G_{\Gamma\setminus B}(x,y)\mu(x) = G_{\Gamma\setminus B}(y,x)\mu(y) \tag{3.37}$$

Inserting this into (3.36) and using (3.35) backwards with $D = \{x\}$ and $A = B$, we get

$$\begin{aligned} f(x)\mu(x)e_{B,x}(x) &= \sum_{y\in\Gamma\setminus B} G_{\Gamma\setminus B}(y,x)e_{B,x}(x)\mu(y)g(y) \\ &= \sum_{y\in\Gamma\setminus B} \mu(y)h_{x,B}(y) \end{aligned} \tag{3.38}$$

or

$$f(x) = \sum_{y\in\Gamma\setminus B} \frac{\mu(y)h_{x,B}(y)}{\mu(x)e_{B,x}(x)}g(y) \tag{3.39}$$

Since this is true for all functions g comparing with (3.31) we read off that

Proposition 3.3.3 *The Dirichlet Green's function for any set $B \subset G$ can be represented in terms of the equilibrium potential and capacities as*

$$G_{\Gamma\setminus B}(x,y) = \frac{\mu(y)h_{x,B}(y)}{\mathrm{cap}(B,x)} \tag{3.40}$$

We now get immediately the desired representations for the mean times:

$$\mathbb{E}_x\tau_A = \sum_{y\in\Gamma\setminus A} \frac{\mu(y)h_{x,A}(y)}{\mathrm{cap}(A,x)} \tag{3.41}$$

These formulas will proof to be excessively useful in the sequel.

3.4 Renewal equations

The application of Proposition 3.3.3 may not appear very convincing, as we can actually solve the Dirichlet problems directly. On the other hand, even if we admit that the Dirichlet variational principle gives us a good tool to compute the denominator, i.e. the capacity, we still do not know how to compute the equilibrium potential. We will now show that a surprisingly simple argument provides a tool that allows us to reduce, for our purposes, the computation of the equilibrium potential to that of capacities.

This yields the *renewal bound* for the equilibrium potential.

Lemma 3.4.4 *Let $A, D \subset \Gamma$ be disjoint, and $x \in (A \cup D)^c$. Then*

$$\mathbb{P}_x[\tau_A < \tau_D] = h_{A,D}(x) \leq \frac{\mathrm{cap}(x,A)}{\mathrm{cap}(x,D)} \tag{3.42}$$

Proof The basis of our argument is the trivial observation that if the process starting at a point x wants to realise the event $\{\tau_A < \tau_D\}$, it may do so by going to A immediately and without returning to x again, or it may return to x without either going to A or to D. Clearly, once the process returns to x it is in the same position as at the starting time, and we can use the (strong) Markov property to separate the probability of what happened before the first return to x to whatever will happen later. Formally:

$$\begin{aligned}\mathbb{P}_x[\tau_A < \tau_D] &= \mathbb{P}_x[\tau_A < \tau_{D\cup x}] + \mathbb{P}_x[\tau_x < \tau_{A\cup D} \wedge \tau_A < \tau_D] \\ &= \mathbb{P}_x[\tau_A < \tau_{D\cup x}] + \mathbb{P}_x[\tau_x < \tau_{A\cup D}]\mathbb{P}_x[\tau_A < \tau_D] \end{aligned} \tag{3.43}$$

We call this a renewal equation. We can solve this equation for $\mathbb{P}_x[\tau_A < \tau_D]$:

$$\mathbb{P}_x[\tau_A < \tau_D] = \frac{\mathbb{P}_x[\tau_A < \tau_{D\cup x}]}{1 - \mathbb{P}_x[\tau_x < \tau_{A\cup D}]} = \frac{\mathbb{P}_x[\tau_A < \tau_{D\cup x}]}{\mathbb{P}_x[\tau_{A\cup D} < \tau_x]} \tag{3.44}$$

By elementary monotonicity properties this representation yields the bound

$$\mathbb{P}_x[\tau_A < \tau_D] \le \frac{\mathbb{P}_x[\tau_A < \tau_x]}{\mathbb{P}_x[\tau_D < \tau_x]} = \frac{\mathrm{cap}(x, A)}{\mathrm{cap}(x, D)} \tag{3.45}$$

□

Of course this bound is useful only if $\frac{\mathrm{cap}(x,A)}{\mathrm{cap}(x,D)} < 1$, but since $\mathbb{P}_x[\tau_A < \tau_D] = 1-\mathbb{P}_x[\tau_D < \tau_A]$, the applicability of this bound is quite wide. It is quite astonishing how far the simple use of this renewal bound will take us.

4

Metastability

We come now to a general definition of metastability in the context of discrete Markov chains.

4.1 Metastable points

Definition 4.1.1 Assume that Γ is a discrete set. Then a Markov processes X_t is metastable with respect to the set of points $\mathcal{M} \subset \Gamma$, if

$$\frac{\sup_{x\in\mathcal{M}} \mathbb{P}_x[\tau_{\mathcal{M}\setminus x} < \tau_x]}{\inf_{y\notin\mathcal{M}} \mathbb{P}_y[\tau_{\mathcal{M}} < \tau_y]} \leq \rho \ll 1 \tag{4.1}$$

We will see that Definition 4.1.1 is (at least if Γ is finite) equivalent to an alternative definition involving averaged hitting times.

Definition 4.1.2 Assume that Γ is a finite discrete set. Then a Markov processes X_t is metastable with respect to the set of points $\mathcal{M} \subset \Gamma$, if

$$\frac{\inf_{x\in\mathcal{M}} \mathbb{E}_x\tau_{\mathcal{M}\setminus x}}{\sup_{y\notin\mathcal{M}} \mathbb{E}_y\tau_{\mathcal{M}}} \geq 1/\rho \gg 1 \tag{4.2}$$

We will show that without further assumptions on the particular properties of the Markov chain we consider, the fact that a set of metastable states satisfying the condition of Definition 4.1.1 exists implies a number of structural properties of the chain.

4.2 Ultrametricity

An important fact that allows to obtain general results under our Definition of metastability is the fact that it implies approximate ultrametricity of capacities. This has been noted in [5].

Lemma 4.2.1 *Assume that $x, y \in \Gamma$, $D \subset \Gamma$. Then, if for $0 < \delta < \frac{1}{2}$, $\mathrm{cap}(y, D) \leq \delta\mathrm{cap}(y, x)$, then*

$$\frac{1-2\delta}{1-\delta} \leq \frac{\mathrm{cap}(x,D)}{\mathrm{cap}(y,D)} \leq \frac{1}{1-\delta} \tag{4.3}$$

Proof The key idea of the proof is to use the probabilistic representation of capacities and renewal type arguments involving the strong Markov property. It would be nice to have a purely analytic proof of this lemma.

We first prove the upper bound. We write

$$\mathrm{cap}(x,D) = \mathrm{cap}(D,x) = \sum_{z\in D} \mu(z) e_{x,D}(z) = \sum_{z\in D} \mu(z) \mathbb{P}_z[\tau_x < \tau_D] \tag{4.4}$$

Now

$$\begin{aligned} \mathbb{P}_z[\tau_x < \tau_D] &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_D, \tau_y \geq \tau_D] \\ &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_{D\cup y}] \mathbb{P}_x[\tau_D < \tau_y] \\ &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_{D\cup y}] \frac{\mathbb{P}_x[\tau_D < \tau_{y\cup x}]}{\mathbb{P}_x[\tau_{D\cup y} < \tau_x]} \end{aligned} \tag{4.5}$$

Here we used the Markov property at the optional time τ_x to split the second probability into a product, and then the renewal equation (3.44). Now by assumption,

$$\frac{\mathbb{P}_x[\tau_D < \tau_{y\cup x}]}{\mathbb{P}_x[\tau_{D\cup y} < \tau_x]} \leq \frac{\mathbb{P}_x[\tau_D < \tau_x]}{\mathbb{P}_x[\tau_y < \tau_x]} \leq \delta \tag{4.6}$$

Inserting (4.6) into (4.5) we arrive at

$$\mathbb{P}_z[\tau_x < \tau_D^x] \leq \mathbb{P}_z[\tau_y < \tau_D, \tau_x < \tau_D] + \delta \mathbb{P}_z[\tau_x < \tau_{D\cup y}] \leq \mathbb{P}_z[\tau_y < \tau_D] + \delta \mathbb{P}_z[\tau_x < \tau_D] \tag{4.7}$$

Inserting this inequality into (4.4) implies

$$\mathrm{cap}(x,D) \leq \sum_{z\in D} \mu(z) \mathbb{P}_z[\tau_y < \tau_D] + \delta \sum_{z\in D} \mu(z) \mathbb{P}_z[\tau_x < \tau_D] = \mathrm{cap}(y,D) + \delta \mathrm{cap}(xD) \tag{4.8}$$

which implies the upper bound.

