

Markov Processes and Metastability

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1. 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 distinguished by different colours. This example was instrumental in the development of stochastic models for metastability by Eyring, Kramers and others [Ey,Kr,...]. 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

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

Such systems have been extensively investigated e.g. in the work of Freidlin and Wentzell [FW] and Kifer [Ki1]. They have their origin in the work of Kramers [Kr].

- (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 [OS1,OS2,Ce,BACe] and also in the analysis of stochastic algorithms for the solution of optimisation problems (“simulated annealing”) [Ca,CaCe]. Recent result using the methods outlined here can be found in [BM,BdHN].
- (iii) Glauber dynamics of mean field [CGOV,MP1,MP2,BEGK1] or lattice [SS] 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 [Day].
- (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 [Ko] 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 [HK,HKN,Nie].
- (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 [Mat] and Miclo [Mi].

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.

I plan to structure these lectures as follows.

1. A brief review of basic notions from the theory of Markov processes: transition matrix, generator, stopping times, Kolmogorov’s forward equations, Feynman-Kac formula, invariant and reversible measures.
2. A short course on potential theory (for discrete state space, discrete time Markov chains). Dirichlet problems, Green’s function, Poisson kernel, equilibrium potential, equilibrium measure, capacity, Dirichlet forms and Dirichlet principle.
3. A representation formula for the Greens function.
4. Some attempts towards rigorous definitions of metastability. Induced Markov chains.
5. Metastable exit times in terms of capacities.
6. Computations of capacities in some examples. The Eyring-Kramers formula.
7. Metastability and spectral theory.

2. A short review of 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 $t_1 < \dots < t_n < t \in I$,

$$\mathbb{P}[X_t \in \mathcal{A} | X_{t_n} = x_n, \dots, X_{t_1} = x_1] = \mathbb{P}[X_t \in \mathcal{A} | X_{t_n} = x_n] \quad (2.1)$$

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 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

$$p(s, t, x, dy) \equiv \mathbb{P}(X_t \in dy | X_s = x) \quad (2.2)$$

By (2.1), $p(t, s, x, y)$ determines uniquely the law of the Markov process. Here we have denoted by dy the natural uniform measure on Γ , i.e. if $\Gamma \subset \mathbb{R}^d$ it is Lebesgue measure, and if Γ is discrete it is just the counting measure on Γ . Of course $p(s, t, x, dy)$ is a probability measure for any values of s, t, x . Conversely, any family of probability measures $p(s, t, x, dy)$ satisfying

$$p(s, s, x, dy) = \delta_x(dy) \quad (2.3)$$

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

$$p(s, t, x, dy) = \int p(s, t', x, dz) p(t', t, z, dy) \quad (2.4)$$

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

$$p(s, t, x, dy) \equiv p_{t-s}(x, dy) \quad (2.5)$$

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,

$$p(x, dy) \equiv p_1(x, dy) \quad (2.6)$$

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

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

$$L \equiv \lim_{\tau \downarrow 0} \tau^{-1}(1 - p_\tau) \quad (2.7)$$

It then follows that conversely

$$p_t = e^{-tL} \quad (2.8)$$

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

$$L \equiv 1 - p_1 \quad (2.9)$$

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

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

respectively on measures ρ on Γ , via

$$\rho p_t(dy) \equiv \int_{\Gamma} \rho(dx) p_t(x, dy) \quad (2.11)$$

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

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

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

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

resp., in the discrete case

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

This equation is called the *Fokker-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

$$\mu p_t(dx) = \mu(dx) \quad (2.15)$$

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

$$\mu L = 0 \quad (2.16)$$

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

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. 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

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

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

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

$$\int \mu(dx) g(x) p_t^* f(x) \equiv \int \mu(dx) f(x) p_t g(x) \quad (2.18)$$

respectively

$$\int \mu(dx) g(x) L^* f(x) \equiv \int \mu(dx) f(x) Lg(x) \quad (2.19)$$

for any pair of functions f, g . 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 than 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

$$\tau_D \equiv \inf(t > 0 : X_t \in D) \quad (2.20)$$

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 . The notion of a stopping time is of course fundamental in the theory of Markov processes. There are many interesting times that can be defined that are not stopping times. In particular, the last exit time of a set,

$$\hat{\tau}_D \equiv \sup(t \geq 0 : X_t \in D) \tag{2.21}$$

Clearly, the event $\{\hat{\tau}_D \leq t\}$ depends on whether or not the processes decides to enter D at some time after t and thus is not \mathcal{F}_t measurable. We will very rarely (if ever) work with random times that are not stopping times. Stopping times are sometimes also called *optional* random variables with respect to $\{X_t, \mathcal{F}_t\}$.

The laws of certain hitting times will be the most important objects of our analysis.

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.

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*

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

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: *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.*

Proof: Assuming that (3.4) has two solution implies that there is a non-zero solution of the problem

$$\begin{aligned} Lf(x) &= 0 & \text{for } x \in \Gamma \setminus (A \cup D) \\ f(x) &= 0 & \text{for } x \in D \cup A \end{aligned} \tag{3.6}$$

If f is not zero, it must have a positive maximum (or a negative minimum) somewhere in $\Gamma \setminus D \setminus A$. Let this maximum (or minimum) be taken at the point be x^* . Assume for definiteness that x^* is a positive maximum. But then

$$f(x^*) = \sum_{y \in \Gamma} p(x^*, y) f(y) \leq \max_{y \in \Gamma} f(y) \tag{3.7}$$

where equality can only hold if $f(y) = f(x^*)$ for all y such that $p(x^*, y) > 0$. Thus, by hypothesis, $f(y) = f(x^*)$ on this set. Iterating this argument shows that in fact $f(y) = f(x^*)$ for any y for which $p_n(x^*, y) > 0$, for some n , i.e. for all of Γ . This implies $f(x) \equiv 0$. \diamond

Remark: What we used here is a version of the *maximum principle* for harmonic function. It says that a harmonic function (i.e. a function that solves an equation $Lf = 0$ on some bounded open set where L is the generator of a Markov process) takes its maximum (minimum) on the “boundary” of that set.

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

$$\mathbb{P}_x[\tau_A < \tau_D] = h_{A,D}(x) \tag{3.8}$$

for $x \in \Gamma \setminus (A \cup D)$ 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

$$\mathbb{P}_x[\tau_A < \tau_D] = \sum_{y \in A} p(x, y) + \sum_{y \in \Gamma \setminus (A \cup D)} p(x, y) \mathbb{P}_y[\tau_A < \tau_D] = \sum_{y \in \Gamma} p(x, y) h_{A,D}(y) \tag{3.9}$$

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

$$e_{A,D}(x) \equiv -(Lh_{A,D})(x) \tag{3.10}$$

Then

$$\mathbb{P}_x[\tau_A < \tau_D] = \begin{cases} h_{A,D}(x), & \text{if } x \in \Gamma \setminus (A \cup D) \\ e_{A,D}(x), & \text{if } x \in D \\ 1 - e_{D,A}(x) & \text{if } x \in A \end{cases} \quad (3.11)$$

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

$$\text{cap}(A, D) \equiv \sum_{x \in D} \mu(x) e_{A,D}(x) \quad (3.12)$$

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

$$\begin{aligned} \sum_{x \in D} \mu(x) e_{A,D}(x) &= \sum_{x \in \Gamma} \mu(x) (1 - h_{A,D}(x)) (-Lh_{A,D})(x) \\ &= \sum_{x \in \Gamma} \mu(x) h_{A,D}(x) (Lh_{A,D})(x) - \sum_{x \in \Gamma} \mu(x) Lh_{A,D}(x) \end{aligned} \quad (3.13)$$

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

$$\text{cap}(A, D) = \sum_{x \in \Gamma} \mu(x) h_{A,D}(x) (Lh_{A,D})(x) \equiv \Phi(h_{A,D}) \quad (3.14)$$

where

$$\Phi(h) \equiv \sum_{x \in \Gamma} \mu(x) h(x) Lh(x) = \frac{1}{2} \sum_{x,y} \mu(x) p(x,y) (h(x) - h(y))^2 \quad (3.15)$$

is called the *Dirichlet form* associated to the Markov process with generator L . 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 3.2: Let \mathcal{H}_D^A denote the space of functions

$$\mathcal{H}_D^A \equiv (h : \Gamma \rightarrow [0, 1], h(x) = 1, x \in A, h(x) = 0, x \in D) \quad (3.16)$$

Then

$$\text{cap}(A, D) = \inf_{h \in \mathcal{H}_D^A} \Phi(h) \quad (3.17)$$

Moreover, the variational problem (3.16) has a unique minimizer that is given by the equilibrium potential $h_{A,D}$.

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

$$\frac{\partial}{\partial h(x)} \Phi(h) = 2\mu(x) Lh(x) \quad (3.18)$$

Thus if h minimizes Φ and $h(x) \in (0, 1)$, it must be true that $Lh(x) = 0$. If $h(x) = 0$, then we can at first only deduce that $Lh(x) \geq 0$, but since then $Lh(x) = -\sum_y p(x, y)h(y)$ and h must be non-negative, the only possibility is that $Lh(x) = 0$. Similar reasoning applies in the case $h(x) = 1$, and any minimizer must satisfy $Lh(x) = 0$. Since we have already seen that the Dirichlet problem (3.3) has a unique solution, the theorem is proven. \diamond

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

$$\mathbb{P}_x[\tau_A < \tau_x] = \frac{1}{\mu(x)} \text{cap}(A, x) \quad (3.19)$$

We will call these quantities sometimes *escape probabilities*. We see that they have, by virtue of Theorem 3.2 a direct variational representation. They play a crucial rôle in what will follow. Let us note the fact that $\text{cap}(x, y) = \text{cap}(y, x)$ implies that

$$\mu(x)\mathbb{P}_x[\tau_y < \tau_x] = \mu(y)\mathbb{P}_y[\tau_x < \tau_y] \quad (3.20)$$

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

$$\mathbb{P}_x[\tau_y < \tau_x] \leq \frac{\mu(y)}{\mu(x)} \quad (3.21)$$

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

Monotonicity and inequalities. The Dirichlet principle allows us in a rather trivial manner to get upper bounds on capacities (and hence on escape probabilities). Namely, trivially, if h is any function in \mathcal{H}_D^A , then

$$\text{cap}(A, D) \leq \Phi(h) \quad (3.22)$$

Thus any intuitive guess on how the equilibrium potential may look like will give an upper bound, and the better the guess the better the bound will be. Note that the set over which the infimum is taken has rather simple constraints, so that ones imagination is not restraint be complicated constraints that need to be verified. We will see later how one can systematically work on ones skill on guessing. While the option for upper bounds is a feature of any variational representation, the Dirichlet principle has the most enjoyable feature that it also provides for a simple technique to get *lower bounds*. This feature is a consequence that the Dirichlet form Φ is a *monotone increasing function* of the transition probabilities $p(x, y)$ for $x \neq y$, while it is independent on the values $p(x, x)$. More precisely we have.

Theorem 3.3: Assume that Φ and $\tilde{\Phi}$ are Dirichlet forms associated to two Markov chains P, \tilde{P} with state space Γ . Assume that the transition probabilities p and \tilde{p} are given, for $x \neq y$, by

$$\begin{aligned} p(x, y) &= \sqrt{\frac{\mu(y)}{\mu(x)}} g(x, y) \\ \tilde{p}(x, y) &= \sqrt{\frac{\mu(y)}{\mu(x)}} \tilde{g}(x, y) \end{aligned} \tag{3.23}$$

where $g(x, y) = g(y, x)$, $\tilde{g}(x, y) = \tilde{g}(y, x)$, and for all $x \neq y$,

$$\tilde{g}(x, y) \leq g(x, y) \tag{3.24}$$

Then for any non-intersecting sets $A, D \subset \Gamma$,

$$\text{cap}(A, D) \geq \widetilde{\text{cap}}(A, D) \tag{3.25}$$

Proof: It is obvious that for any function $h \in \mathcal{H}_D^A$,

$$\Phi(h) \geq \tilde{\Phi}(h) \tag{3.26}$$

Thus

$$\text{cap}(A, D) = \Phi(h_{A,D}) \geq \tilde{\Phi}(h_{A,D}) \geq \inf_{h \in \mathcal{H}_D^A} \tilde{\Phi}(h) = \widetilde{\text{cap}}(A, D) \tag{3.27}$$

which proves the theorem. \diamond

Theorem 3.3 will mostly be used by simply setting some of the transition probabilities $p(x, y)$ equal to zero. It is clear that if enough of these are set to zero, we obtain a chain where everything can be, computed easily. But then it is likely that the lower bound obtained will be very bad (like zero). The trick will be to guess which transitions can be switched off without altering the capacities too much, and still to simplify enough to be able to compute it. How to do this is quite an art, just as the choice of a good test function is for the upper bound. We will see how one can somewhat systematically use both bounds iteratively to arrive at good guesses that in some cases lead to (almost) coinciding upper and lower bounds.

It is now time that we learn how to compute things in at least one simple setting, the one-dimensional nearest neighbor random walk.

4. 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

$$p(x, y) = \begin{cases} \sqrt{\frac{\mu(y)}{\mu(x)}}g(x, y), & \text{if } y = x \pm \epsilon, \\ 1 - p(x, x + \epsilon) - p(x, x - \epsilon), & \text{if } x = y, \\ 0, & \text{else} \end{cases} \quad (4.1)$$

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

Exercise 4.1: Show that any nearest neighbor walk can be written in this form, i.e. show that $\mu(x)$ can be expressed in terms of the transition rates $p(x, y)$.

Exercise 4.2: Show that a possible choice is (for $x \neq y$)

$$p(x, y) = \begin{cases} \frac{1}{2}, & \text{if } y = x \pm \epsilon \text{ and } \mu(y) > \mu(x) \\ \frac{1}{2} \frac{\mu(y)}{\mu(x)}, & \text{if } y = x \pm \epsilon \text{ and } \mu(y) \leq \mu(x) \\ 0, & \text{else} \end{cases} \quad (4.2)$$

What is special about this choice?

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

$$h_{b,a}(x) = \mathbb{P}_x[\tau_b < \tau_a] \quad (4.3)$$

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

$$\begin{aligned} p(x, x + \epsilon)(h(x + \epsilon) - h(x)) + p(x, x - \epsilon)(h(x - \epsilon) - h(x)) &= 0, & a < x < b \\ h(a) &= 0 \\ h(b) &= 1 \end{aligned} \quad (4.4)$$

Note that the first equation can be conveniently written as

$$p(x, x + \epsilon)(h(x + \epsilon) - h(x)) = p(x, x - \epsilon)(h(x) - h(x - \epsilon)) \quad (4.5)$$

Setting $d(x) = h(x) - h(x - \epsilon)$, we get that

$$d(x + \epsilon) = \frac{p(x, x - \epsilon)}{p(x, x + \epsilon)}d(x) \quad (4.6)$$

so that

$$d(x) = \prod_{z=a+\epsilon}^{x-\epsilon} \frac{p(z, z-\epsilon)}{p(z, z+\epsilon)} d(a+\epsilon) \quad (4.7)$$

Using reversibility, the product can be written as

$$\prod_{z=a+\epsilon}^{x-\epsilon} \frac{p(z, z-\epsilon)}{p(z, z+\epsilon)} = \prod_{z=a+\epsilon}^{x-\epsilon} \frac{\mu(z)}{\mu(x+\epsilon)} \frac{p(z, z-\epsilon)}{p(z+\epsilon, z)} = \frac{\mu(a+\epsilon)}{\mu(x)} \frac{p(a+\epsilon, a)}{p(x, x-\epsilon)} \quad (4.8)$$

But

$$h(x) = d(x) + d(x-\epsilon) + d(x-2\epsilon) + \cdots + d(a+\epsilon) + h(a) \quad (4.9)$$

so that

$$h(x) = \sum_{y=a+\epsilon}^x \frac{\mu(a+\epsilon)}{\mu(y)} \frac{p(a+\epsilon, a)}{p(y, y-\epsilon)} d(a+\epsilon) + h(a) \quad (4.10)$$

Now $h(a) = 0$, it remains to determine $d(a+\epsilon)$ from the condition $h(b) = 1$, i.e.

$$1 = \sum_{y=a+\epsilon}^b \frac{\mu(a+\epsilon)}{\mu(y)} \frac{p(a+\epsilon, a)}{p(y, y-\epsilon)} d(a+\epsilon) \quad (4.11)$$

i.e.

$$d(a+\epsilon) = \frac{1}{\sum_{y=a+\epsilon}^b \frac{\mu(a+\epsilon)}{\mu(y)} \frac{p(a+\epsilon, a)}{p(y, y-\epsilon)}} \quad (4.12)$$

Hence

$$\begin{aligned} h(x) &= \frac{\sum_{y=a+\epsilon}^x \frac{\mu(a+\epsilon)}{\mu(y)} \frac{p(a+\epsilon, a)}{p(y, y-\epsilon)}}{\sum_{y=a+\epsilon}^b \frac{\mu(a+\epsilon)}{\mu(y)} \frac{p(a+\epsilon, a)}{p(y, y-\epsilon)}} \\ &= \frac{\sum_{y=a+\epsilon}^x \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}}{\sum_{y=a+\epsilon}^b \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}} \end{aligned} \quad (4.13)$$

Example. Let the transition rates be defined as in Exercise 2, and let

$$\mu(x) = \exp(-f(x)/\epsilon) \quad (4.14)$$

with e.g.

$$f(x) = \frac{1}{4}x^4 - \frac{1}{2}c^2x^2 + k(\epsilon) \quad (4.15)$$

f has its two (local and global) minima at $\pm c$ and for $0 < \epsilon \ll 1$, this implies that μ is concentrated near the two points $\pm c$. Note that with this choice of rates, if $f(x+\epsilon) > f(x)$,

$$p(x, x+\epsilon) = \frac{1}{2}e^{(f(x)-f(x+\epsilon))/\epsilon} \approx \frac{1}{2}e^{-f'(x)} \quad (4.16)$$

that is, the probability to make a step upwards in the “landscape” described by f is exponentially decreasing in the slope of f . These are thus reasonable transition probabilities for a walker in a mountainous landscape.

One of the most interesting questions is then to compute $\mathbb{P}_x[\tau_c < \tau_{-c}]$. (We assume that $c \in \epsilon\mathbb{Z}$). Obviously, due to the simple geometry of our problem, $\mathbb{P}_x[\tau_c < \tau_{-c}] = 0$, if $x < -c$, and $\mathbb{P}_x[\tau_c < \tau_{-c}] = 1$, if $x > c$. If $-c < x < c$, Eq. (4.13) gives

$$\mathbb{P}_x[\tau_c < \tau_{-c}] = \frac{\sum_{y=-c+\epsilon}^x e^{+f(y)/\epsilon}}{\sum_{y=-c+\epsilon}^0 e^{+f(y)/\epsilon} + \sum_{y=\epsilon}^c e^{+f(y-\epsilon)/\epsilon}} \quad (4.17)$$

for $x \leq 0$. For small ϵ , such integrals can easily be analysed using simple saddle point approximations. Looking at the denominator, it is clear that its main contribution comes from the terms in the sum where $f(x)$ is maximal, i.e. from a small neighborhood of 0. A simple way to estimate such sums is by approximating with integrals.

$$\mathbb{P}_x[\tau_c < \tau_{-c}] \approx \frac{\int_{-c}^x \exp\left(+\left(\frac{y^4}{4} - \frac{c^2 y^2}{2}\right)/\epsilon\right) dy}{\int_{y=-c}^c \exp\left(+\left(\frac{y^4}{4} - \frac{c^2 y^2}{2}\right)/\epsilon\right) dy} \quad (4.18)$$

The quality of this approximation by integrals differs: If the integrand has its maximum in the interior of the domain of integration, the sum and the integral differ by at most a factor $(1 + O(\sqrt{\epsilon}))$. If the integrand has its maximum at the boundary, they differ by a constant depending on the derivative of f at the boundary. In the latter case one can however estimate the sum itself quite easily. More details on how to compute integrals and sums of this form are given in Appendix 1.

The integral in the denominator is easily estimated

$$\int_{-c}^c \exp\left(+\left(\frac{y^4}{4} - \frac{c^2 y^2}{2}\right)/\epsilon\right) dy = \sqrt{\frac{2\pi\epsilon}{c^2}}(1 + O(\epsilon)) \quad (4.19)$$

The treatment of the numerator depends a little on the values of x . If $x < 0 - \delta$, for $\delta >$, independent of ϵ , the integral is dominated by the contribution from a neighborhood of size $\epsilon^{1-\gamma}$, for any $\gamma > 0$. Thus a first order expansion in the exponent gives the leading value, and one finds that

$$\int_{y=-c}^x \exp\left(+\left(\frac{x^4}{4} - \frac{c^2 x^2}{2}\right)/\epsilon\right) dy = \exp\left(+\left(\frac{x^4}{4} - \frac{c^2 x^2}{2}\right)/\epsilon\right) \frac{\epsilon}{x^3 - c^2 x} (1 + O(\epsilon)) \quad (4.20)$$

so that we have

$$\mathbb{P}_x[\tau_c < \tau_{-c}] \approx \exp\left(+\left(\frac{x^4}{4} - \frac{c^2 x^2}{2}\right)/\epsilon\right) \frac{c\sqrt{2\epsilon}}{\sqrt{\pi}(x^3 - c^2 x)} \quad (4.21)$$

A more precise evaluation of the actual discrete sum gives that actually

$$\mathbb{P}_x[\tau_c < \tau_{-c}] \approx \exp\left(\left(\frac{x^4}{4} - \frac{c^2 x^2}{2}\right)/\epsilon\right) \frac{c\sqrt{2\epsilon}}{\sqrt{\pi}(1 - e^{-x^3 + c^2 x})} \quad (4.22)$$

We see that this probability is exponentially small, since $(\frac{x^4}{4} - \frac{c^2 x^2}{2}) < 0$, and up to the prefactor behaves just like $\mu(0)/\mu(x)$.

By the same argument, for $x > 0$, we get that

$$\mathbb{P}_x[\tau_c < \tau_{-c}] = 1 - \exp\left(\left(\frac{x^4}{4} - \frac{c^2 x^2}{2}\right)/\epsilon\right) \frac{c\sqrt{2\epsilon}}{\sqrt{\pi}(1 - e^{-x^3 + c^2 x})} (1 + O(\sqrt{\epsilon})) \quad (4.23)$$

Being a bit more careful, one can show that the formulas (4.22) and (4.23) still hold if $|x| \gg \epsilon^{1/2}$, while for $|x| \sim \epsilon^{1/2}$, we can expand the exponent around zero to second order and get effectively

$$\mathbb{P}_{\epsilon^{1/2}z}[\tau_c < \tau_{-c}] = \sqrt{\frac{2c^2}{\pi}} \int_{-\infty}^z e^{-c^2 z^2/2} dz \quad (4.24)$$

Similarly, if x is close to $-c$ we have to modify formula (4.23) and take the quadratic term in the Taylor expansion of f into account. Since we will soon compute this probability for $x = -c$, we will not do the computation here.

We have seen in our example that the formulas obtained for the equilibrium potential in the one-dimensional model yield quite explicit and precise answers in some cases.

Aside: A diffusion approximation. It is instructive to compare at this point the discrete Markov chain with its diffusion counterpart. Without going into details, we may consider a continuous state continuous time Markov process on \mathbb{R} with generator

$$L_\epsilon = -\epsilon \frac{d^2}{dx^2} + f'(x) \frac{d}{dx} \quad (4.25)$$

Also for this process it is true that, for $x \in (a, b)$,

$$\mathbb{P}_x[\tau_a < \tau_b] = h_{b,a}(x) \quad (4.26)$$

where $h_{b,a}$ solves the boundary value problem

$$\begin{aligned} L_\epsilon h_{b,a}(x) &= 0, x \in (a, b) \\ h_{b,a}(x) &= 0, x \leq a \\ h_{b,a}(x) &= 1, x \geq b \end{aligned} \quad (4.27)$$

Since we are in dimension one, this problem is reduced to solving an ordinary second order differential equation of a particularly nice form, namely

$$\left(-\epsilon \frac{d}{dx} + f'(x)\right) h'(x) = 0 \quad (4.28)$$

If we solve first for h' , we see that the general solution is

$$h'(x) = ce^{f(x)/\epsilon} \quad (4.29)$$

and hence

$$h(x) = c \int_d^x \exp(f(y)/\epsilon) dy \quad (4.30)$$

it remains to determine the two integration constants c and d from the boundary conditions $h(a) = 0, h(b) = 1$. The first condition implies readily $d = a$, and the second $c = \frac{1}{\int_a^b \exp(f(x)/\epsilon)}$, so that we get

$$h_{b,a}(x) = \frac{\int_a^x \exp(f(y)/\epsilon) dy}{\int_a^b \exp(f(y)/\epsilon) dy} \quad (4.31)$$

We see that this is the same as the approximation to the equilibrium potential in the discrete case, after we approximated the sums in (4.17) by integrals. The diffusion process generated by L_ϵ is thus similar to our Markov chain. It is usually called the *diffusion approximation* to the random walk. Note that there is a difference here from the more familiar limit theorems (law of large numbers, central limit theorem): we do not really take a limit, but we compare two processes with finite values of ϵ . As one sees, some computations are more easily done in the continuous case, and this model is somehow *the* standard toy model for a metastable system.