The lower bound follows by observing that from the upper bound we get that $\mathrm{cap}(x,D) \leq \frac{\delta}{1-\delta}\mathrm{cap}(x,y)$. Thus reversing the rôle of x and y, the resulting upper bound for $\frac{\mathrm{cap}(y,D)}{\mathrm{cap}(x,D)}$ is precisely the claimed lower bound. □

Lemma 4.2.1 has the following immediate corollary, which is the version of the ultrametric triangle inequality we are looking for:

Corollary 4.2.2 *Let $x, y, z \in \mathcal{M}$. Then*

$$\mathrm{cap}(x,y) \geq \frac{1}{3} \min\left(\mathrm{cap}(x,z), \mathrm{cap}(y,z)\right) \tag{4.9}$$

Valleys. In the sequel it will be useful to have the notion of a "valley" or "attractor" of a point in $\mathcal{M}$. We set for $x \in \mathcal{M}$,

$$A(x) \equiv \left\{ z \in \Gamma \,|\, \mathbb{P}_z[\tau_x = \tau_{\mathcal{M}}] = \sup_{y \in \mathcal{M}} \mathbb{P}_z[\tau_y = \tau_{\mathcal{M}}] \right\} \tag{4.10}$$

Note that valleys may overlap, but from Lemma 4.2.1 it follows easily that the intersection has a vanishing invariant mass. The notion of a valley in the case of a process with invariant measure $\exp(-f(x)/\epsilon)$ coincides with this notion.

More precisely, the next Lemma will show that if y belongs to the valley of $m \in \mathcal{M}$, then either the capacity $\mathrm{cap}(y, \mathcal{M}\backslash m)$ is essentially the same as $\mathrm{cap}(m, \mathcal{M}\backslash m)$, or the invariant mass of y is excessively small. That is to say that within each valley there is a subset that "lies below the barrier defined by the capacity $\mathrm{cap}(m, \mathcal{M}\backslash m)$, while the rest has virtually no mass, i.e. the process never really gets there.

Lemma 4.2.3 *Let $m \in \mathcal{M}$, $y \in A(m)$, and $D \subset \mathcal{M}\backslash m$. Then either*

$$\frac{1}{2} \leq \frac{\mathrm{cap}(m, D)}{\mathrm{cap}(y, D)} \leq \frac{3}{2}$$

or

$$\mu(y) \leq 3|\mathcal{M}| \frac{\mu(y)}{\mathrm{cap}(y, \mathcal{M})} \mathrm{cap}(m, D)$$

Proof Lemma 4.2.1 implies that *if* $\mathrm{cap}(m, y) \geq 3\mathrm{cap}(m, D)$, then (4.2.3) holds. Otherwise,

$$\frac{\mu(y)}{\mu(m)} \leq 3 \frac{\mu(y)}{\mathrm{cap}(y, m)} \frac{\mathrm{cap}(m, D)}{\mu(m)} \tag{4.11}$$

Since $y \in A(m)$, we have that $\mathbb{P}_y[\tau_m \leq \tau_{\mathcal{M}}] \geq 1/|\mathcal{M}|$. On the other hand, the renewal estimate yields

$$\mathbb{P}_y[\tau_m \leq \tau_{\mathcal{M}}] \leq \frac{\mathrm{cap}(y, m)}{\mathrm{cap}(y, \mathcal{M})} \tag{4.12}$$

Hence

$$\mathrm{cap}(y, \mathcal{M}) \leq |\mathcal{M}| \mathrm{cap}(y, m) \tag{4.13}$$

which yields (4.2.3). □

4.3 Mean entrance times

We will now derive a very convenient expression for the mean time of arrival in a subset $J \subset \mathcal{M}$ of the metastable points. This will be based on our general representation formula for mean arrival times (3.41) together with the renewal

based inequality for the equilibrium potential and the ultrametric inequalities for the capacities that we just derived under the hypothesis of Definition 4.1.1.

Let $x \in \mathcal{M}$, $x \notin J \subset \mathcal{M}$. We want to compute $\mathbb{E}_x \tau_J$. Our starting point is the following equation, that is immediate from (3.41)

$$\mathbb{E}_x \tau_J = \frac{\mu(x)}{\mathrm{cap}(x,J)} \sum_{y \in J^c} \frac{\mu(y)}{\mu(x)} h_{x,J\setminus x}(y) \tag{4.14}$$

We want to estimate the summands in the sum (4.14). We will set $\inf_y \mu(y)^{-1}\mathrm{cap}(y,\mathcal{M}) = a$. The following lemma provides the necessary control over the equilibrium potentials appearing in the sum.

Lemma 4.3.4 *Let $x \in \mathcal{M}$ and $J \subset \mathcal{M}$ with $x \notin J$. Then:*

(i) If $x = m$, either

$$h_{x,J}(y) \geq 1 - \frac{3}{2}|\mathcal{M}|a^{-1}\frac{\mathrm{cap}(x,J)}{\mu(y)} \tag{4.15}$$

or

$$\mu(y) \leq 3|\mathcal{M}|a^{-1}\mathrm{cap}(m,J) \tag{4.16}$$

(ii) If $m \in J$, then

$$\mu(y)h_{x,J}(y) \leq \frac{3}{2}|\mathcal{M}|a^{-1}\mathrm{cap}(m,x) \tag{4.17}$$

(iii) If $m \notin J \cup x$, then either

$$h_{x,J}(y) \leq 3\frac{\mathrm{cap}(m,x)}{\mathrm{cap}(m,J)} \tag{4.18}$$

and

$$h_{x,J}(y) \geq 1 - 3\frac{\mathrm{cap}(m,J)}{\mathrm{cap}(m,x)} \tag{4.19}$$

or

$$\mu(y) \leq 3|\mathcal{M}|a^{-1}\max\left(\mathrm{cap}(m,J), \mathrm{cap}(m,x)\right) \tag{4.20}$$

We will skip the somewhat tedious proof of this lemma. With its help one can give rather precise expressions for the mean hitting times (4.14) that only involve capacities and the invariant measure. We will only consider a special case of particular interest, namely when J contains all points in $\mathcal{M}$ that 'lie lower than' x, i.e. if $J = \mathcal{M}_x \equiv \{m \in \mathcal{M} : \mu(m) \geq \delta\mu(x)\}$, for some $\delta \ll 1$ to be chosen. We will call the corresponding time $\tau_{\mathcal{M}_x}$ the *metastable exit time* from x. In fact, it is reasonable to consider this the time when the process has definitely left x, since the mean time to return to x from $\mathcal{M}_x$ is definitely larger than (or at most equal in degenerate cases) $\mathbb{E}_x \tau_{\mathcal{M}_x}$. Nicely enough, these mean times can be computed very precisely:

Theorem 4.3.5 *Let $x \in \mathcal{M}$ and $J \subset \mathcal{M}\backslash x$ be such a that for all $m \notin J \cup x$ either $\mu(m) \ll \mu(x)$ or $\mathrm{cap}(m, J) \gg \mathrm{cap}(m, x)$, then*

$$\mathbb{E}_x \tau_J = \frac{\mu(A(x))}{\mathrm{cap}(x, J)} \left(1 + O(\rho)\right) \tag{4.21}$$

Proof Left to the reader. □

Finally we want to compute the mean time to reach $\mathcal{M}$ starting from a general point.

Lemma 4.3.6 *Let $z \notin \mathcal{M}$. Then*

$$\mathbb{E}_z \tau_{\mathcal{M}} \leq a^{-2} \left(|\{y : \mu(y) \geq \mu(z)|\} + C\right) \tag{4.22}$$

Proof Using Lemma 4.1.2, we get that

$$\begin{aligned}
\mathbb{E}_z \tau_{\mathcal{M}} &\leq \frac{\mu(z)}{\mathrm{cap}(z, \mathcal{M})} \sum_{y \in \mathcal{M}^c} \frac{\mu(y)}{\mu(z)} \max\left(1, \frac{\mathrm{cap}(y, z)}{\mathrm{cap}(y, \mathcal{M})}\right) \\
&= \frac{\mu(z)}{\mathrm{cap}(z, \mathcal{M})} \sum_{y \in \mathcal{M}^c} \frac{\mu(y)}{\mu(z)} \max\left(1, \frac{\mathbb{P}_y[\tau_z < \tau_y]}{\mathbb{P}_y[\tau_{\mathcal{M}} < \tau_y]}\right) \\
&\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\mathrm{cap}(y, \mathcal{M})}\right)^2 \sum_{y \in \mathcal{M}^c} \max\left(\frac{\mu(y)}{\mu(z)}, \mathbb{P}_z[\tau_y < \tau_z]\right) \\
&\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\mathrm{cap}(y, \mathcal{M})}\right)^2 \left(\sum_{y : \mu(y) \leq \mu(z)} \frac{\mu(y)}{\mu(z)} + \sum_{y : \mu(y) > \mu(z)} 1\right) \\
&\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\mathrm{cap}(y, \mathcal{M})}\right)^2 \left(C + |\{y : \mu(y) > \mu(z)\}|\right)
\end{aligned} \tag{4.23}$$

which proves the lemma. □

Remark 4.3.1 If Γ is finite (resp. not growing to fast with ϵ), the above estimate combined with Theorem 4.3.5 shows that the two definitions of metastability we have given in terms of mean times rep. capacities are equivalent. On the other hand, in the case of infinite state space Γ, we cannot expect the supremum over $\mathbb{E}_z \tau_{\mathcal{M}}$ to be finite, which shows that our first definition was somewhat naive.

5

Upper and lower bounds for capacities

In this lecture we will introduce some powerful, though simple ideas that allow to compute upper and lower bounds for capacities that are relevant for metastability. We will do this with a concrete model, the Glauber dynamics for the Curie-Weiss model, at hand, but the methods we will use are also applicable in other situations.