Capacities. We now continue the analysis of this model by computing capacities. We consider

$$\mathbb{P}_a[\tau_b < \tau_a] \equiv e_{b,a}(a) \quad (4.32)$$

Eq. (3.10) becomes in this case

$$\begin{aligned} e_{b,a}(a) &= p(a, a + \epsilon)h(a + \epsilon) + p(a, a - \epsilon)h(a - \epsilon) \\ &= p(a, a + \epsilon)h(a + \epsilon) \end{aligned} \quad (4.33)$$

since $h(a - \epsilon) = 0$. Inserting the formula (4.13) for h , we get

$$\begin{aligned}
 e_{b,a}(a) &= p(a, a + \epsilon) \frac{\sum_{y=a+\epsilon}^{a+\epsilon} \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}}{\sum_{y=a+\epsilon}^b \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}} \\
 &= \frac{\frac{p(a, a+\epsilon)}{\mu(a+\epsilon)p(a+\epsilon, a)}}{\sum_{y=a+\epsilon}^b \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}} \\
 &= \frac{1}{\sum_{y=a+\epsilon}^b \frac{\mu(a)}{\mu(y)} \frac{1}{p(y, y-\epsilon)}}
 \end{aligned} \tag{4.34}$$

Consequently, we get for the capacity

$$\text{cap}(a, b) = \frac{1}{\sum_{y=a+\epsilon}^b \frac{1}{\mu(y)} \frac{1}{p(y, y-\epsilon)}} \tag{4.35}$$

Remark: Formula (4.35) 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 (4.35) 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 Snell². I will not overly insist on this interpretation in these lectures, since all what is ever used about it are the inequalities that follow from the Dirichlet principle, but whoever likes to think in terms of electric networks may of course do so.

Example. *In our example, we see that*

$$\text{cap}(-c, c) = \frac{1}{2 \sum_{y=-c+\epsilon}^0 e^{+f(y)/\epsilon} + 2 \sum_{y=\epsilon}^c e^{+f(y-\epsilon)/\epsilon}} \tag{4.36}$$

Note that the capacity depends on the choice of the invariant measure (while the probabilistic quantities will not). A natural choice here is to choose μ as a probability measure. That means that $k(\epsilon)$ must be chosen such that

$$\sum_{x \in \epsilon\mathbb{Z}} \exp(-f(x)/\epsilon) = 1 \tag{4.37}$$

²P.G. Doyle and J.L. Snell, “Random walks and electrical networks”, Carus Mathematical Monographs, 22, Mathematical Association of America, Washington, DC, 1984; note that there is a reprint available for free on the Internet: <http://front.math.ucdavis.edu/math.PR/0001057>.

But

$$\begin{aligned}
\sum_{x \in \epsilon\mathbb{Z}} \exp(-f(x)/\epsilon) &\approx \epsilon^{-1} \int dx \exp(-f(x)/\epsilon) \\
&\approx 2 \exp\left(-k(\epsilon)/\epsilon + \frac{c^4}{4\epsilon}\right) \epsilon^{-1} \int dx \exp\left(-\frac{2c^2x^2}{2\epsilon}\right) \\
&= 2e^{-k(\epsilon)/\epsilon + \frac{c^4}{4\epsilon}} \epsilon^{-1} \sqrt{\frac{2\epsilon\pi}{2c^2}} \\
&= 2 \exp\left(-k(\epsilon)/\epsilon + \frac{c^4}{4\epsilon}\right) \sqrt{\frac{2\pi}{2c^2\epsilon}}
\end{aligned} \tag{4.38}$$

or

$$e^{k(\epsilon)/\epsilon} = 2 \exp\left(\frac{c^4}{4\epsilon}\right) \sqrt{\frac{2\pi}{2c^2\epsilon}} \tag{4.39}$$

For later reference, we write the ensuing explicit form for the invariant measure

$$\mu(x) = \frac{1}{2} \exp\left(-\frac{x^4}{4} - \frac{c^2x^2}{2} + \frac{c^4}{4}\right) \sqrt{\frac{2c^2\epsilon}{2\pi}} (1 + O(\sqrt{\epsilon})) \tag{4.40}$$

Note that it is easy to remember the factor $\sqrt{\epsilon}$: The sum over $\mu(x)$ is dominated by the about $1/\sqrt{\epsilon}$ terms that fall in a neighborhood of size $\sqrt{\epsilon}$ of the positions of the absolute minima of $f(x)$; also, the absolute minimum of f is essentially zero.

Combining this with the estimate (4.19), we see that

$$\text{cap}(-c, c) = \frac{1}{\sqrt{2}} \frac{c^2\epsilon}{4\pi} \exp\left(-\frac{c^4}{4\epsilon}\right) (1 + O(\sqrt{\epsilon})) \tag{4.41}$$

Consequently we get for the escape probability from $-c$:

$$\mathbb{P}_{-c}[\tau_c < \tau_{-c}] = \sqrt{\frac{c^2\epsilon}{8\pi}} \exp\left(-\frac{c^4}{4\epsilon}\right) \tag{4.42}$$

Exercise 4.3: Show that the same formula holds for $\text{cap}(-a, b)$ whenever $a, b > 0$!

It is instructive to look at what we could easily get as an upper bound from the variational representation of the capacity. This just requires us to guess a candidate for the equilibrium potential. We have to find a function h that equals 0 at $-c$ and 1 at c . Clearly it will be optimal to set $h(x) = 0$ for all $x \leq -c$ and $h(x) = 1$ for all $x \geq c$. Between $-c$ and c h has to go from 0 to 1. The Dirichlet form basically counts the square of the gradient weighted with the measure μ . Thus it will be good to concentrate the gradient where the measure $\mu(u)$ is small, which is near zero. The simplest choice would then be $h(x) = 0$, for $x < 0$, and $h(x) = 1$, for $x \geq 0$. This yields the bound

$$\text{cap}(-c, c) \leq \mu(-\epsilon)p(-\epsilon, 0) = \mu(0) = \exp\left(-\frac{c^4}{4\epsilon}\right) \sqrt{\frac{c^2\epsilon}{4\pi}} \tag{4.43}$$

Comparing with the true answer, this is not such a bad bound; in fact, it is off only by about a factor of $1/\sqrt{\epsilon}$. Being a little more careful, one can get a bound that differs from the correct answer only by a multiplicative constant:

Exercise 4.4: Choose a test function

$$h(x) = \begin{cases} 0, & x \leq \sqrt{\epsilon} \\ \epsilon^{-1/2}(x + \sqrt{\epsilon})/2, & -\sqrt{\epsilon} < x < \sqrt{\epsilon} \\ 1, & x \geq \sqrt{\epsilon} \end{cases} \quad (4.44)$$

and show that this yields an upper bound for the capacity that has the correct behaviour as a function of ϵ .

We conclude our example by computing the capacity $\text{cap}(-c, -a)$ for $a > 0$. Then

$$\text{cap}(-c, -a) = \frac{1}{\sum_{y=-c+\epsilon}^{-a} e^{+f(y)/\epsilon}} \quad (4.45)$$

In that case the sum is dominated by the contribution from terms close to $x = -a$, and the same arguments that lead to (4.20) show that

$$\text{cap}(-c, -a) = \frac{1}{(1 - e^{-a^3+c^2a})} \sqrt{\frac{2c^2\epsilon}{2\pi}} \exp\left(\left(-\frac{a^4}{4} + \frac{c^2a^2}{2}\right)/\epsilon\right) (1 + O(\sqrt{\epsilon})) \quad (4.46)$$

Hence

$$\mathbb{P}_{-c}[\tau_{-a} < \tau_{-c}] = \frac{1}{(1 - e^{-a^3+c^2a})} \exp\left(\left(-\frac{a^4}{4} + \frac{c^2a^2}{2}\right)/\epsilon\right) (1 + o(\sqrt{\epsilon})) \quad (4.47)$$

5. Mean hitting times.

We now return to the general setting of Section 3. Our next task is to derive formulas for the mean values of hitting times τ_A . As in Section 3 we first derive a forward equation for $\mathbb{E}_x \tau_A$ by considering what can happen in the first step:

$$\mathbb{E}_x \tau_A = \sum_{y \in A} p(x, y) + \sum_{y \notin A} p(x, y)(1 + \mathbb{E}_y \tau_A) \quad (5.1)$$

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

$$w_A(x) \equiv \begin{cases} \mathbb{E}_x \tau_A, & \text{if } x \in \Gamma \setminus A \\ 0, & \text{if } x \in A \end{cases} \quad (5.2)$$

we see that (5.1) can be written in the nicer form

$$w_A(x) = \sum_{y \in \Gamma} p(x, y)w_A(y) + 1 \quad (5.3)$$

we see that (5.1) can be written in the nicer form

$$w_A(x) = \sum_{y \in \Gamma} p(x, y)w_A(y) + 1 \quad (5.4)$$

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

$$\begin{aligned} Lw_A(x) &= 1, & x \in G \setminus A \\ w_A(x) &= 0, & x \in A \end{aligned} \quad (5.5)$$

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

$$\mathbb{E}_x \tau_A = \sum_{y \in A} p(x, y) + \sum_{y \notin A} p(x, y)(1 + \mathbb{E}_y \tau_A) \quad (5.6)$$

or in compact form

$$\mathbb{E}_x \tau_A = Pw_A(x) + 1 = -Lw_A(x) + 1 \quad (5.7)$$

We will sometimes have to consider mean hitting times under the condition that some other set is avoided, e.g. for $A \cap D = \emptyset$, we consider $\mathbb{E}_x \tau_A \mathbb{1}_{\tau_A < \tau_D}$. Using the same reasoning as before, we see that the function

$$w_{A,D}(x) \equiv \begin{cases} \mathbb{E}_x \tau_A \mathbb{1}_{\tau_A < \tau_D}, & \text{if } x \in \Gamma \setminus (A \cup D) \\ 0, & \text{if } x \in A \cup D \end{cases} \quad (5.8)$$

satisfies the Dirichlet problem

$$\begin{aligned} Lw_{A,D}(x) &= h_{A,D}(x), & x \in G \setminus (A \cup D) \\ w_{A,D}(x) &= 0, & x \in A \cup D \end{aligned} \quad (5.9)$$

where $h_{A,D}$ is the equilibrium potential.

Equations (5.5) and (5.9) are special cases of the general Dirichlet problem

$$\begin{aligned} Lf(x) &= g(x), & x \in \Gamma \setminus B \\ f(x) &= 0 \end{aligned} \quad (5.10)$$

for some set B and some function f . We have seen in Proposition 3.1 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 (5.10) has a unique solution that can (by linearity) be represented in the form

$$f(x) = \sum_{y \in \Gamma \setminus B} G_{\Gamma \setminus B}(x, y)g(y) \quad (5.11)$$

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

$$\begin{aligned} L^{\Gamma \setminus B}(x, y) &= L(x, y), \quad x, y \in \Gamma \setminus B \\ L^{\Gamma \setminus B}(x, y) &= 0, \quad x \in B \vee y \in B \end{aligned} \quad (5.12)$$

We will call $L^{\Gamma \setminus B}$ the Dirichlet operator on $\Gamma \setminus B$. Note that while L is a positive operator, due to Proposition 3.1, $L^{\Gamma \setminus B}$ is *strictly positive* whenever $B \neq \emptyset$. The inverse operator $G_{\Gamma \setminus B}(x, y)$ 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 (3.10) 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 $h_{A,D}(x) = 1 - h_{D,A}(x)$, (3.10) can also be written as

$$e_{A,D}(x) = Lh_{D,A}(x) \quad (5.13)$$

This can be rewritten as

$$\begin{aligned} Lh_{D,A}(x) &= 0, \quad x \in \Gamma \setminus (A \cup D) \\ Lh_{D,A}(x) &= e_{A,D}(x), \quad x \in D \\ h_{D,A}(x) &= 0, \quad x \in A \end{aligned} \quad (5.14)$$

Thus we can write

$$h_{D,A}(x) = \sum_{y \in D} G_{\Gamma \setminus A}(x, y) e_{A,D}(y) \quad (5.15)$$

Now consider a solution of the Dirichlet problem (5.10). Multiplying $f(x)$ by $\mu(x)e_{B,x}(x)$, for $x \in \Gamma \setminus B$, and then using the representation (5.11) we get

$$f(x)\mu(x)e_{B,x}(x) = \sum_{y \in \Gamma \setminus B} G_{\Gamma \setminus B}(x, y)g(y)\mu(x)e_{B,x}(x) \quad (5.16)$$

Now due to the symmetry of L ,

$$G_{\Gamma \setminus B}(x, y)\mu(x) = G_{\Gamma \setminus B}(y, x)\mu(y) \quad (5.17)$$

Inserting this into (5.16) and using (5.15) backwards with $D = \{x\}$ and $A = B$, we get

$$\begin{aligned} f(x)\mu(x)e_{B,x}(x) &= \sum_{y \in \Gamma \setminus B} G_{\Gamma \setminus B}(y, x)e_{B,x}(x)\mu(y)g(y) \\ &= \sum_{y \in \Gamma \setminus B} \mu(y)h_{x,B}(y) \end{aligned} \quad (5.18)$$

or

$$f(x) = \sum_{y \in \Gamma \setminus B} \frac{\mu(y) h_{x,B}(y)}{\mu(x) e_{B,x}(x)} g(y) \quad (5.19)$$

Since this is true for all functions g comparing with (5.11) we read off that

Proposition 5.1: *The Dirichlet Green's function for any set $B \subset G$ can be represented in terms of the equilibrium potential and capacities as*

$$G_{\Gamma \setminus B}(x, y) = \frac{\mu(y) h_{x,B}(y)}{\text{cap}(B, x)} \quad (5.20)$$

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

$$\mathbb{E}_x \tau_A = \sum_{y \in \Gamma \setminus A} \frac{\mu(y) h_{x,A}(y)}{\text{cap}(A, x)} \quad (5.21)$$

and

$$\mathbb{E}_x \tau_A \mathbb{1}_{\tau_A < \tau_D} = \sum_{y \in \Gamma \setminus A \cup D} \frac{\mu(y) h_{x,A \cup D}(y)}{\text{cap}(A \cup D, x)} h_{A,D}(y) \quad (5.22)$$

or

$$\mathbb{E}_x [\tau_A | \tau_A < \tau_D] = \frac{1}{h_{A,D}(x)} \sum_{y \in \Gamma \setminus A \cup D} \frac{\mu(y) h_{x,A \cup D}(y)}{\text{cap}(A \cup D, x)} h_{A,D}(y) \quad (5.23)$$

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

The one-dimensional chain. In the case of the one-dimensional chain of Section 4 we have all the ingredients to compute the mean arrival times explicitly. In fact, inserting (4.13) and (4.35) into (5.21), we get in this case (w.r.g. let $a < x$)

$$\begin{aligned} \mathbb{E}_x \tau_a &= \sum_{z=a+\epsilon}^x \frac{1}{\mu(z)} \frac{1}{p(z, z-\epsilon)} \left(\sum_{y=a+\epsilon}^{x-\epsilon} \frac{\sum_{z=a+\epsilon}^y \frac{\mu(y)}{\mu(z)} \frac{1}{p(z, z-\epsilon)}}{\sum_{z=a+\epsilon}^x \frac{1}{\mu(z)} \frac{1}{p(z, z-\epsilon)}} + \sum_{y=x}^{\infty} \mu(y) \right) \\ &= \sum_{y=a+\epsilon}^{x-\epsilon} \sum_{z=a+\epsilon}^y \frac{\mu(y)}{\mu(z)} \frac{1}{p(z, z-\epsilon)} + \sum_{y=x}^{\infty} \sum_{z=a+\epsilon}^x \frac{\mu(y)}{\mu(z)} \frac{1}{p(z, z-\epsilon)} \end{aligned} \quad (5.24)$$

Exercise 5.1: *Verify by explicit computation that the formula (5.24) provides a solution for the boundary value problem (5.2).*

Diffusion approximation. *In the particular case $\mu(x) = e^{f(x)/\epsilon}$, we can verify that if we approximate the solution (5.24) by*

$$w_a(x) = \int_a^x dy \int_a^y e^{(f(z)-f(y))/\epsilon} dz + \int_x^\infty dy \int_a^x e^{(f(z)-f(y))/\epsilon} dz \quad (5.25)$$

$x < a$, then $w_a(x)$ solves the boundary value problem

$$\begin{aligned} L_\epsilon w_a(x) &= 1, \quad , x < a \\ w_a(x) &= 0, \quad x = a \end{aligned} \tag{5.26}$$

with the additional boundary condition that $\frac{d}{dx}w_a(x) \downarrow 0$, as $x \rightarrow \infty$. Here L_ϵ is the operator defined in (4.26). In fact it is not very difficult to find this solution directly. The first step is to guess a particular solution of the equation

$$-\epsilon \frac{d}{dx}g(x) + f'(x)g(x) = 1 \tag{5.27}$$

One easily verifies that $g(x) = \epsilon^{-1} \int_x^\infty e^{(f(x)-f(y))/\epsilon} dy$ solves this equation. Thus the general solution of (5.27) is

$$g(x) + Ce^{f(x)/\epsilon} \tag{5.28}$$

Hence w_a must be of the form

$$w_a(x) = \int_a^x \left(g(y) + Ce^{f(y)/\epsilon} \right) dy \tag{5.29}$$

where the choice of the lower integration boundary already ensures the correct boundary condition $w_a(a) = 0$. The choice $C = 0$ is then imposed by the natural condition that while it is natural that the mean hitting time should tend to infinity with x , the derivative should not blow up, and actually go to zero, if the drift $f'(x)$ tends to infinity. It is a small exercise to verify that (5.29) with $C = 0$ and (5.25) are the same.

It is instructive to go back to our 'double well example' and investigate the behaviour of e.g. $\mathbb{E}_x \tau_{-c}$. Our formula in the diffusion approximation yields then

$$\mathbb{E}_x \tau_{-c} = \epsilon^{-1} \int_{-c}^x dy e^{f(y)/\epsilon} \int_y^\infty dz e^{-f(z)/\epsilon} \tag{5.30}$$

We see that as long as $x > 0$, there is essentially no dependence on x : The first integral is always dominated by the contribution from a small neighborhood of zero, while the second gets its contribution from a neighborhood of $-c$. Using the Laplace asymptotics as explained before and in the appendix, we obtain

i) For $-c < y < c$,

$$\int_y^\infty dz e^{-f(z)/\epsilon} = e^{-f(c)/\epsilon} \sqrt{\frac{2\pi\epsilon}{|f''(c)|}} (1 + O(\epsilon)) \tag{5.31}$$

ii) For $x > 0$,

$$\int_{-c}^x dy e^{f(y)/\epsilon} = e^{f(0)/\epsilon} \sqrt{\frac{2\pi\epsilon}{|f''(0)|}} (1 + O(\epsilon)) \quad (5.32)$$

Therefor we get in particular

$$\mathbb{E}_c \tau_{-c} = e^{(f(0)-f(c))/\epsilon} \sqrt{\frac{(2\pi)^2}{|f''(c)f''(0)|}} (1 + O(\epsilon)) \quad (5.33)$$

This is (particular case of) the celebrated Eyring-Kramers formula for the transition time between two metastable states in the case of the one-dimensional chain (resp. the one-dimensional diffusion) in a double well potential. Note that only properties of f at the start point c and at the “saddle point”, 0 , enter the formula.

As $x < 0$, the expected time begins to decrease: The first integral picks up only a contribution of $e^{f(x)/\epsilon}$, and the mean time is of order $\exp((f(x) - f(c))/\epsilon)$. This may still appear surprisingly long: should the process not simply go in at time of order $1/\epsilon$ to $-c$? Of course we know that the process will do just that with enormous probability. Nonetheless, with probability of order $\exp((f(x) - f(0))/\epsilon)$ it will decide to go to c first; but in this case the mean time of arrival is given by (5.33). Multiplying this with the probability of doing things this way yields the result. We see here a first instance of what we will have to beware of all the time: events of extremely small probability may often dominate mean values.

This interpretation is supported by the observation that the mean time to reach either $-c$ or c from any point x is very small. In fact, in the diffusion approximation we have now to solve the boundary value problem of the form (5.26) with zero boundary conditions in both $-c$ and c . Since the general form of the solution of the equation $L_\epsilon w_{\{-c,c\}}(x)$ is of the form given in (5.29), the second boundary condition (we consider the case $-c < x < c$) allows to determine C . In fact we must have

$$w_{\{-c,c\}}(c) = \int_{-c}^c (g(y) + C e^{f(y)/\epsilon}) dy = 0 \quad (5.34)$$

i.e.

$$C = -\frac{\int_{-c}^c dy g(y)}{\int_{-c}^c dy e^{f(y)/\epsilon}} \quad (5.35)$$

so that

$$\begin{aligned} w_{\{-c,c\}}(x) &= \epsilon^{-1} \int_{-c}^x dy e^{f(y)/\epsilon} \left(\int_y^\infty dz e^{-f(z)/\epsilon} - \frac{\int_{-c}^c dz e^{f(z)/\epsilon} \int_z^\infty dw e^{-f(w)/\epsilon}}{\int_{-c}^c dz e^{f(z)/\epsilon}} \right) \\ &= \frac{\int_{-c}^c dz e^{f(z)/\epsilon} \int_{-c}^x dy e^{f(y)/\epsilon} \int_y^z dw e^{-f(w)/\epsilon}}{\epsilon \int_{-c}^c e^{f(z)/\epsilon}} \end{aligned} \quad (5.36)$$

The computation of this integral using the Laplace method is somewhat tedious (as there are a number of cases to distinguish), and I will not write down the details of the computation.

The result is:

$$w_{\{-c,c\}}(c) = \begin{cases} |\ln \epsilon| \left(\frac{1}{|f''(-c)|} + \frac{1}{|f''(0)|} \right) + O(1), & \text{if } x = 0 \\ |\ln \epsilon| \frac{1}{|f''(-c)|} + O(1), & \text{if } -c < x < 0 \end{cases} \quad (5.37)$$

Here we assume x fixed independent of ϵ . Of course, in a neighborhood of order $\sqrt{\epsilon}$ about 0, the function interpolates between the two domains, and in a neighborhood of order $\sqrt{\epsilon}$ of $-c$, the function behaves like $|x - c|\sqrt{\epsilon}$.

The $\ln \epsilon$ behaviour of the mean time is clearly related to the difficulty the process has to move in a neighborhood of the critical points. Starting at 0, it takes a time of order $|\ln \epsilon|$ to “get away from 0” by a distance considerably larger than $\sqrt{\epsilon}$. Then the gradient of f is strong enough to impose a ballistic motion towards a neighborhood of order $\sqrt{\epsilon}$ of c or $-c$. There again the process slows down and needs time of order $|\ln \epsilon|$ to actually hit the minimum of f .

Exercise 5.2: Interpret our results on the mean transition time in light of the formula (5.23).

Exercise 5.3: Derive a formula for $\mathbb{E}_x[\tau_{-c} | \tau_{-c} < \tau_c]$. Interpret the result in terms of the behaviour of the process.

Renewal equations. The application of Proposition 5.1 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.

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:

$$\begin{aligned}\mathbb{P}_x[\tau_A < \tau_D] &= \mathbb{P}_x[\tau_A < \tau_{D \cup x}] + \mathbb{P}_x[\tau_x < \tau_{A \cup D} \wedge \tau_A < \tau_D] \\ &= \mathbb{P}_x[\tau_A < \tau_{D \cup x}] + \mathbb{P}_x[\tau_x < \tau_{A \cup D}] \mathbb{P}_x[\tau_A < \tau_D]\end{aligned}\tag{5.38}$$

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

$$\mathbb{P}_x[\tau_A < \tau_D] = \frac{\mathbb{P}_x[\tau_A < \tau_{D \cup x}]}{1 - \mathbb{P}_x[\tau_x < \tau_{A \cup D}]} = \frac{\mathbb{P}_x[\tau_A < \tau_{D \cup x}]}{\mathbb{P}_x[\tau_{A \cup D} < \tau_x]}\tag{5.39}$$

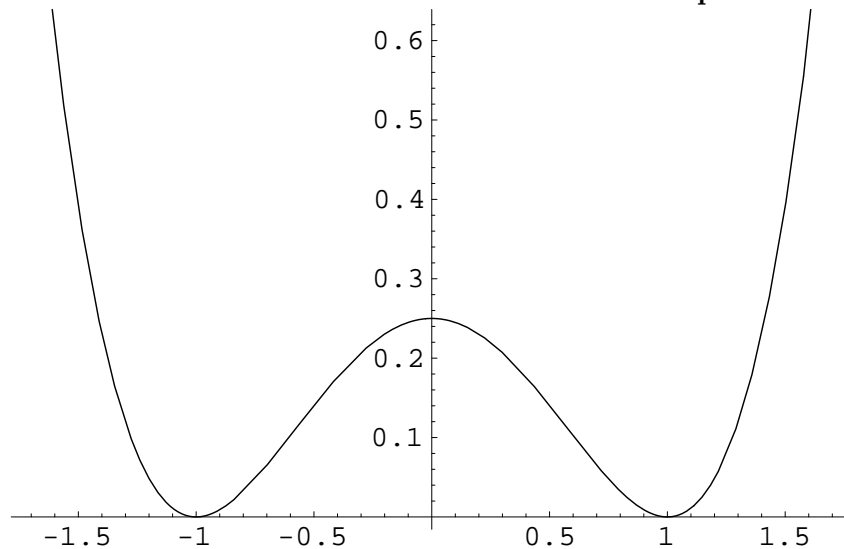
By elementary monotonicity properties this representation yields the bound

$$\mathbb{P}_x[\tau_A < \tau_D] \leq \frac{\mathbb{P}_x[\tau_A < \tau_x]}{\mathbb{P}_x[\tau_D < \tau_x]} = \frac{\text{cap}(x, A)}{\text{cap}(x, D)}\tag{5.40}$$