Let me therefore first of all recall this model and its dynamics.

5.1 The Curie-Weiss model

The Curie-Weiss model is the simplest model for a ferromagnet. Here the state space is the hypercube $\mathcal{S}_N \equiv \{-1,1\}^N$, and the Hamiltonian of the Curie–Weiss model is

$$H_N(\sigma) = -\frac{1}{N}\sum_{1\le i,j\le N}\sigma_i\sigma_j - h\sum_{i=1}^N \sigma_i \tag{5.1}$$

The crucial feature of the model is that the Hamiltonian is a function of the *macroscopic variable*, the magnetization as a *function* on the configuration space: we will call

$$m_N(\sigma) \equiv N^{-1}\sum_{i=1}^N \sigma_i \tag{5.2}$$

the *empirical magnetization*. Here we divided by N to have a specific magnetization. A function of this type is called a *macroscopic* function, because it depends on all spin variables. We can indeed write

$$H_N(\sigma) = -\frac{N}{2}\left[m_N(\sigma)\right]^2 - hNm_N(\sigma) \equiv N\Psi_h(m_N(\sigma)) \tag{5.3}$$

The computation of the partition function is then very easy: We write

$$Z_{\beta,h,N} = \sum_{m\in\mathcal{M}_N} e^{N\beta(\frac{m^2}{2}+mh)} z_{m,N} \tag{5.4}$$

where $\mathcal{M}_N$ is the set of possible values of the magnetization, i.e.,

$$\begin{aligned}\mathcal{M}_N &\equiv \{m \in \mathbb{R} : \exists \sigma \in \{-1,1\}^N : m_N(\sigma) = m\} \\ &= \{-1, -1+2/N, \ldots, 1-2/N, 1\}\end{aligned} \tag{5.5}$$

and

$$z_{m,N} \equiv \sum_{\sigma \in \{-1,1\}^N} \mathbb{I}_{m_N(\sigma)=m} \tag{5.6}$$

is a 'micro-canonical partition function'. Fortunately, the computation of this micro-canonical partition function is easy. In fact, all possible values of m are of the form $m = 1 - 2k/N$, and for these

$$z_{m,N} = \binom{N}{N(1-m)/2} \equiv \frac{N!}{[N(1-m)/2]![N(1+m)/2]!} \tag{5.7}$$

It is always useful to know the asymptotics of the logarithm of the binomial coefficients. If we set, for $m \in \mathcal{M}_N$

$$N^{-1} \ln z_{m,N} \equiv \ln 2 - I_N(m) \equiv \ln 2 - I(m) - J_N(m) \tag{5.8}$$

where

$$I(m) = \frac{1+m}{2} \ln(1+m) + \frac{1-m}{2} \ln(1-m) \tag{5.9}$$

then

$$\begin{aligned}J_N(m) = \frac{1}{2N} \ln \frac{1-m^2}{4} + \frac{\ln N + \ln(2\pi)}{2N} \\ + O\left(N^{-2}\left(\frac{1}{1-m} + \frac{1}{1+m}\right)\right)\end{aligned} \tag{5.10}$$

(5.10) is obtained using the asymptotic expansion for the logarithm of the Gamma function. The function $I(x)$ is called *Cramèr's entropy function* and worth memorizing. Note that by its nature it is a relative entropy. The function J_N is of lesser importance, since it is very small.

The Gibbs measure is then

$$\mu_{\beta,N} \equiv \frac{\exp\left(\beta N \left[m_N(\sigma)^2/2 + h m_N(\sigma)\right]\right)}{Z_{\beta,N}}. \tag{5.11}$$

an important role is played by the measure induced by the map m_N,

$$\mathbb{Q}_{\beta,N}(m) \equiv \mu_{\beta,N} \circ m_N^{-1}(m) = \frac{\exp\left(\beta N \left[m_N(\sigma)^2/2 + h m_N(\sigma)\right] - N I_N(m)\right)}{Z_{\beta,N}}. \tag{5.12}$$

Note that this measure concentrates sharply, as N goes to infinity, on the minimizers of the function $f_{\beta,N} \equiv \Phi(m) - \beta^{-1} I(m)$.

5.2 Glauber dynamics

Typical dynamics studied for such models are Glauber dynamics, i.e. (random) Markov chains $\sigma(t)$, defined on the configuration space $\mathcal{S}^N$ that are reversible with respect to the (random) Gibbs measures $\mu_{\beta,N}(\sigma)$ and in which the transition rates are non-zero only if the final configuration can be obtained from the initial one by changing the value of one spin only. A particular choice of transition rates are given by the Metropolis algorithm:

$$p_N(\sigma,\sigma') \equiv \begin{cases} 0, & \text{if } \|\sigma-\sigma'\| > 2, \\ \frac{1}{N} e^{-\beta[H_N(\sigma')-H_N(\sigma)]_+}, & \text{if } \|\sigma-\sigma'\| = 2, \\ , & \text{if } \sigma = \sigma'. \end{cases} \tag{5.13}$$

Here $[f]_+ \equiv \max(f,0)$.

There is a simple way of analysing this dynamics which is based on the observation that in this particular model, if $\sigma(t)$ is the Markov process with the above transition rates, then the stochastic process $\tilde{m}_N(t) \equiv m_N(\sigma(t))$ is again a Markov process with state space $\mathcal{M}_N$ and invariant measure $\mathbb{Q}_{\beta,N}$.

Here we do not want to follow this course, but we will use more generally applicable bounds that will, however, reproduce the exact results in this simple case.

As a first problem that we encounter in this way it the proper definition of metastable state. Since the invariant (Gibbs) measure is constant on the sets of configurations with given value of m_N, clearly looking for configurations that are local minima of the energy, H_N, is not a good idea. In fact, since the induces measure $\mathbb{Q}_{\beta,N}$ has local maxima at the minima of the function $f_{\beta,N}$, and given the symmetries of the problem, it seems far more natural to consider as metastable sets the sets

$$M_\pm \equiv \{\sigma : m_N(\sigma) = m_\pm^*\}, \tag{5.14}$$

where $m_\pm^*$ are the largest, respectively smallest local minimizer of $f_{\beta,N}(m) = 0$.

We may come back to the question whether this is a feasible definition later. For the moment, we want to see how in such a situation we can compute the relevant capacity, $\mathrm{cap}(M_+, M--)$.

5.3 Upper bounds

Our task is to compute

$$\mathrm{cap}(M_+, M_-) = \inf_{h\in\mathcal{H}} \frac{1}{2} \sum_{\sigma,\tau\in\mathcal{S}_N} \mu(\sigma) p_N(\sigma,\tau) \left[h(\sigma) - h(\tau)\right]^2, \tag{5.15}$$

where

$$\mathcal{H} = \{h : \Sigma_N \to [0,1] : h(\sigma) = 0, \sigma \in M_+, h(\sigma) = 1, \sigma \in M_-\}. \tag{5.16}$$

The general strategy is to prove an upper bound by guessing some a-priori properties of the minimizer, h, and then to find the minimizers within this class. There are no limits to one's imagination here, but of course some good physical insight will be helpful. The good thing is that, whatever we will guess here, will be put to the test later when we will or will not be able to come up with a matching lower bound. Quite often it is not a bad idea to try to assume that the minimizer (i.e. the equilibrium potential) depends on σ only through some *order parameter*. In our case this can only be the magnetisation, $m_N(\sigma)$. As a matter of fact, due to symmetry, in our case we can know a priori that this will be true for a fact, but, even if it may not be true, it may give a good bound for the capacity: it is really only necessary that this assumption holds in those places where the sum in (5.15) gives a serious contribution!

Let us see where this gets us:

$$\mathrm{cap}(M_+, M_-) = \inf_{g\in\widetilde{\mathcal{H}}} \frac{1}{2} \sum_{\sigma,\tau\in\mathcal{S}_N} \mu(\sigma) p_N(\sigma,\tau) \left[g(m_N(\sigma)) - g(m_N(\tau))\right]^2, \tag{5.17}$$

where

$$\mathcal{H} = \left\{g : [m_-^*, m_+^*] \to [0,1] : g(m_-^*) = 0, g(m_+^*) = 1\right\}. \tag{5.18}$$

But

$$\begin{aligned} &\frac{1}{2} \sum_{\sigma,\tau\in\mathcal{S}_N} \mu(\sigma) p_N(\sigma,\tau) \left[g(m_N(\sigma)) - g(m_N(\tau))\right]^2 \qquad (5.19)\\ &= \frac{1}{2} \sum_{m,m'} [g(m) - g(m')]^2 \sum_{\sigma: m_N(\sigma)=m, \tau: m_N(\tau)=m'} \mu(\sigma) p_N(\sigma,\tau)\\ &= \frac{1}{2} \sum_{m,m'} \mathcal{Q}_{\beta,N}(m) r_N(m.m') [g(m) - g(m')]^2, \end{aligned}$$

where

$$r_N(x,y) \equiv \frac{1}{\mathbb{Q}_{\beta,N}(x)} \sum_{\sigma: m(\sigma)=x} \sum_{\tau: m(\sigma')=y} \mu_{\beta_N}(\sigma) p_N(\sigma,\tau) \tag{5.20}$$

In our special case of the Metropolis dynamics, $p_N(\sigma,\tau)$ depends only on $m_N(\sigma)$ and $m_N(\tau)$

$$r_N(x,y) = \begin{cases} 0, & \text{if } |x-y| > 2/N,\\ (1-x)/2 \exp(\beta N |\Psi_N(x+2/N) - \Psi(x)]_*, & \text{if } y = x+2/N,\\ (1+x)/2 \exp(\beta N |\Psi_N(x-2/N) - \Psi(x)]_*, & \text{if } y = x-2/N,\\ 1 - \frac{(1-x)}{2} \exp(\beta N |\Psi_N(x+2/N) - \Psi(x)]_* & \\ -\frac{(1+x)}{2} \exp(\beta N |\Psi_N(x-2/N) - \Psi(x)]_*, & \text{if } x = y. \end{cases} \tag{5.21}$$

The main point is that the remaining one-dimensional variational problem

involving the quadratic form (5.19) can be solved exactly. The answer is given in the form

$$\inf_{g\in\widetilde{\mathcal{H}}} \frac{1}{2}\sum_{m,m'} \mathcal{Q}_{\beta,N} r_N(m.m')[g(m)-g(m')]^2 \tag{5.22}$$
$$= \left[\sum_{\ell=0}^{N(m_+-m_-)/2-1} \frac{1}{\mathcal{Q}_{\beta,N}(\ell/N) r_N(2\ell/N,(2\ell+2)/N)}\right]^{-1}$$

The sum appearing in the denominator can be further analysed using the Laplace method, but this shall be not our main concern at the moment.

The question we want to address now is how to get a corresponding lower bound.

5.4 Lower bounds

The real art in analysing metastability in our approach lies in the judicious derivation of lower bounds for the capacity. There are two ways of seeing how this can be done. First, we may use the monotonicity of the Dirichlet form in the parameters $p(_N(\sigma,\tau)$. This means that we may, in particular, set a number of the $p_N((\sigma,\tau)$ to zero to obtain a simpler system for which we may be able to find the solution of our variational problem more easily. In many cases, this strategy has provided good results.

There is, however, a more general approach that gives us far more flexibility. To this end, consider a countable set I, and a let $\mathcal{G} \equiv \{g_{xy}, x, y \in \Gamma\}$, be a collection of sub-probability measures on I, i.e. for each (x,y), $g_{xy}(\alpha) \geq 0$, and $\sum_{\alpha\in I} g_{xy}(\alpha) \leq 1$. Then

$$\begin{aligned}
\mathrm{cap}(A,B) &= \inf_{h\in\mathcal{H}_{A,D}} \sum_{\alpha\in I}\frac{1}{2}\sum_{x,y} \mathbb{Q}(y) g_{xy}(\alpha) p(x,y) \left\|h_{A,D}(x)-h_{A,D}(y)\right\|^2 \\
&\geq \sum_{\alpha\in I} \inf_{h\in\mathcal{H}_{A,D}} \sum_{\alpha\in I}\frac{1}{2}\sum_{x,y} \mathbb{Q}(y) g_{xy}(\alpha) p(x,y) \left\|h_{A,D}(x)-h_{A,D}(y)\right\|^2 \\
&\equiv \sum_{\alpha\in I} \inf_{h\in\mathcal{H}_{A,D}} \Phi^{\mathcal{G}(x)}(h) \equiv \sum_{\alpha\in I} \mathrm{cap}^{\mathcal{G}(\alpha)}(A,D)
\end{aligned} \tag{5.23}$$

As this it true for all $\mathcal{G}$, we get the variational principle

$$\mathrm{cap}(A,D) = \sup_{\mathcal{G}} \sum_{\alpha\in I} \mathrm{cap}^{\mathcal{G}(a)}(A,D) \tag{5.24}$$

Note that this may look trivial, as of course the supremum is realised for the trivial case $I=\{1\}$, $g_{xy}(1)=1$, for all (x,y). The interest in the principle arises from the fact that there may be other choices that still realise the supremum (or

at least come very close to it). If we denote by $h_{A,D}^{\mathcal{G}(\alpha)}$ the minimizer of $\Phi^{\mathcal{G}(x)}(h)$, then $\mathcal{G}$ realises the supremum, whenever

$$h_{A,D}^{\mathcal{G}(\alpha)}(x) = h_{A,D}(x), \quad \forall x : g_{xy}(\alpha) \neq 0 \tag{5.25}$$

Of course we do not know $h_{A,D}(x)$, but this observation suggest a very good strategy to prove lower bounds, anyhow: guess a plausible test function h for the upper bound, then try to construct $\mathcal{G}$ such that the minimizers, $h^{\mathcal{G}(\alpha)}$, are computable, and are similar to h! If this succeeds, the resulting upper and lower bounds will be at least very close. Remarkably, this strategy actually does work in many cases.

Lower bounds through one-dimensional paths The following approach was developed in this context with D. Ioffe [7]. It can be seen as a specialisation of a more general approach by Berman and Konsowa [2]. We describe it first in an abstract context and then apply it to the Curie-Weiss model. Let $\Gamma \equiv \Gamma_0 \cup \dots \Gamma_K$ be the vertex set of a graph. We call a graph layered, if for any edge, $e \equiv (v, u)$, there exists ℓ such that $u \in \Gamma_\ell$ and $v \in \Gamma_{\ell-1}$ or $v \in \Gamma_{\ell+1}$. Let $p(u, v)$ be a Markov transition matrix whose associated graph is a layered graph on Γ, and whose unique reversible measure is given by μ. We are interested in computing the capacity from Γ_0 to Γ_K, i.e.

$$\begin{aligned} C_{0,K} \equiv & \frac{1}{2} \inf_{h:h(\Gamma_0)=1,h(\Gamma_K)=0} \sum_{\sigma,\sigma' \in \Gamma} \mu(\sigma) p(\sigma, \sigma') \left[h(\sigma) - h(\sigma')\right]^2 \\ = & \inf_{h:h(\Gamma_0)=1,h(\Gamma_K)=0} \sum_{\ell=0}^{K-1} \sum_{\sigma_\ell \in \Gamma_\ell, \sigma_{\ell+1} \in \Gamma_{\ell+1}} \mu(\sigma_\ell) p(\sigma_\ell, \sigma_{\ell+1}) \left[h(\sigma_\ell) - h(\sigma_{\ell+1})\right]^2 \end{aligned} \tag{5.26}$$

Let us introduce a probability measure ν_0 on Γ_0. Let q be a Markov transition matrix on Γ whose elements, $q(\sigma.\sigma')$, are non-zero only if, for some ℓ, $\sigma \in \Gamma_\ell$ and $\sigma' \in \Gamma_{\ell+1}$, and if $p(\sigma, \sigma') > 0$. Define, for $\ell \geq 0$,

$$\nu_{\ell+1}(\sigma_{\ell+1}) = \sum_{\sigma_\ell \in \Gamma_\ell} \nu_\ell(\sigma_\ell) q(\sigma_\ell, \sigma_{\ell+1}). \tag{5.27}$$

Let $\mathcal{T}$ denote the set of all directed paths form Γ_0 to Γ_K on our graph. Note that the Markov chain with transition matrix q and initial distribution ν_0 defines a probability measure on $\mathcal{T}$, which we will denote by $\mathbb{Q}$.

We now associate for any $T \in \mathcal{T}$ and any edge, $b = (\sigma_\ell, \sigma_{\ell+e})$ in our graph the weight

$$w_T(b) \equiv \begin{cases} 0, & \text{if } b \notin T \\ Q(T)/(q(b)\nu_\ell(\sigma_\ell)), & \text{if } b = (\sigma_\ell, \sigma_{\ell+1}) \in T \end{cases} \tag{5.28}$$

Lemma 5.4.1 *For all b in our graph,*

$$\sum_T w_T(b) = 1 \tag{5.29}$$

Proof Note that, if $T = (\sigma - 1, \ldots, \sigma_K)$, and $b = (\sigma_\ell, \sigma_{\ell+e})$

$$Q(T)/(q(b)\nu_\ell(\sigma_\ell)) = \nu_0(\sigma_0)q(\sigma_0,\sigma_1)\ldots q(\sigma_{\ell-1},\sigma_\ell)\frac{1}{\nu_\ell}q(\sigma_{\ell+1},\sigma_{\ell+2})\ldots q(\sigma_{k-1},\sigma_K) \tag{5.30}$$

Summing over all T containing b means to sum this expression over $\sigma_0, \sigma_1, \ldots, \sigma_{\ell-1}$, and over $\sigma_{\ell+1}, \ldots, \sigma_K$. Using the definition of ν_k is is easy to see that this gives exactly one. □

Theorem 5.4.2 *With the definition above we have that*

$$C_{0,K} \geq \sum_{T\in\mathcal{T}} \mathbb{Q}(T) \left[\sum_{\ell=0}^{K-1} \frac{\nu_\ell(\sigma_\ell)q(\sigma_\ell,\sigma_{\ell+1})}{\mu(\sigma_\ell)p(\sigma_\ell,\sigma_{\ell+1})}\right]^{-1} \tag{5.31}$$