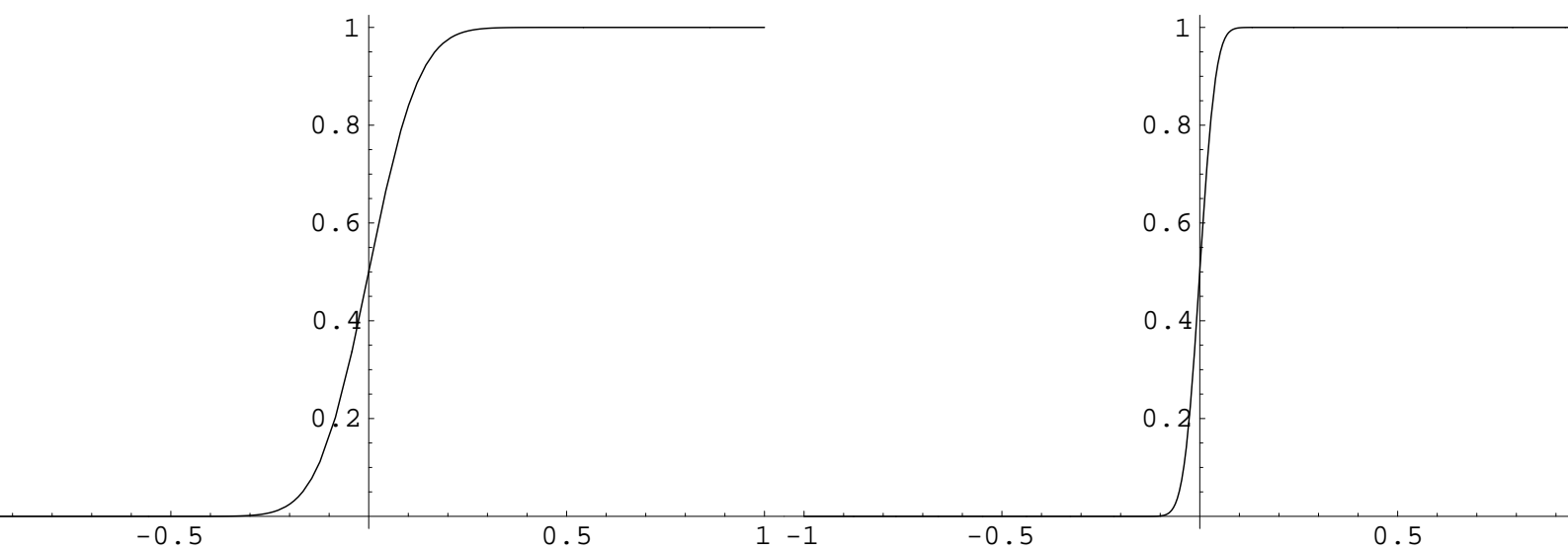
Of course this bound is useful only if $\frac{\text{cap}(x, A)}{\text{cap}(x, D)} < 1$, but since $\mathbb{P}_x[\tau_A < \tau_D] = 1 - \mathbb{P}_x[\tau_D < \tau_A]$, the applicability of this bound is quite wide. It is quite astonishing how far the simple use of this renewal bound will take us.

Exercise 5.4. Use the bound (5.40) in the case of the one dimensional chain with invariant measure $\exp(-\epsilon^{-1}f(x))$ and compare with the exact value. When is the approximation good?

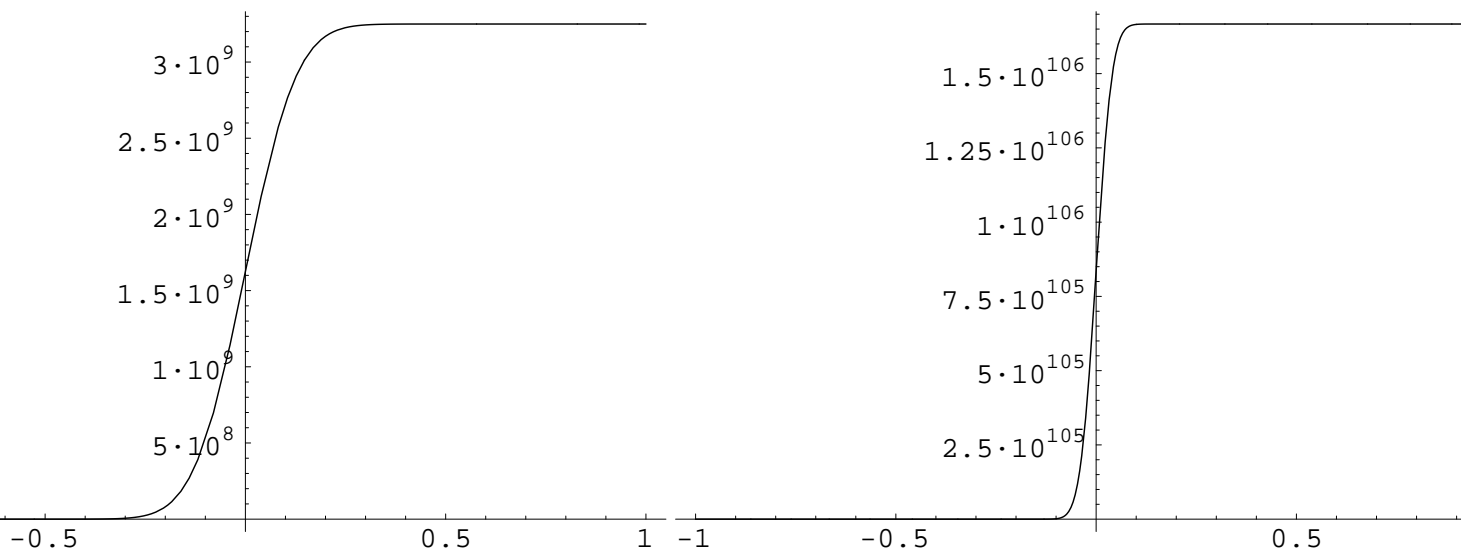
Some numerical illustrations in our one-dimensional example.



The function $f(x)$ with $c = 1$.

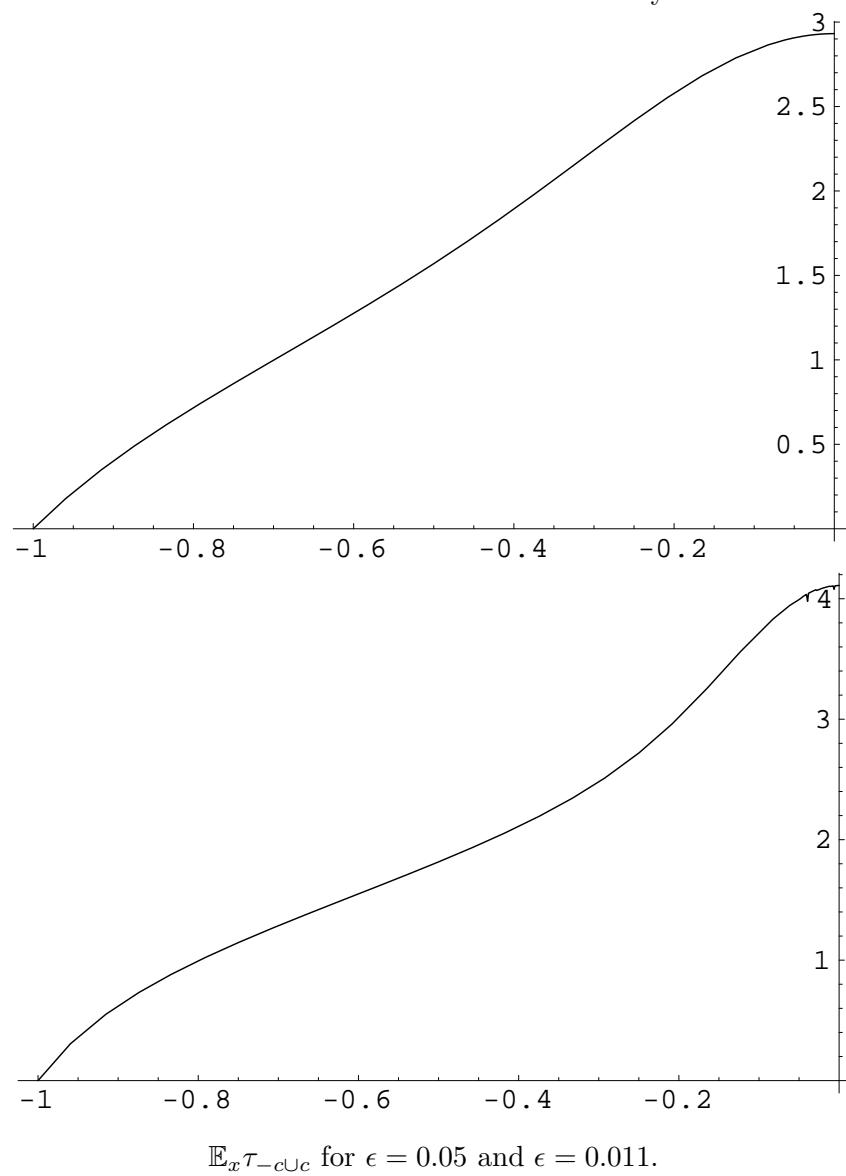


Equilibrium potential $h_{-c,c}(x)$ in the case $c = 1$ for $\epsilon = 0.01$ and $\epsilon = 0.001$

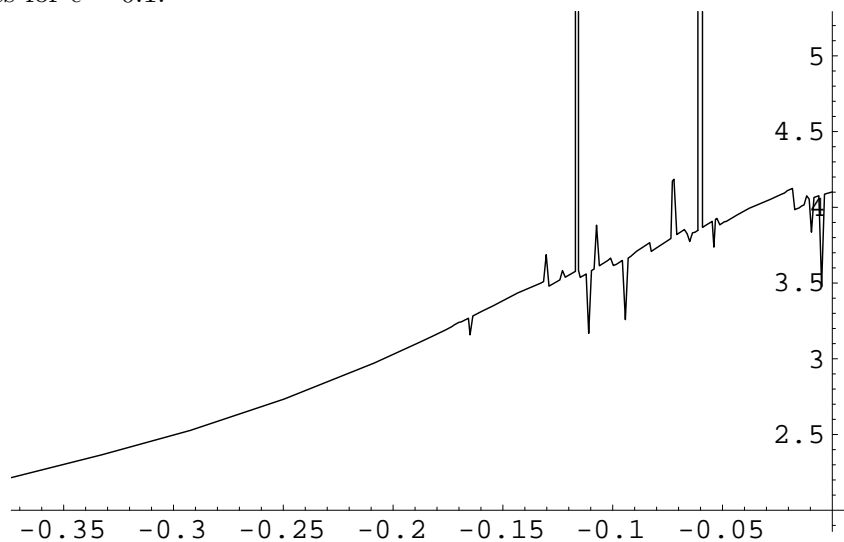


Mean hitting time $\mathbb{E}_x \tau_{-c}$ in the case $c = 1$ for $\epsilon = 0.01$ and $\epsilon = 0.001$

The times to reach either of the two minima are dramatically shorter:



The numerical evaluation of these quantities is rather tricky. Here is what standard Mathematica gives for $\epsilon = 0.1$.



6. Metastability.

We come now to a general definition of metastability in the context of discrete Markov chains. We may draw some intuition from the example of the one-dimensional chain with invariant measure $\exp(-\epsilon^{-1}f(x))$. Assume that $f(x)$ has a set of local minima $\mathcal{M} \equiv \{x_1, \dots, x_n\}$. Then obviously there exists a local maximum z_i between any two neighboring minima x_i and x_{i+1} . This leads to a natural partition of the real line (resp. $\epsilon\mathbb{Z}$) into *valleys*

$$A_i = (z_i, z_{i+1}) \quad (6.1)$$

containing the minimum x_i . The following facts are easily checked from our explicit formulae:

(i) For any $y \in A_i$,

$$\mathbb{P}_y[\tau_{x_i} < \tau_{\mathcal{M} \setminus x_i}] > \frac{1}{2} \quad (6.2)$$

(ii) For any $y \in \Gamma$,

$$\mathbb{E}_y \tau_{\mathcal{M}} \leq C\epsilon^{-1} |\ln \epsilon| \quad (6.3)$$

and

$$\mathbb{P}_y[\tau_{\mathcal{M}} < \tau_y] \geq C\epsilon^{1/2} \quad (6.4)$$

(iii) For any $x_i \in \mathcal{M}$,

$$\mathbb{E}_{x_i} \tau_{\mathcal{M} \setminus x_i} \approx e^{(\min(f(z_i), f(z_{i+1})) - f(x_i))/\epsilon} \quad (6.5)$$

respectively

$$\mathbb{P}_{x_i}[\tau_{\mathcal{M} \setminus x_i} < \tau_{x_i}] \approx e^{-(\min(f(z_i), f(z_{i+1})) - f(x_i))/\epsilon} \quad (6.6)$$

In simple terms, wherever the process starts, it will go quickly to one minimum (and more precisely to the one in the valley it started in) and then take a very long time to go to another minimum. This corresponds to our intuitive notion of metastability. We shall see that it is quite reasonable to define metastability in general by simply requiring properties like this above.

Definition 6.1: *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*

$$\frac{\sup_{x \in \mathcal{M}} \mathbb{P}_x[\tau_{\mathcal{M} \setminus x} < \tau_x]}{\inf_{y \notin \mathcal{M}} \mathbb{P}_y[\tau_{\mathcal{M}} < \tau_y]} \leq \rho \ll 1 \quad (6.7)$$

Remark: More properly we should speak of ρ -metastability. However, in most cases we will think of metastability of an asymptotic property of a *family* of Markov processes indexed by a parameter ϵ such that the corresponding constant $\rho(\epsilon)$ tends to zero with ϵ .

We will see that Definition 6.1 is (at least if Γ is finite) equivalent to an alternative definition involving averaged hitting times.

Definition 6.2: *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*

$$\frac{\inf_{x \in \mathcal{M}} \mathbb{E}_x \tau_{\mathcal{M} \setminus x}}{\sup_{y \notin \mathcal{M}} \mathbb{E}_y \tau_{\mathcal{M}}} \geq 1/\rho \gg 1 \quad (6.8)$$

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 6.1 exists implies a number of structural properties of the chain.