Proof In view of the preceding lemma, we have clearly that

$$\begin{aligned} C_{0,K} &= \inf_{h:h(\Gamma_0)=1,h(\Gamma_K)=0} \sum_{\ell=0}^{K-1} \sum_{\sigma_\ell\in\Gamma_\ell,\sigma_{\ell+1}\in\Gamma_{\ell+1}} \sum_{T\in\mathcal{T}} w_T(\sigma_\ell,\sigma_{\ell+1})\mu(\sigma_\ell)p(\sigma_\ell,\sigma_{\ell+1})\left[h(\sigma_\ell)-h(\sigma_{\ell+1})\right]^2 \\ &= \inf_{h:h(\Gamma_0)=1,h(\Gamma_K)=0} \sum_{T\in\mathcal{T}} \mathbb{Q}(T) \sum_{\ell=0}^{K-1} \frac{\mu(\sigma_\ell)p(\sigma_\ell,\sigma_{\ell+1})}{\nu_\ell(\sigma_\ell)q(\sigma_\ell,\sigma_{\ell+1})}\left[h(\sigma_\ell)-h(\sigma_{\ell+1})\right]^2 \\ &\geq \sum_{T\in\mathcal{T}} \mathbb{Q}(T) \inf_{h:h(\sigma_0)=1,h(\sigma_K)=0} \sum_{\ell=0}^{K-1} \frac{\mu(\sigma_\ell)p(\sigma_\ell,\sigma_{\ell+1})}{\nu_\ell(\sigma_\ell)q(\sigma_\ell,\sigma_{\ell+1})}\left[h(\sigma_\ell)-h(\sigma_{\ell+1})\right]^2 \end{aligned} \tag{5.32}$$

Solving the one-dimensional variational problems in the last line gives the well-known expression that is given in the statement of the theorem. □

Remark 5.4.1 The quality of the lower bound depends on to what extend the interchange of the summation over paths and the infimum over the functions h is introducing errors. If the minimizers are the same for all paths, then no error what so ever is made. This will be the case if the effective capacities

$$\frac{\mu(\sigma_\ell)p(\sigma_\ell,\sigma_{\ell+1})}{\nu_\ell(\sigma_\ell)q(\sigma_\ell,\sigma_{\ell+1})}$$

are independent of the particular path.

Remark 5.4.2 Berman and Konsowa [2] prove a more general lower bound where the space of paths contains all self-avoiding paths, without the restriction of directedness we have made. In this class, they show the the supremum over all probability distributions on the space of paths yields exactly the capacity.

Application to the Curie-Weiss model. In the Curie-Weiss model, it is a very simple matter to achieve the objective stated in the remark above. Clearly, we chose for the layers Γ_ℓ the sets $\{\sigma : m_N(\sigma) = m *_- +2\ell/N\}$.

Since $\mu(\sigma)$ depends only on $m_N(\sigma)$, and $p_N(\sigma, \tau)$ depends only on $m_N(\sigma)$, $m_N(\tau)$, and the fact whether or not τ is reachable from σ by a single spin flip, it is enough to chose for ν_ℓ the uniform measure on the sets Γ_ℓ, and for $q(\sigma_\ell, \sigma_{\ell+1}) = \frac{2}{N-Nm_-^*-2\ell}$. It then follows that

$$\frac{\nu_\ell(\sigma_\ell)}{\mu(\sigma_\ell)} = \frac{1}{\mu(\Gamma_\ell)} = \frac{1}{\mathcal{Q}_{\beta,N}(m_-^* + 2\ell/N)}, \tag{5.33}$$

and

$$\frac{p_N(\sigma_\ell, \sigma_{\ell+1})}{q(\sigma_\ell, \sigma_{\ell+1})} = r_N(\sigma_\ell, \sigma_{\ell+1}). \tag{5.34}$$

Thus, the lower bound from Theorem 5.4.2 reproduces the upper bound exactly.

6

Metastability and spectral theory

We now turn to the characterisation of metastability through spectral data. The connection between metastable behaviour and the existence of small eigenvalues of the generator of the Markov process has been realised for a very long time. Some key references are [13, 14, 15, 19, 20, 23, 27, 29, 34, 36, 35].

We will show that Definition 4.1.1 implies that the spectrum of L decomposes into a cluster of $|\mathcal{M}|$ very small real eigenvalues that are separated by a gap from the rest of the spectrum. To avoid complications we will assume that $|\Gamma|$ s finite throughout this section.

6.1 Basic notions

Let $\Delta \subset \Gamma$. We say that $\lambda \in \mathbb{C}$ is an *eigenvalue* for the Dirichlet problem, resp. the Dirichlet operator L^D, with boundary conditions in D if the equation

$$\begin{aligned} Lf(x) &= \lambda f(x), \quad x \in \Gamma \backslash D \\ f(x) &= 0, \quad x \in D \end{aligned} \tag{6.1}$$

has a non-zero solution f. $f \equiv f_\lambda$ is then called an eigenfunction. If $D = \emptyset$ we call the corresponding values eigenvalues of L. From the symmetry of the operator L it follows that any eigenvalue must be real; moreover, since L is positive, all eigenvalues are positive. If Γ is finite and $D \neq \emptyset$, the eigenvalues of the corresponding Dirichlet problem are *strictly* positive, while zero is an eigenvalue of L itself with the constant function the corresponding (right) eigenfunction.

If λ is not an eigenvalue of L^D, the Dirichlet problem

$$\begin{aligned} (L - \lambda) f(x) &= g(x), \quad x \in \Gamma \backslash D \\ f(x) &= 0, \quad x \in D \end{aligned} \tag{6.2}$$

has a unique solution and the solution can be represented in the form

$$f(x) = \sum_{y \in \Gamma \setminus D} G^{\lambda}_{\Gamma \setminus D}(x,y) g(y) \tag{6.3}$$

where $G^{\lambda}_{\Gamma \setminus D}(x,y)$ is called the Dirichlet Green's for $L - \lambda$.

Equally, the boundary value problem

$$\begin{aligned} (L-\lambda) f(x) &= 0, \quad x \in \Gamma \setminus D \\ f(x) &= \phi(x), \quad x \in D \end{aligned} \tag{6.4}$$

has a unique solution in this case Of particular importance will be the λ-equilibrium potential (of the capacitor (A, D)), $h^{\lambda}_{A,D}$, defined as the solution of the Dirichlet problem

$$\begin{aligned} (L-\lambda) h^{\lambda}_{A,D}(x) &= 0, \quad x \in (A \cup D)^c \\ h^{\lambda}_{A,D}(x) &= 1, \quad x \in A \\ h^{\lambda}_{A,D}(x) &= 0, \quad x \in D \end{aligned} \tag{6.5}$$

We may define analogously the λ-equilibrium measure

$$e^{\lambda}_{D,A}(x) \equiv (L-\lambda) h^{\lambda}_{A,D}(x) \tag{6.6}$$

Alternatively, $e^{\lambda}_{A,D}$ on A, is the unique measure on A, such that

$$h^{\lambda}_{A,D}(x) = \sum_{y \in A} G^{\lambda}_{D^c}(x,y) e^{\lambda}_{A,D}(y) \tag{6.7}$$

If $\lambda \neq 0$, the equilibrium potential still has a probabilistic interpretation in terms of the Laplace transform of the hitting time τ_A of the process starting in x and killed in D. Namely, we have for general λ, that, with $u(\lambda) \equiv -\ln(1-\lambda)$,

$$h^{\lambda}_{A,D}(x) = \mathbb{E}_x e^{u(\lambda)\tau_A} \mathbb{1}_{\tau_A < \tau_D}$$

for $x \in (A \cup D)^c$, whenever the right-hand side exists. Note that the left hand side is in general the meromorphic extension (in $\lambda \in \mathbb{C}$) of the probabilistically defined right-hand side.

6.2 A priori estimates

The first step of our analysis consists in showing that the matrix $L^{\mathcal{M}}$ that has Dirichlet conditions in all the points of $\mathcal{M}$ has a minimal eigenvalue that is not smaller than $O(a^2)$.

The basis for a priori estimates of eigenvalues is the variational representation of the principle eigenvalue:

Lemma 6.2.1 *The principal (smallest) eigenvalue, λ_D, of the Dirichlet operator L^D satisfies*

$$\lambda_D = \inf_{f:f(x)=0,x\in D} \frac{\Phi(f)}{\|f\|_{2,\mu}^2} \tag{6.8}$$

where $\|f\|_{2,\mu} \equiv \left(\sum_{x\in\Gamma} \mu(x) f(x)^2\right)^{1/2}$

Proof Since L^D is a positive operator, there exists A such that $L = A^*A$. If λ is the smallest eigenvalue of L^D, then $\sqrt{\lambda}$ is the smallest eigenvalue of A and vice versa. But

$$\begin{aligned}\lambda &= \left(\inf_{f:f(x)=0,x\in D} \frac{\|Af\|_{2,\mu}}{\|f\|_{2,\mu}}\right)^2 \\ &= \inf_{f:f(x)=0,x\in D} \frac{\|Af\|_{2,\mu}^2}{\|f\|_{2,\mu}^2} = \inf_{f:f(x)=0,x\in D} \frac{\Phi(f)}{\|f\|_{2,\mu}^2}\end{aligned} \tag{6.9}$$

□

The following is a simple application due to Donsker and Varadhan [12]

Lemma 6.2.2 *Let λ_D denote the infimum of the spectrum of L^D. Then*

$$\lambda_D \geq \frac{1}{\sup_{z\in\Gamma\setminus D} \mathbb{E}_z \tau_D} \tag{6.10}$$

Proof Consider any function $\phi : \Gamma \to \mathbb{R}$ satisfying $\phi(x) = 0$ for $x \in \Delta$. We will use the elementary fact that for all $x, y \in \Gamma$ and $C > 0$

$$\phi(y)\phi(x) \leq \frac{1}{2}(\phi(x)^2 C + \phi(y)^2/C) \tag{6.11}$$

with $C \equiv \psi(y)/\psi(x)$, for some positive function ψ to get a lower bound on $\Phi(\phi)$:

$$\begin{aligned}\Phi(\phi) &= \frac{1}{2}\sum_{x,y} \mu(x)p(x,y)\left(\phi(x)-\phi(y)\right)^2 \\ &= \|\phi\|_{2,\mu}^2 - \sum_{x,y\notin D} \mu(x)p(x,y)\phi(x)\phi(y) \\ &\geq \|\phi\|_{2,\mu}^2 - \sum_{x,y} \mu(x)p(x,y)\frac{1}{2}\left(\phi(x)^2\psi(y)/\psi(x) + \phi(y)^2\psi(x)/\psi(y)\right) \\ &= \|\phi\|_{2,\mu}^2 - \sum_{x\notin D} \mu(x)\phi(x)^2 \frac{\sum_y p(x,y)\psi(y)}{\psi(x)}\end{aligned} \tag{6.12}$$

Now chose $\psi(x) = w_D(x)$ (defined in (3.25)). By (3.26), this yields

$$\begin{aligned}\Phi(\phi) &\geq \|\phi\|_{2,\mu}^2 - \|\phi\|_{2,\mu}^2 + \sum_{x\notin D} \mu(x)\phi(x)^2 \frac{1}{w_D(x)} \\ &= \sum_{x\notin D} \mu(x)\phi(x)^2 \frac{1}{w_D(x)} \geq \|\phi\|_{2,\mu}^2 \sup_{x\in D^c} \frac{1}{w_D(x)} = \|\phi\|_{2,\mu}^2 \frac{1}{\inf_{x\in D^c} \mathbb{E}_x \tau_D}\end{aligned} \tag{6.13}$$

Since this holds for all ϕ that vanish on D,

$$\lambda_D = \inf_{\phi:\phi(x)=0, x\in D} \frac{\Phi(\phi)}{\|\phi\|^2_{2,\mu}} \geq \frac{1}{\inf_{x\in D^c} \mathbb{E}_x \tau_D} \tag{6.14}$$

as claimed. □

If we combine this result with the estimate from Lemma 4.3.6, we obtain the following proposition.

Proposition 6.2.3 *Let λ^0 denote the principal eigenvalue of the operator $L^{\mathcal{M}}$. Then there exists a constant $C > 0$, independent of ϵ, such that for all ϵ small enough,*

$$\lambda^0 \geq Ca^2 \tag{6.15}$$

Remark 6.2.1 Proposition 6.2.3 links the fast time scale to the smallest eigenvalue of the Dirichlet operator, as should be expected. Note that the relation is not very precise. We will soon derive a much more precise relation between times and eigenvalues for the cluster of small eigenvalues.

6.3 Characterization of small eigenvalues

We will now obtain a representation formula for all eigenvalues that are smaller than λ^0. It is clear that there will be precisely $|\mathcal{M}|$ such eigenvalues. This representation was exploited in [5], but already in 1973 Wentzell put forward very similar ideas (in the case of general Markov processes). As will become clear, this is extremely simple in the context of discrete processes (see [8] for the more difficult continuous case).

The basic idea is to use the fact that the solution of the Dirichlet problem

$$\begin{aligned} (L-\lambda)f(x) &= 0, \quad x \notin \mathcal{M} \\ f(x) &= \phi_x, \quad x \in \mathcal{M} \end{aligned} \tag{6.16}$$

which exists uniquely if $\lambda < \lambda^0$, already solves the eigenvalue equation $L\phi(x) = \lambda\phi(x)$ everywhere, except possibly on $\mathcal{M}$. It is natural to try to choose the boundary conditions ϕ_x, $x \in \mathcal{M}$ carefully in such a way that $(L-\lambda)f(x) = 0$ holds also for all $x \in \mathcal{M}$. Note that there are $|\mathcal{M}|$ free parameters (ϕ_x, $x \in \mathcal{M}$) for just as many equations. Moreover, by linearity,

$$f(y) = \sum_{x\in\mathcal{M}} \phi_x h^{\lambda}_{x,\mathcal{M}\setminus x}(y) \tag{6.17}$$

Thus the system of equations to be solved can be written as

$$0 = \sum_{x\in\mathcal{M}} \phi_x L h^{\lambda}_{x,\mathcal{M}\setminus x}(m) \equiv \sum_{x\in\mathcal{M}} \phi_x e^{\lambda}_{x,\mathcal{M}\setminus x}(m), \quad \forall\, m \in \mathcal{M} \tag{6.18}$$

Thus, if these equations have a non-zero solution $\phi_x x \in \mathcal{M}$, then λ is an eigenvalue. On the other hand, if λ is an eigenvalue smaller than λ^0 with eigenfunction ϕ_λ, then we may take $\phi_x \equiv \phi_\lambda(x)$ in (6.16). Then, obviously, $f(y) = \phi_\lambda(y)$ solves (6.16) uniquely, and it must be true that (6.18) has a non-zero solution.

Let us denote by $\mathcal{E}_\mathcal{M}(\lambda)$ the $|\mathcal{M}| \times |\mathcal{M}|$- matrix with elements

$$(\mathcal{E}_\mathcal{M}(\lambda))_{xy} \equiv e^\lambda_{z,\mathcal{M}\setminus z}(x) \tag{6.19}$$

Since the condition for (6.16) to have a non-zero solution is precisely the vanishing of the determinant of $\mathcal{E}^\lambda_\mathcal{M}$, we can now conclude that:

Lemma 6.3.4 *A number $\lambda < \lambda^0$ is an eigenvalue of L if and only if*

$$\det \mathcal{E}_\mathcal{M}(\lambda) = 0 \tag{6.20}$$

In the following we need a useful expression for the matrix elements of $\mathcal{E}_\mathcal{M}(\lambda)$. Since we anticipate that λ will be small, we set

$$h^\lambda_x(y) \equiv h_x(y) + \psi^\lambda_x(y) \tag{6.21}$$

where $h_x(y) \equiv h^0_x(y)$ and consequently $\psi^\lambda_x(y$ solves the inhomogeneous Dirichlet problem

$$\begin{aligned} (L-\lambda)\psi^\lambda_x(y) &= \lambda h_x(y), \quad y \in \Gamma\setminus\mathcal{M} \\ \psi^\lambda_x(y) &= 0, \quad y \in \mathcal{M} \end{aligned} \tag{6.22}$$

A reorganisation of terms allows to express the matrix $\mathcal{E}_\mathcal{M}(\lambda)$ in the following form:

Lemma 6.3.5

$$(\mathcal{E}_\mathcal{M}(\lambda))_{xz} = \mu(x)^{-1}\Big(\Phi(h_z, h_x) - \lambda((h_z, h_x)_\mu + (h_x, \psi^\lambda_z)_\mu\Big) \tag{6.23}$$

Proof Note that

$$(L-\lambda)h^\lambda_z(x) = (L-\lambda)h_z(x) + (L-\lambda)\psi^\lambda_z(x) = Lh_z(x) - \lambda h_z(x) + (L-\lambda)\psi^\lambda_z(x) \tag{6.24}$$

Now,

$$Lh_z(x) = \frac{\mu(x)}{\mu(x)} h_x(x) Lh_z(x) \tag{6.25}$$

The function $\mu^{-1}(y')h_x(y')Lh_z(y')$ vanishes for all $y' \neq x$. Thus, by adding a huge zero,

$$\begin{aligned} Lh_z(x) &= \mu(x)^{-1} \sum_{y'\in\Gamma} \mu(y')h_x(y')Lh_z(y') \\ &= \mu(x)^{-1}\frac{1}{2} \sum_{y,y'\in\Gamma} \mu(y')p(y',y))[h_z(y') - h_z(y)][h_x(y') - h_x(y)] \end{aligned} \tag{6.26}$$

there the second inequality is obtained just as in the derivation of the representation of the capacity through the Dirichlet form. Similarly,

$$(L-\lambda)\psi_z^\lambda(x) = \mu(x)^{-1}\sum_{y'\in\Gamma}\mu(y')\left(h_x(y')(L-\lambda)\psi_z^\lambda(y') - \lambda\mathbb{1}_{y'\neq x}h_x(y')h_z(y')\right) \tag{6.27}$$

Since $\psi_z^\lambda(y) = 0$ whenever $y \in \mathcal{M}$, and $Lh_x(y)$ vanishes whenever $y \notin \mathcal{M}$, using the symmetry of L, we get that the right-hand side of (6.27) is equal to

$$-\lambda\mu(x)^{-1}\sum_{y'\in\Gamma}\left(\mu(y')h_x(y')(\psi_z^\lambda(y') + \mathbb{1}_{y'\neq x}h_x(y')h_z(y')\right) \tag{6.28}$$

Adding the left-over term $-\lambda h_z(x) = -\lambda h_x(x)h_z(x)$ from (6.24) to (6.27), we arrive at (6.23). □

Expanding in λ. Anticipating that we are interested in small λ, we want to control the λ-dependent terms ψ^λ in the formula for the matrix $\mathcal{E}_{\mathcal{M}}(\Lambda)$. From (6.22) we can conclude immediately that ψ_x^λ is small compared to h_x in the $L_2(\Gamma,\mu)$ sense when λ is small, since

$$\psi_x^\lambda = \lambda(L^{\mathcal{M}} - \lambda)^{-1}h_x \tag{6.29}$$

Using that for symmetric operators, $\|(L-a)^{-1}\| \leq \frac{1}{\mathrm{dist}(\,\mathrm{spec(L)},\mathrm{a})}$, we see that

$$\|\psi_x^\lambda\|_{2,\mu} \leq \frac{\lambda}{\lambda^0-\lambda}\|h_x\|_{2,\mu} \tag{6.30}$$

We are now in a position to relate the small eigenvalues of L to the eigenvalues of the classical capacity matrix. Let us denote by $\|\cdot|_2 \equiv \|\cdot\|_{2,\mu}$.