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 [BEGK2].

Lemma 6.3: *Assume that $x, y \in \Gamma$, $D \subset \Gamma$. Then, if for $0 < \delta < \frac{1}{2}$, $\text{cap}(y, D) \leq \delta \text{cap}(y, x)$, then*

$$\frac{1 - 2\delta}{1 - \delta} \leq \frac{\text{cap}(x, D)}{\text{cap}(y, D)} \leq \frac{1}{1 - \delta} \quad (6.9)$$

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

$$\text{cap}(x, D) = \text{cap}(D, x) = \sum_{z \in D} \mu(z) e_{x, D}(z) = \sum_{z \in D} \mu(z) \mathbb{P}_z[\tau_x < \tau_D] \quad (6.10)$$

Now

$$\begin{aligned} \mathbb{P}_z[\tau_x < \tau_D] &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_D, \tau_y \geq \tau_D] \\ &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_{D \cup y}] \mathbb{P}_x[\tau_D < \tau_y] \\ &= \mathbb{P}_z[\tau_x < \tau_D, \tau_y < \tau_D] + \mathbb{P}_z[\tau_x < \tau_{D \cup y}] \frac{\mathbb{P}_x[\tau_D < \tau_{y \cup x}]}{\mathbb{P}_x[\tau_{D \cup y} < \tau_x]} \end{aligned} \quad (6.11)$$

Here we used the Markov property at the optimal time τ_x to split the second probability into a product, and then the renewal equation (5.39). Now by assumption,

$$\frac{\mathbb{P}_x[\tau_D < \tau_{y \cup x}]}{\mathbb{P}_x[\tau_{D \cup y} < \tau_x]} \leq \frac{\mathbb{P}_x[\tau_D < \tau_x]}{\mathbb{P}_x[\tau_y < \tau_x]} \leq \delta \quad (6.12)$$

Inserting (6.12) into (6.11) we arrive at

$$\mathbb{P}_z[\tau_x < \tau_D^x] \leq \mathbb{P}_z[\tau_y < \tau_D, \tau_x < \tau_D] + \delta \mathbb{P}_z[\tau_x < \tau_{D \cup y}] \leq \mathbb{P}_z[\tau_y < \tau_D] + \delta \mathbb{P}_z[\tau_x < \tau_D] \quad (6.13)$$

Inserting this inequality into (6.10) implies

$$\text{cap}(x, D) \leq \sum_{z \in D} \mu(z) \mathbb{P}_z[\tau_y < \tau_D] + \delta \sum_{z \in D} \mu(z) \mathbb{P}_z[\tau_x < \tau_D] = \text{cap}(y, D) + \delta \text{cap}(x, D) \quad (6.14)$$

which implies the upper bound.

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

Lemma 6.3 has the following immediate corollary, which is the version of the ultrametric triangle inequality we are looking for:

Corollary 6.4: *Let $x, y, z \in \mathcal{M}$. Then*

$$\text{cap}(x, y) \geq \frac{1}{3} \min(\text{cap}(x, z), \text{cap}(y, z)) \quad (6.15)$$

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 $x \in \mathcal{M}$,

$$A(x) \equiv \left\{ z \in \Gamma \mid \mathbb{P}_z[\tau_x = \tau_{\mathcal{M}}] = \sup_{y \in \mathcal{M}} \mathbb{P}_z[\tau_y = \tau_{\mathcal{M}}] \right\} \quad (6.16)$$

Note that valleys may overlap, but from Lemma 6.3 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 Corollary will show that if y belongs to the valley of $m \in \mathcal{M}$, then either the capacity $\text{cap}(y, \mathcal{M} \setminus m)$ is essentially the same as $\text{cap}(m, \mathcal{M} \setminus m)$, 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 $\text{cap}(m, \mathcal{M} \setminus m)$, while the rest has virtually no mass, i.e. the process never really gets there.

Corollary 6.5: *Let $m \in \mathcal{M}$, $y \in A(m)$, and $D \subset \mathcal{M} \setminus m$. Then either*

$$\frac{1}{2} \leq \frac{\text{cap}(m, D)}{\text{cap}(y, D)} \leq \frac{3}{2} \quad (6.17)$$

or

$$\mu(y) \leq 3|\mathcal{M}| \frac{\mu(y)}{\text{cap}(y, \mathcal{M})} \text{cap}(m, D) \quad (6.18)$$

Proof: Lemma 6.3 implies that if $\text{cap}(m, y) \geq 3\text{cap}(m, D)$, then (6.17) holds. Otherwise,

$$\frac{\mu(y)}{\mu(m)} \leq 3 \frac{\mu(y)}{\text{cap}(y, m)} \frac{\text{cap}(m, D)}{\mu(m)} \quad (6.19)$$

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

$$\mathbb{P}_y[\tau_m \leq \tau_{\mathcal{M}}] \leq \frac{\text{cap}(y, m)}{\text{cap}(y, \mathcal{M})} \quad (6.20)$$

Hence

$$\text{cap}(y, \mathcal{M}) \leq |\mathcal{M}| \text{cap}(y, m) \quad (6.21)$$

which yields (6.18). \diamond

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 (5.21) 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 6.1.

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 (5.21)

$$\mathbb{E}_x \tau_J = \frac{\mu(x)}{\text{cap}(x, J)} \sum_{y \in J^c} \frac{\mu(y)}{\mu(x)} h_{x, J \setminus x}(y) \quad (6.22)$$

We want to estimate the summands in the sum (6.22). We will set $\inf_y \mu(y)^{-1} \text{cap}(y, \mathcal{M}) = a$. The following lemma provides the necessary control over the equilibrium potentials appearing in the sum.

Lemma 6.6: *Let $x \in \mathcal{M}$ and $J \subset \mathcal{M}$ with $x \notin J$. Then:*

(i) *If $x = m$, either*

$$h_{x,J}(y) \geq 1 - \frac{3}{2}|\mathcal{M}|a^{-1} \frac{\text{cap}(x, J)}{\mu(y)} \quad (6.23)$$

or

$$\mu(y) \leq 3|\mathcal{M}|a^{-1} \text{cap}(m, J) \quad (6.24)$$

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

$$\mu(y)h_{x,J}(y) \leq \frac{3}{2}|\mathcal{M}|a^{-1} \text{cap}(m, x) \quad (6.25)$$

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

$$h_{x,J}(y) \leq 3 \frac{\text{cap}(m, x)}{\text{cap}(m, J)} \quad (6.26)$$

and

$$h_{x,J}(y) \geq 1 - 3 \frac{\text{cap}(m, J)}{\text{cap}(m, x)} \quad (6.27)$$

or

$$\mu(y) \leq 3|\mathcal{M}|a^{-1} \max(\text{cap}(m, J), \text{cap}(m, x)) \quad (6.28)$$

Proof: We make use of the fact that by Lemma 6.2,

$$0 \leq h_{x,J}(y) \leq \frac{\text{cap}(y, x)}{\text{cap}(y, J)} \quad (6.29)$$

and

$$1 \geq h_{x,J}(y) \geq 1 - \frac{\text{cap}(y, J)}{\text{cap}(y, x)} \quad (6.30)$$

In case (i), we anticipate that only (6.30) will be useful. To get the first dichotomy, we use Corollary 6.5 to replace the numerator by $\text{cap}(m, J)$. To get the second assertion, note simply that

$$\frac{\text{cap}(m, J)}{\text{cap}(y, m)} \leq \frac{\mu(y)\text{cap}(m, J)}{\text{cap}(y, x)\mu(m)} \frac{\mu(m)}{\mu(y)} \quad (6.31)$$

and rewrite this inequality for $\frac{\mu(y)}{\mu(m)}$.

In case (ii), we use (6.29) and apply Corollary 6.5 to $\text{cap}(y, x)$.

In case (iii), we admit both possibilities and apply the corollary to both the numerators and the denominators. \diamond

Remark: Case (iii) in the preceding lemma is special in as much as it will not always give sharp estimates, namely whenever $\text{cap}(m, J) \sim \text{cap}(m, y)$. If this situation occurs, and the corresponding terms contribute to leading order, we cannot get sharp estimates with the tools we are exploiting here, and better estimates on the equilibrium potential will be needed.

Let us now apply this lemma to the computation of the sum (6.22) (we ignore the fact that the sets $A(m)$ may not be disjoint, as the overlaps give no significant contribution).

$$\sum_{y \in \mathcal{M}^c} \frac{\mu(y)}{\mu(x)} h_{x, J}(y) = \sum_{m \in \mathcal{M}} \frac{\mu(m)}{\mu(x)} \sum_{y \in A(m) \setminus J} \frac{\mu(y)}{\mu(m)} h_{x, J}(y) \equiv \sum_{m \in \mathcal{M}} \frac{\mu(m)}{\mu(x)} L(m) \quad (6.32)$$

(we ignore the fact that the sets $A(m)$ may not be disjoint, as the overlaps give no significant contribution).

We now estimate the terms $L(m)$ with the help of Lemma 6.6.

Lemma 6.7: *Let us assume that either $|\Gamma|$ is finite, or that $\mu(y)$ has the property that $\sum_{y: \mu(y) \leq \delta} \mu(y) \leq C\delta$, for some finite C . With the notation introduced above and the assumptions of Lemma 6.6, we have that*

(i) If $m = x$

$$L(x) \leq \frac{\mu(A(x))}{\mu(x)} \quad (6.33)$$

and

$$L(x) \geq \frac{\mu(A(x))}{\mu(x)} \left(1 - 6C|\mathcal{M}|a^{-1} \frac{\text{cap}(x, J)}{\mu(A(x))} \right) \quad (6.34)$$

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

$$L(m) \leq Ca^{-1}|\mathcal{M}| \frac{\text{cap}(m, x)}{\mu(m)} |\{y \in A(m) : \mu(y) \geq a^{-1}|\mathcal{M}|\text{cap}(m, x)\}| \quad (6.35)$$

for some constant C independent of ϵ .

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

$$L(m) \leq \frac{\mu(A(m))}{\mu(m)} \quad (6.36)$$

Moreover,

(iii.1) if $\text{cap}(m, J) \leq \frac{1}{3}\text{cap}(m, x)$, then

$$L(m) \geq \frac{\mu(A(m))}{\mu(m)} \left(1 - 3 \frac{\text{cap}(m, J)}{\text{cap}(m, x)} \right) \left(1 - C|\mathcal{M}|a^{-1} \frac{\text{cap}(m, x)}{\mu(A(m))} \right) \quad (6.37)$$

and

(iii.2) if $\text{cap}(m, J) \geq \frac{1}{3}\text{cap}(m, x)$, then

$$L(m) \leq \frac{\mu(A(m))}{\mu(m)} \frac{\text{cap}(m, x)}{\text{cap}(m, J)} + C|\mathcal{M}|a^{-1} \frac{\text{cap}(m, J)}{\mu(m)} \quad (6.38)$$

Proof: Basically the proof consists in inserting the estimates for the equilibrium potentials from Lemma 6.6 into the formulae for $L(m)$. In case (i) we obtain the upper bound trivially from the fact that $h_{x,J}(y) \leq 1$. For the lower bound we use that, for any $\epsilon > 0$,

$$\begin{aligned} L(x) &\geq \sum_{y:\mu(y) \geq 3|\mathcal{M}|\epsilon^{-1}a^{-1}\text{cap}(x,J)} \frac{\mu(y)}{\mu(x)} \left(1 - \frac{3}{2}|\mathcal{M}| \frac{\text{cap}(x, J)}{\mu(x)}\right) \\ &\geq \left(1 - \frac{a}{2}\right) \left(\frac{\mu(A(x))}{\mu(x)} - \sum_{y:\mu(y) < 3|\mathcal{M}|\epsilon^{-1}a^{-1}\text{cap}(x,J)} \frac{\mu(y)}{\mu(x)}\right) \\ &\geq \frac{\mu(A(x))}{\mu(x)} \left(1 - C3|\mathcal{M}|\epsilon^{-1}a^{-1} \frac{\text{cap}(x, J)}{\mu(A(x))}\right) \left(1 - \frac{\epsilon a}{2}\right) \end{aligned} \quad (6.39)$$

If ρ is sufficiently small one may choose ϵ such as to obtain the claimed estimate (6.34).