Theorem 6.3.6 *If $\lambda < \lambda^0$ is an eigenvalue of L, then there exists an eigenvalue μ of the $|\mathcal{M}| \times |\mathcal{M}|$-matrix $\mathcal{K}$ whose matrix elements are given by*

$$\begin{aligned}\mathcal{K}_{zx} &= \frac{\frac{1}{2}\sum_{y\neq y'}\mu(y')p(y',y)[h_z(y')-h_z(y)][h_x(y')-h_x(y)]}{\|h_z\|_2\|h_x\|_2} \\ &\equiv \frac{\Phi(h_z,h_x)}{\|h_z\|_2\|h_x)\|_2}\end{aligned} \tag{6.31}$$

such that $\lambda = \mu\,(1+O(\rho))$, where $\rho = \lambda/\lambda_0$.

We will skip the proof of this theorem since it is not really needed.

In fact we will prove the following theorem.

Proposition 6.3.7 *Assume that there exists $x \in \mathcal{M}$ such that, for some*

$d \ll 1$

$$\delta^2\frac{\mathrm{cap}(x,\mathcal{M}\backslash x)}{\|h_x\|_2^2} \geq \max_{z\in\mathcal{M}\backslash x}\frac{\mathrm{cap}(z,\mathcal{M}\backslash z)}{\|h_z\|_2^2} \tag{6.32}$$

Then the largest eigenvalue of L below λ_0 is given by

$$\lambda_x = \frac{\mathrm{cap}(x, \mathcal{M}\backslash x)}{\|h_x\|_2^2}(1 + O(\delta^2 + \rho^2)) \tag{6.33}$$

Moreover, the eigenvector, ϕ, corresponding to the largest eigenvalues normalized s.t. $\phi_x = 1$ satisfies $\phi_z \leq C(\delta + \rho)$, for $z \neq x$.

Proof Let x be the point in $\mathcal{M}$ specified in the hypothesis. Denote by $\bar{\lambda}_1$ the Dirichlet eigenvalue with respect the the set $\mathcal{M}\backslash x$. It is not very hard to verify that $\bar{\lambda}_1 \sim \frac{\mathrm{cap}(x,\mathcal{M}\backslash x)}{\|h_x\|_2^2}$. Moreover, one can easily verify that there will be exactly $|\mathcal{M}| - 1$ eigenvalues below $\bar{\lambda}_1$. Thus, there must be one eigenvalue, λ_x, between $\bar{\lambda}_1$ and λ_0. We are trying to compute the precise value of this one, i.e. we look for a root of the determinant of $\mathcal{E}_M(\lambda)$ that is of order at least $\frac{\mathrm{cap}(x,\mathcal{M}\backslash x)}{\|h_x\|_2^2}$.

The determinant of $\mathcal{E}_{\mathcal{M}}(\lambda)$ vanishes together with that of the matrix $\mathcal{K}$ whose elements are

$$\mathcal{K}_{xz} = \frac{\mu(x)}{\|h_x\|_2\|h_z\|_2}\left(\mathcal{E}_{\mathcal{M}}(\lambda)\right)_{xz} = \frac{\Phi(h_x, h_z)}{\|h_x\|_2\|h_z\|_2} - \lambda\left(\frac{(h_x, h_z)_\mu + (\psi_x^\lambda, h_z)_\mu}{\|h_x\|_2\|h_z\|_2}\right) \tag{6.34}$$

We will now control al the elements of this matrix. We first deal with the off-diagonal elements of this matrix.

Lemma 6.3.8 *There is a constant $C < \infty$ such that*

$$\max_{x\neq z\in\mathcal{M}} \frac{(h_x, h_z)_\mu}{\|h_x\|_2\|h_z\|_2} \leq Ca^{-1} \max_{m\in\mathcal{M}} \mu(m)^{-1}\mathrm{cap}(m, \mathcal{M}\backslash m) \leq \rho \tag{6.35}$$

Proof Note first by the estimate (3.45) the equilibrium potentials $h_x(y)$ are essentially equal to one on $A(x)$. Namely,

$$1 \geq h_x(y) \geq 1 - \frac{\mathrm{cap}(y, \mathcal{M}\backslash x)}{\mathrm{cap}(y, x)} \tag{6.36}$$

By Corollary 4.2.2, $\mathrm{cap}(y, \mathcal{M}\backslash x) \leq 2\mathrm{cap}(x, \mathcal{M}_x)$, or $\mu(y) \leq 3\|\mathcal{M}|a^{-1}\mathrm{cap}(x, \mathcal{M}_x)$. Thus

$$\begin{aligned}
\sum_{y\in A(x)} \mu(y)h_x(y)^2 &\geq \sum_{\substack{y\in A(x)\\ \mu(y)\geq 3\|\mathcal{M}|a^{-1}\mathrm{cap}(x,\mathcal{M}_x)}} \left(1 - \frac{\mathrm{cap}(x, \mathcal{M}\backslash x)}{\mathrm{cap}(y, x)}\right)^2 \\
&\geq \sum_{\substack{y\in A(x)\\ \mu(y)\geq 3\|\mathcal{M}|a^{-1}\mathrm{cap}(x,\mathcal{M}_x)}} \mu(y) - \sum_{y\in A(x)} 2\frac{\mu(y)}{\mathrm{cap}(y, x)}\mathrm{cap}(x, \mathcal{M}\backslash x) \\
&= \mu(A(m))\left(1 - 3|A(m)||\mathcal{M}\|a^{-1}\frac{\mathrm{cap}(x, \mathcal{M}\backslash x)}{\mu(A(m))}\right) \\
&\geq \mu(A(m))\left(1 - O(\rho)\right)
\end{aligned} \tag{6.37}$$

Thus the denominator in (6.35) is bounded from below by

$$\sqrt{\sum_{y\in A(x)}\mu(y)h_x^2(y)\sum_{y\in A(y)}\mu(y)h_z^2(y)} \geq \sqrt{\mu(A(x))\mu(A(z))}(1-O(\rho)) \tag{6.38}$$

To bound the numerator, we use that, for any $x \neq z \in \mathcal{M}$,

$$\sum_{y\in\Gamma}\mu(y)h_x(y)h_z(y) \leq C\rho\sqrt{\mu(x)\mu(z)} \tag{6.39}$$

Using this bound we arrive at the assertion of the lemma. □

Next we bound the terms involving ψ^λ.

Lemma 6.3.9 *If λ^0 denotes the principal eigenvalue of the operator L with Dirichlet boundary conditions in $\mathcal{M}$, then*

$$\begin{aligned}&\left|\sum_{y\in\Gamma}\mu(y)\left(h_z(y)\psi_x^\lambda(y)\right)\right| \\ &\leq \frac{\lambda}{(\lambda^0-\lambda)}\|h_z\|_2\|h_x\|_2\end{aligned} \tag{6.40}$$

Proof Recall that ψ_x^λ solves the Dirichlet problem (6.22). But the Dirichlet operator $L^{\mathcal{M}}-\lambda$ is invertible for $\lambda<\lambda^0$ and is bounded as an operator on $\ell^2(\Gamma,\mu)$ by $1/(\lambda^0-\lambda)$. Thus

$$\|\psi_x^\lambda|_2^2 \leq \left(\frac{\lambda}{\lambda^0-\lambda}\right)^2\|h_x\|_2^2 \tag{6.41}$$

The assertion of the lemma now follows from the Cauchy-Schwartz inequality. □

Finally we come to the control of the terms involving $\Phi(h_x,h_z)$. By the Cauchy-Schwartz inequality,

$$\begin{aligned}\Phi(h_z,h_x) &= \left|\frac{1}{2}\sum_{y,y'}\mu(y')p(y',y)[h_x(y')-h_x(y)][h_z(y')-h_z(y)]\right| \\ &\leq \sqrt{\Phi(h_x)\Phi(h_z)}\end{aligned} \tag{6.42}$$

Thus

$$\left|\frac{\Phi(h_x,h_z)}{\|h_x\|_2\|h_z\|_2}\right| \leq \sqrt{\frac{\Phi(h_x)}{\|h_x\|_2^2}}\sqrt{\frac{\Phi(h_z)}{\|h_z\|_2^2}} \tag{6.43}$$