In the case we just use (6.25), unless $\mu(y)$ is so small that the bound $h \leq 1$ is even better, to get

$$L(m) \leq \sum_{y \in A(m) \setminus m: \mu(y) \geq \text{cap}(m, x)} \frac{3}{2}|\mathcal{M}|a^{-1} \frac{\text{cap}(m, x)}{\mu(m)} + C \frac{\text{cap}(m, x)}{\mu(m)} \quad (6.40)$$

In case (iii), the upper bound (6.36) is trivial, but only sensible if $\text{cap}(m, x) \leq \text{cap}(m, J)$. In this case the corresponding lower bound follows very much like in case (i). In the opposite case we use (6.26) resp. (6.28) to arrive at our conclusion. \diamond

Remark: The statement of Lemma 6.7 looks a little complicated due to the rather explicit error terms. Ignoring all small factors, its statement boils down to:

(i) There is always the term

$$L(x) \approx \frac{\mu(A(x))}{\mu(x)}$$

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

$$L(m) \leq \frac{\text{cap}(m, x)}{\mu(m)}$$

(iii) If $m \notin J \cup x$, it is always true that

$$L(m) \leq \frac{\mu(A(m))}{\mu(m)}$$

i.e. roughly of order one. This bound is achieved, if

(iii.1) $\text{cap}(m, J) \ll \text{cap}(m, x)$, whereas in the opposite case

(iii.2) $\text{cap}(m, J) \gg \text{cap}(m, x)$,

$$L(m) \leq \max\left(\frac{\text{cap}(m, x)}{\mu(m)}, \frac{\text{cap}(m, J)}{\text{cap}(m, J)}\right)$$

Of course these arguments use that quantities like $\frac{\mu(m)}{\mu(A(m))}$ are not too small, i.e. that the most massive points in a metastable set have a reasonably large mass (compared to say, $\rho(\epsilon)$). If this condition is violated, the idea to represent metastable sets by single points is clearly mislead. We will discuss later what has to be done in such cases.

Taking into account that the $L(m)$ appear with the prefactor $\mu(m)/\mu(x)$ in the expression (6.32), we see that contributions from case (ii) are always sub-dominant; in particular, when $J = \mathcal{M} \setminus x$, the term $m = x$ gives always the main contribution. The terms from case (iii) have a chance to contribute only if $\mu(m) \geq \mu(x)$. If that is the case, and we are in sub-case (iii.1), they indeed contribute, and potentially dominate the sum. In sub-case (iii.2) they may still contribute, if

$$\frac{\mu(m)\text{cap}(m, x)}{\mu(x)\text{cap}(m, J)} = \frac{\mathbb{P}_x[\tau_m < \tau_x]}{\mathbb{P}_m[\tau_J < \tau_m]}$$

is not small, which is to say when the process typically visits m often before it visits J .

We summarise these results in the following proposition:

Proposition 6.8: *With the notation and under the assumptions of Lemma 6.7,*

$$\begin{aligned} \mathbb{E}_x \tau_J &= \frac{\mu(A(x))}{\text{cap}(x, J)} (1 + O(\rho)) \\ &+ \sum_{\substack{m \in \mathcal{M} \setminus J \setminus x \\ \text{cap}(m, J) \leq \frac{1}{3} \text{cap}(m, x)}} \frac{\mu(A(m))}{\text{cap}(x, J)} \left(1 - O\left(\frac{\text{cap}(m, J)}{\text{cap}(m, x)}\right)\right) \\ &+ \sum_{\substack{m \in \mathcal{M} \setminus J \setminus x \\ \text{cap}(m, J) > \frac{1}{3} \text{cap}(m, x)}} O\left(\frac{\mu(A(m))}{\text{cap}(x, J)} \frac{\text{cap}(m, x)}{\text{cap}(m, J)} + \frac{\mu(x)}{\text{cap}(x, J)} \frac{\text{cap}(m, J)}{\mu(x)}\right) \\ &+ \sum_{m \in J} O(Ca^{-1} |\mathcal{M}| |\{y \in A(m) : \mu(y) \geq a^{-1} |\mathcal{M}| \text{cap}(m, x)\}|) \end{aligned}$$

where here all $O(\cdot)$ terms are to be understood as upper bounds.

A case of special interest occurs 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 6.9: *Let $x \in \mathcal{M}$ and $J \subset \mathcal{M} \setminus x$ be such a that for all $m \notin J \cup x$ either $\mu(m) \ll \mu(x)$ or $\text{cap}(m, J) \gg \text{cap}(m, x)$, then*

$$\mathbb{E}_x \tau_J = \frac{\mu(A(x))}{\text{cap}(x, J)} (1 + O(\rho)) \quad (6.41)$$

Proof: The proof of this result is straightforward from (6.22), (6.32) and Lemma 6.6. \diamond

Remark: In much the same way one can compute conditional mean times such as $\mathbb{E}_x[\tau_J | \tau_J \leq \tau_I]$. Formulae are given in [BEGK1, BEGK2] and we will not go into these issues any further here.

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

Lemma 6.10: *Let $z \notin \mathcal{M}$. Then*

$$\mathbb{E}_z \tau_{\mathcal{M}} \leq a^{-2} (|\{y : \mu(y) \geq \mu(z)\}| + C) \quad (6.42)$$

Proof: Using Lemma 6.2, we get that

$$\begin{aligned} \mathbb{E}_z \tau_{\mathcal{M}} &\leq \frac{\mu(z)}{\text{cap}(z, \mathcal{M})} \sum_{y \in \mathcal{M}^c} \frac{\mu(y)}{\mu(z)} \max \left(1, \frac{\text{cap}(y, z)}{\text{cap}(y, \mathcal{M})} \right) \\ &= \frac{\mu(z)}{\text{cap}(z, \mathcal{M})} \sum_{y \in \mathcal{M}^c} \frac{\mu(y)}{\mu(z)} \max \left(1, \frac{\mathbb{P}_y[\tau_z < \tau_y]}{\mathbb{P}_y[\tau_{\mathcal{M}} < \tau_y]} \right) \\ &\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\text{cap}(y, \mathcal{M})} \right)^2 \sum_{y \in \mathcal{M}^c} \max \left(\frac{\mu(y)}{\mu(z)}, \mathbb{P}_z[\tau_y < \tau_z] \right) \\ &\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\text{cap}(y, \mathcal{M})} \right)^2 \left(\sum_{y: \mu(y) \leq \mu(z)} \frac{\mu(y)}{\mu(z)} + \sum_{y: \mu(y) > \mu(z)} 1 \right) \\ &\leq \sup_{y \in \mathcal{M}^c} \left(\frac{\mu(y)}{\text{cap}(y, \mathcal{M})} \right)^2 (C + |\{y : \mu(y) > \mu(z)\}|) \end{aligned} \quad (6.43)$$

which proves the lemma. \diamond

Remark: If Γ is finite (resp. not growing too fast with ϵ), the above estimate combined with Theorem 6.9 shows that the two definitions of metastability we have given in terms of mean times resp. 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. We will later see that this definition can be rectified in the context of spectral estimates.

7. 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 [D1,D2,D3,FW,GS,HKS,KoMak,Ma,Mi,Sc,W1,W2].

We will show that Definition 6.1 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 $|\Gamma|$ is finite throughout this section.

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

$$\begin{aligned} Lf(x) &= \lambda f(x), & x \in \Gamma \setminus D \\ f(x) &= 0, & x \in D \end{aligned} \tag{7.1}$$

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 0 is an eigenvalue of L itself with the constant function the corresponding eigenfunction.

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

$$\begin{aligned} (L - \lambda)f(x) &= g(x), & x \in \Gamma \setminus D \\ f(x) &= 0, & x \in D \end{aligned} \tag{7.2}$$

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

$$f(x) = \sum_{y \in \Gamma \setminus D} G_{\Gamma \setminus D}^\lambda(x, y)g(y) \tag{7.3}$$

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

Equally, the boundary value problem

$$\begin{aligned} (L - \lambda)f(x) &= 0, & x \in \Gamma \setminus D \\ f(x) &= \phi(x), & x \in D \end{aligned} \tag{7.4}$$

has a unique solution in this case and we denote by H_Ω^λ the associated solution operator. Of particular importance will be the λ -equilibrium potential (of the capacitor (A, D)), $h_{A,D}^\lambda$, defined as the solution of the Dirichlet problem

$$\begin{aligned} (L - \lambda)h_{A,D}^\lambda(x) &= 0, & x \in (A \cup D)^c \\ h_{A,D}^\lambda(x) &= 1, & x \in A \\ h_{A,D}^\lambda(x) &= 0, & x \in D \end{aligned} \tag{7.5}$$

We may define analogously the λ -equilibrium measure

$$e_{D,A}^\lambda(x) \equiv (L - \lambda)h_{A,D}^\lambda(x) \tag{7.6}$$

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

$$h_{A,D}^\lambda(x) = \sum_{y \in A} G_{D^c}^\lambda(x, y) e_{A,D}^\lambda(y) \tag{7.7}$$

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 $u(\lambda) \equiv -\ln(1 - \lambda)$,

$$h_{A,D}^\lambda(x) = \mathbb{E}_x e^{u(\lambda)\tau_A} \mathbb{I}_{\tau_A < \tau_D} \tag{7.8}$$

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.

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

$$\lambda_D = \inf_{f: f(x)=0, x \in D} \frac{\Phi(f)}{\|f\|_{2,\mu}^2} \tag{7.9}$$

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

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

$$\begin{aligned} \lambda &= \left(\inf_{f:f(x)=0, x \in D} \frac{\|Af\|_{2,\mu}}{\|f\|_{2,\mu}} \right)^2 \\ &= \inf_{f:f(x)=0, x \in D} \frac{\|Af\|_{2,\mu}^2}{\|f\|_{2,\mu}^2} = \inf_{f:f(x)=0, x \in D} \frac{\Phi(f)}{\|f\|_{2,\mu}^2} \end{aligned} \quad (7.10)$$

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

Lemma 7.2: Let λ_D denote the infimum of the spectrum of L^D . Then

$$\lambda_D \geq \frac{1}{\sup_{z \in \Gamma \setminus D} \mathbb{E}_z \tau_D} \quad (7.11)$$

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

$$\phi(y)\phi(x) \leq \frac{1}{2}(\phi(x)^2 C + \phi(y)^2 / C) \quad (7.12)$$

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

$$\begin{aligned} \Phi(\phi) &= \frac{1}{2} \sum_{x,y} \mu(x)p(x,y) (\phi(x) - \phi(y))^2 \\ &= \|\phi\|_{2,\mu}^2 - \sum_{x,y \notin D} \mu(x)p(x,y) \phi(x)\phi(y) \\ &\geq \|\phi\|_{2,\mu}^2 - \sum_{x,y} \mu(x)p(x,y) \frac{1}{2} (\phi(x)^2 \psi(y)/\psi(x) + \phi(y)^2 \psi(x)/\psi(y)) \\ &= \|\phi\|_{2,\mu}^2 - \sum_{x \notin D} \mu(x) \phi(x)^2 \frac{\sum_y p(x,y) \psi(y)}{\psi(x)} \end{aligned} \quad (7.13)$$

Now chose $\psi(x) = w_D(x)$ (defined in (5.2)). By (5.4), this yields

$$\begin{aligned} \Phi(\phi) &\geq \|\phi\|_{2,\mu}^2 - \|\phi\|_{2,\mu}^2 + \sum_{x \notin D} \mu(x) \phi(x)^2 \frac{1}{w_D(x)} \\ &= \sum_{x \notin D} \mu(x) \phi(x)^2 \frac{1}{w_D(x)} \geq \|\phi\|_{2,\mu}^2 \sup_{x \in D^c} \frac{1}{w_D(x)} = \|\phi\|_{2,\mu}^2 \frac{1}{\inf_{x \in D^c} \mathbb{E}_x \tau_D} \end{aligned} \quad (7.14)$$

Since this holds for all ϕ that vanish on D ,

$$\lambda_D = \inf_{\phi:\phi(x)=0, x \in D} \frac{\Phi(\phi)}{\|\phi\|_{2,\mu}^2} \geq \frac{1}{\inf_{x \in D^c} \mathbb{E}_x \tau_D} \quad (7.15)$$

as claimed. \diamond

In the case when Γ is a finite set, (7.11) together with the estimate of Lemma 6.10 will yield a sufficiently good estimate.

If we combine this result with the estimate from Lemma 6.10, we obtain the following proposition.

Proposition 7.3: *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,*

$$\lambda^0 \geq C\epsilon^2 \tag{7.16}$$

Remark: Proposition 7.3 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.

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 [BEGK2], 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 [BGK] for the more difficult continuous case).