Therefore, by assumption, there exists one $x\in\mathcal{M}$ such that for any $(z,y)\neq(x,x)$,

$$\left|\frac{\Phi(h_x,h_z)}{\|h_x\|_2\|h_z\|_2}\right| \leq \delta\frac{\Phi(h_x)}{\|h_x\|_2^2} \tag{6.44}$$

If we collect all our results:

(i) The matrix $\mathcal{K}$ has one diagonal element

$$\mathcal{K}_{xx} = \frac{\Phi(h_x)}{\|h_x\|_2^2} - \lambda(1 + O(\lambda)) \equiv A - \lambda(1 + O(\lambda)), \tag{6.45}$$

(ii) all other diagonal elemement, $\mathcal{K}_{yy}$, satisfy

$$\mathcal{K}_{yy} = O(\delta^2)A - \lambda(1 + O(\lambda)) \approx -\lambda. \tag{6.46}$$

(iii) All off-diagonal elements satisfy

$$|\mathcal{K}_{yz}\| \leq C\delta\frac{\Phi(h_x)}{\|h_x\|_2^2} + C\lambda\rho \equiv C(\delta A + \lambda\rho). \tag{6.47}$$

One can now look for non-zero solutions of the equations

$$\sum_y \mathcal{K}_{zy}c_y = 0, \quad y \in \mathcal{M}. \tag{6.48}$$

In the sequal C denotes a numerical connstant whose value changes from line to line. We may choose the vector c in such a wa that $\max_{y\in\mathcal{M}} |c_y| = 1$, and this component realising the maximum to be equal to $+1$. We will first show that $c_x = 1$. To do so, assume that $c_z = 1$ for $z \neq x$. Then the equation (6.48) can be written

$$-\mathcal{K}_{zz} = \sum_{y\neq z} c_y\mathcal{K}_{zy} \tag{6.49}$$

Using our bounds, this implies

$$\lambda \leq C(\delta A + \rho\lambda) \Leftarrow \lambda \leq \frac{C\delta A}{1 - C\rho}, \tag{6.50}$$

in contradiction with the fact that $\lambda \geq A$. Thus $c_x = 1 \geq |c_z|$, for all $z \neq x$. Let us return to equation (6.48) for $z \neq x$. It now reads

$$-\mathcal{K}_{zz}c_z = \sum_{y\neq z} c_y\mathcal{K}_{zy} \tag{6.51}$$

and hence

$$|c_z| \leq C\frac{\delta A + \rho\lambda}{\lambda} \tag{6.52}$$

Finally, we consider equation (6.48) with $z = x$,

$$\mathcal{K}_{xx} = \sum_{y\neq x} c_y\mathcal{K}_{xy} \tag{6.53}$$

In view of our bounds on $\mathcal{K}_{xy}$ and on c_y, this yields

$$|\mathcal{K}_{xx}| \leq C\frac{(\delta A + \rho\lambda)^2}{\lambda} \leq C\delta^2 A + C\rho^2\lambda, \tag{6.54}$$

that is, we otain that

$$\|A - \lambda| \leq C\delta^2 A + \rho^2\lambda \tag{6.55}$$

which implies

$$\lambda = A\left(1 + O(\delta^2 + \rho^2)\right), \tag{6.56}$$

which is the first claim of the proposition. The assertion on the eigenvector follows from our estimates on the vector c. □

Theorem 6.3.7 has the following simple corollary, that allows in many situations a complete characterization of the small eigenvalues of L.

Theorem 6.3.10 *Assume that we can construct a sequence of metastable sets $\mathcal{M}_k \supset \mathcal{M}_{k-1} \supset \cdots \supset \mathcal{M}_2 \supset \mathcal{M}_1 = x_0$, such that for any i, $\mathcal{M}_i \backslash \mathcal{M}_{i-1} = x_i$ is a single point, and that each $\mathcal{M}_i$ satisfies the assumptions of Theorem 6.3.7. Then L has k eigenvalues*

$$\lambda_i = \frac{\mathrm{cap}(x_i, \mathcal{M}_{i-1})}{\mu(A(x_i))}\,(1 + O(\delta)) \tag{6.57}$$

As a consequence,

$$\lambda_i = \frac{1}{\mathbb{E}_{x_i}\tau_{\mathcal{M}_{x_i}}}(1 + O(\delta)) \tag{6.58}$$

The corresponding normalized eigenfunction is given by

$$\psi_i(y) = \frac{h_{x_i,\mathcal{M}_{i-1}}(y)}{\|h_{x_i,\mathcal{M}_{i-1}}\|_2} + \sum_{j=1}^{i-1} O(\delta)\frac{h_{x_i,\mathcal{M}_{j-1}}(y)}{\|h_{x_i,\mathcal{M}_{j-1}}\|_2} \tag{6.59}$$

Proof The idea behind this theorem is simple. Let the sets $\mathcal{M}_i$ of the corollary be given by $\mathcal{M}_i = \{x_1, \ldots, x_i\}$. Having computed the largest eigenvalue, λ_k, of L, we only have to search for eigenvalues smaller than λ_k. If we could be sure that the principal Dirichlet eigenvalue $\Lambda_{\mathcal{M}_{k-1}}$ is (much) larger than $k-1$st eigenvalue of L, then we could do so as before but replacing the set $\mathcal{M} \equiv \mathcal{M}_k$ by $\mathcal{M}_{k-1}$ everywhere. λ_{k-1} would then again be the largest eigenvalue of a capacity matrix involving only the points in $\mathcal{M}_{k-1}$. Iterating this procedure we arrive at the conclusion of the theorem.

The theorem is now immediate except for the statement (6.58). To conclude, we need to show that $\mathrm{cap}(x_{\ell+1}, \mathcal{M}_\ell) = \mathrm{cap}(x_\ell, \mathcal{M}_{x_\ell})$. To see this, note first that $\mathcal{M}_\ell \supset \mathcal{M}_{x_\ell}$. For if there was $x \in \mathcal{M}_{x_\ell}$ that is not contained in $\mathcal{M}_\ell$, then $\mathrm{cap}(x, \mathcal{M}_\ell \backslash x) \sim \mathrm{cap}(x_{\ell+1}, \mathcal{M}_\ell)$, while $\|h_{x_{\ell+1},\mathcal{M}_\ell}\_2 \leq \|h_{x,\mathcal{M}_{\ell+1}\backslash x}\_2$, contradicting the assumption in the construction of the set $\mathcal{M}_\ell$. Thus $\mathrm{cap}(x_{\ell+1}, \mathcal{M}_\ell) \geq \mathrm{cap}(x_\ell, \mathcal{M}_{x_\ell})$.

Similarly, if there was any point $x \in \mathcal{M}_\ell$ for which $\mathrm{cap}(x_{\ell+1}, \mathcal{M}_\ell) < \mathrm{cap}(x_\ell, \mathcal{M}_{x_\ell})$, then this point would have been associated to a larger eigenvalue in an earlier stage of the construction and thus would have already been removed from $\mathcal{M}_{\ell+1}$ before $x_{\ell+1}$ is being removed.

This observation allows us to finally realize that the k smallest eigenvalues of L

are precisely the inverses of the mean (metastable) exit times from the metastable points $\mathcal{M}$. □

6.4 Exponential law of the exit time

The spectral estimates can be used to show that the law of the metastable exit times are close to exponential, provided the non-degeneracy hypothesis of Theorem 6.3.7 hold. Note that

$$\mathbb{P}_x[\tau_{\mathcal{M}_x} > t] = \sum_{x_1,\ldots,x_t \notin \mathcal{M}_x} p(x,x_1) \prod_{i=1}^{t-1} p(x_i,x_{i+1}) = \sum_{y \notin \mathcal{M}_x} \left(P^{\mathcal{M}_x}\right)^t_{xy} \tag{6.60}$$

To avoid complications, let us assume that the P is positive (in particular that P has no eigenvalues close to -1. This can be avoided e.g. by imposing that $p(x,x) > 0$). We now introduce the projection operators Π on the eigenspace of the principal eigenvalue of $P^{\mathcal{M}_\ell}$. Then

$$\left(P^{\mathcal{M}_x}\right)^t_{xy} = \sum_{y \notin \mathcal{M}_x} \left(\left(P^{\mathcal{M}_x}\right)^t \Pi\right)_{xy} + \sum_{y \notin \mathcal{M}_x} \left(\left(P^{\mathcal{M}_x}\right)^t \Pi^c\right)_{xy} \tag{6.61}$$

Using our estimate for the principal eigenfunction of $L^{\mathcal{M}_x}$ the first term in (6.61) equals

$$\left(1-\lambda^{\mathcal{M}_x}\right)^t \sum_{y \notin \mathcal{M}_x} \frac{h_{x,\mathcal{M}_x}(y)}{\|h_{x,\mathcal{M}_x}(y)\|_2}(1+O(\lambda^{\mathcal{M}_x})) \sim e^{-\lambda^{\mathcal{M}_x} t} \tag{6.62}$$

The remaining term is bounded in turn by

$$e^{-\lambda_2^{\mathcal{M}_x} t} \tag{6.63}$$

which under our assumptions decays much faster to zero than the first term.

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