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

$$\begin{aligned} (L - \lambda)f(x) &= 0, & x \notin \mathcal{M} \\ f(x) &= \phi_x, & x \in \mathcal{M} \end{aligned} \tag{7.17}$$

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 to achieve that $(L - \lambda)f(x) = 0$ holds also on \mathcal{M} . Note that we have $|\mathcal{M}|$ free parameters for as many equations. Moreover, by linearity,

$$f(y) = \sum_{x \in \mathcal{M}} \phi_x h_{x, \mathcal{M} \setminus x}^\lambda(y) \tag{7.18}$$

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

$$0 = \sum_{x \in \mathcal{M}} \phi_x Lh_{x, \mathcal{M} \setminus x}^\lambda(m) \equiv \sum_{x \in \mathcal{M}} \phi_x e_{x, \mathcal{M} \setminus x}^\lambda(m), \quad \forall m \in \mathcal{M} \tag{7.19}$$

Thus, if this equations have a solution $\phi_x \in \mathcal{M}$ other than $\phi_x \equiv 0$, 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 (7.17). Then, obviously, $f(y) = \phi_\lambda(y)$ solves (7.17) uniquely, and it must be true that (7.19) has a non-zero solution. From this we can conclude that

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

$$(\mathcal{E}_\mathcal{M}(\lambda))_{xy} \equiv e_{z, \mathcal{M} \setminus z}^\lambda(x) \quad (7.20)$$

Since the condition for (7.17) to have a non-zero solution is precisely the vanishing of the determinant of $\mathcal{E}_\mathcal{M}^\lambda$, we can now conclude that:

Lemma 7.4: *A number $\lambda < \lambda^0$ is an eigenvalue of L if and only if*

$$\det \mathcal{E}_\mathcal{M}(\lambda) = 0 \quad (7.21)$$

Expanding in λ . Anticipating that we are interested in small λ , we want to re-write the matrix $\mathcal{E}_\mathcal{M}$ in a more convenient form. To do so let us set

$$h_x^\lambda(y) \equiv h_x(y) + \psi_x^\lambda(y) \quad (7.22)$$

where $h_x(y) \equiv h_x^0(y)$ and consequently $\psi_x^\lambda(y)$ solves the inhomogeneous Dirichlet problem

$$\begin{aligned} (L - \lambda)\psi_x^\lambda(y) &= \lambda h_x(y), \quad y \in \Gamma \setminus \mathcal{M} \\ \psi_x^\lambda(y) &= 0, \quad y \in \mathcal{M} \end{aligned} \quad (7.23)$$

From (7.23) 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

$$\psi_x^\lambda = \lambda(L^\mathcal{M} - \lambda)^{-1}h_x \quad (7.24)$$

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

$$\|\psi_x^\lambda\|_{2, \mu} \leq \frac{\lambda}{\lambda^0 - \lambda} \|h_x\|_{2, \mu} \quad (7.25)$$

We are however not content with this, since this implies only very poor *pointwise* estimates. To get much better pointwise comparison estimates we proceed differently. Note first that equation (7.23) implies also

$$\begin{aligned} L\psi_x^\lambda(y) &= \lambda h_x^\lambda(y), \quad y \in \Gamma \setminus \mathcal{M} \\ \psi_x^\lambda(y) &= 0, \quad y \in \mathcal{M} \end{aligned} \quad (7.26)$$

Thus

$$\frac{h_x^\lambda(y)}{h_x(y)} = 1 + \lambda \sum_{z \notin \mathcal{M}} \frac{1}{h_x(y)} G_{\Gamma \setminus \mathcal{M}}(y, z) h_x(z) \frac{h_x^\lambda(z)}{h_x(z)} \quad (7.27)$$

Now put $M \equiv \max_{z \in \Gamma \setminus \mathcal{M}} \frac{h_x^\lambda(z)}{h_x(z)}$. Note that $M < \infty$ since by the maximum principle, $h_x(y) > 0$ for all $y \in \Gamma \setminus \mathcal{M}$. We get from (7.27) that

$$M \leq 1 + \lambda M \max_{y \in \Gamma \setminus \mathcal{M}} \sum_{z \notin \mathcal{M}} \frac{1}{h_x(y)} G_{\Gamma \setminus \mathcal{M}}(y, z) h_x(z) \quad (7.28)$$

Now by symmetry of $G_{\setminus \mathcal{M}}$,

$$\begin{aligned} \frac{1}{h_x(y)} G_{\Gamma \setminus \mathcal{M}}(y, z) h_x(z) &= \frac{\mu(z)}{\mu(y)} \frac{1}{h_x(y)} G_{\Gamma \setminus \mathcal{M}}(z, y) h_x(z) \\ &= \mu(z) \frac{1}{h_x(y)} \frac{h_{z, \mathcal{M}}(y) h_x(z)}{\text{cap}(z, \mathcal{M})} \\ &= \frac{\mu(z)}{\text{cap}(z, \mathcal{M})} \mathbb{P}_y [\tau_z < \tau_{\mathcal{M}} | \tau_x = \tau_{\mathcal{M}}] \end{aligned} \quad (7.29)$$

Note that we used (5.20) to represent the Green's function and then the Markov property to get that

$$\mathbb{P}_y [\tau_z \tau_{\mathcal{M}}, \tau_x = \tau_{\mathcal{M}}] = \mathbb{P}_y [\tau_z < \tau_{\mathcal{M}}] \mathbb{P}_z [\tau_x = \tau_{\mathcal{M}}] \quad (7.30)$$

Inserting this identity yields

$$\sum_{z \notin \mathcal{M}} \frac{1}{h_x(y)} G_{\Gamma \setminus \mathcal{M}}(y, z) h_x(z) = (\mathbb{E}_y [\tau_x | \tau_x = \tau_{\mathcal{M}}]) \leq a^{-1} |\Gamma| \quad (7.31)$$

Therefore, $M \leq 1 + \lambda a^{-1} |\Gamma| M$ or

$$M \leq \frac{1}{1 - \lambda a^{-1} |\Gamma|} \quad (7.32)$$

where a is defined after (6.22) and by hypothesis not too small. Thus we conclude that

Lemma 7.5: *assume that $0 \leq \lambda \ll a^{-1} |\Gamma|$. Then for all $y \in \Gamma$,*

$$0 \leq h_x^\lambda(y) - h_x(y) \leq h_x(y) \frac{\lambda a^{-1} |\Gamma|}{1 - \lambda a^{-1} |\Gamma|} \quad (7.33)$$

Lemma 7.6:

$$\begin{aligned} (\mathcal{E}_{\mathcal{M}}(\lambda))_{xz} &= \mu(x)^{-1} \left(\frac{1}{2} \sum_{y \neq y'} \mu(y') p(y', y) [h_z(y') - h_z(y)] [h_x(y') - h_x(y)] \right. \\ &\quad \left. - \lambda \sum_y \mu(y) (h_z(y) h_x(y) + h_x(y) \psi_z^\lambda(y)) \right) \end{aligned} \quad (7.34)$$

Proof: Note that

$$(L - \lambda)h_z^\lambda(x) = (L - \lambda)h_z(x) + (L - \lambda)\psi_z^\lambda(x) = Lh_z(x) - \lambda h_z(x) + (L - \lambda)\psi_z^\lambda(x) \quad (7.35)$$

Now,

$$Lh_z(x) = \frac{\mu(x)}{\mu(x)} h_x(x) Lh_z(x) \quad (7.36)$$

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

$$\begin{aligned} Lh_z(x) &= \mu(x)^{-1} \sum_{y' \in \Gamma} \mu(y') h_x(y') Lh_z(y') \\ &= \mu(x)^{-1} \frac{1}{2} \sum_{y, y' \in \Gamma} \mu(y') p(y', y) [h_z(y') - h_z(y)] [h_x(y') - h_x(y)] \end{aligned} \quad (7.37)$$

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

$$(L - \lambda)\psi_z^\lambda(x) = \mu(x)^{-1} \sum_{y' \in \Gamma} \mu(y') (h_x(y') (L - \lambda)\psi_z^\lambda(y') - \lambda \mathbb{1}_{y' \neq x} h_x(y') h_z(y')) \quad (7.38)$$

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 (7.38) is equal to

$$-\lambda \mu(x)^{-1} \sum_{y' \in \Gamma} (\mu(y') h_x(y') (\psi_z^\lambda(y') + \mathbb{1}_{y' \neq x} h_x(y') h_z(y')) \quad (7.39)$$

Adding the left-over term $-\lambda h_z(x) = -\lambda h_x(x) h_z(x)$ from (7.35) to (7.38), we arrive at (7.34).

◇

Remark: Note that we get an alternative probabilistic interpretation of $Lh_z(x)$ as

$$Lh_z(x) = \begin{cases} -\mathbb{P}_x[\tau_z \leq \tau_{\mathcal{M}}], & \text{if } z \neq x \\ \mathbb{P}_x[\tau_{\mathcal{M} \setminus x} < \tau_x] & \text{if } z = x \end{cases} \quad (7.40)$$

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 7.7: *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*

$$\begin{aligned} \mathcal{K}_{zx} &= \frac{\frac{1}{2} \sum_{y \neq y'} \mu(y') p(y', y) [h_z(y') - h_z(y)] [h_x(y') - h_x(y)]}{\|h_z\|_2 \|h_x\|_2} \\ &\equiv \frac{\Phi(h_z, h_x)}{\|h_z\|_2 \|h_x\|_2} \end{aligned} \quad (7.41)$$

such that $\lambda = \mu(1 + O(\rho))$.

Proof: The proof will rely on the following general fact.

Lemma 7.8: *Let A be a finite dimensional self-adjoint matrix. Let $B(\lambda)$ be a Lipschitz continuous family of bounded operators on the same space that satisfies the bound $\|B(\lambda)\| \leq \delta + \lambda C$, and $\|B(\lambda) - B(\lambda')\| \leq C|\lambda - \lambda'|$ for $0 \leq \delta \ll 1$, and $0 \leq C < \infty$. Assume that A has k eigenvalues $\lambda_1, \dots, \lambda_k$ in an interval $[0, a]$ with $a < \delta/C$. Then*

(i) *Any solution of the equation*

$$\det(A - \lambda(\mathbb{I} + B(\lambda))) = 0 \quad (7.42)$$

λ'_1 *satisfies* $|\lambda'_1 - \lambda_1| \leq 4\delta\lambda_1$, *for some* $i \in 1, \dots, k$.

(ii) *There exists* $\delta_0 > 0$ *and* $a_0 > 0$, *such that for all* $\delta < \delta_0$, *and* $a \leq a_0$, *equation (7.42) has exactly* k *solutions* $\lambda'_1, \dots, \lambda'_k$ *and each solution satisfies* $|\lambda'_i - \lambda_i| \leq 4\delta\lambda_i$.

(iii) *If the eigenvalue* λ_i *is simple and isolated with* $\min_{j \neq i} |\lambda_i - \lambda_j| \geq b\lambda_i$ *with* $b > 2\delta$, *then if* λ'_i *is a solution of (7.42) with* $|\lambda'_i - \lambda_i| \leq 4\delta\lambda_i$, *then there exists a unique solution* c *of the equation*

$$(A - \lambda'_i(\mathbb{I} + B(\lambda'_i)))c = 0 \quad (7.43)$$

Moreover, if c_i *denotes the normalized eigenfunction of* A *with eigenvalue* λ_i , *then*

$$\|c - c_0\|_2 \leq \frac{2\lambda'_i\delta}{(b - 6\delta)} \quad (7.44)$$

Proof: We first show (ii). If (7.42) holds, then there exist a non-zero vector c such that

$$(A - \lambda)c = \lambda B(\lambda)c \quad (7.45)$$

or

$$c = \frac{\lambda}{A - \lambda} B(\lambda)c \quad (7.46)$$

Thus

$$\|c\|_2 \leq \lambda \|(A - \lambda)^{-1}\| \|B(\lambda)\| \|c\|_2 \quad (7.47)$$

Since c is non-zero, this means that

$$\lambda \|(A - \lambda)^{-1}\| \|B(\lambda)\| \geq 1 \quad (7.48)$$

Now since A is symmetric, we have that

$$\|(A - \lambda)^{-1}\| \leq \max_i \frac{1}{|\lambda_i - \lambda|} \quad (7.49)$$

and so

$$\min_{i=1}^k |\lambda_i - \lambda| \leq \lambda \|B(\lambda)\| \leq \lambda(\delta + C\lambda) \quad (7.50)$$

which implies (i).

To prove (ii), Let us consider the operator $A(\lambda) \equiv A(1 + B(\lambda))^{-1}$. It is plain that λ solves (7.42) if and only if λ is an eigenvalue of $A(\lambda)$. Since $A(\lambda) = A + AB(\lambda)(1 + B(\lambda))^{-1}$, and $\|AB(\lambda')(1 + B(\lambda'))^{-1}\| \leq a \frac{2\delta}{1-2\delta}$, by standard perturbation theory, $A(\lambda)$ has k eigenvalues that satisfy $|\lambda_i(\lambda') - \lambda_i| \leq 4\delta$. Moreover, by the Lipschitz continuity of $B(\lambda)$, it follows that

$$|\lambda_i(\lambda') - \lambda_i(\lambda'')| \leq Ca|\lambda' - \lambda''| \quad (7.51)$$

But now, if $Ca < 1$, (7.51) implies the existence of a fix-point λ that satisfies $\lambda_i(\lambda) = \lambda$. This yields (ii).

To prove (iii) note first that the existence of a solution of (7.43) is obvious. The remaining properties follow from the assumption that the eigenspace of λ_i is one-dimensional. Namely, let c be of the form $c_i + \delta c$, with $(c_i, \delta c) = 0$. Inserting this into Eq. (7.43) and multiplying with $\delta c >$ from the left yields

$$(\delta c, (A - \lambda)c_i) + (\delta c, (A - \lambda)\delta c) = \lambda(\delta c, B(\lambda)c) \quad (7.52)$$

wich implies that

$$\|\delta c\|_2^2 (b - 4\delta\lambda_i) \leq \lambda_i(1 + 4\delta)2\delta(\|\delta c\|_2^2 + \|\delta c\|_2) \quad (7.53)$$

resp.

$$\|\delta c\|_2 \leq \frac{\lambda_i(1 - 4\delta)2\delta}{b - 7\delta\lambda_i} \quad (7.54)$$

Uniqueness of c follows from the fact that the operator $A - \lambda'_i(1 - B(\lambda'_i))$ restricted to the subspace orthogonal to c_i is bounded from below by $(b - 6\delta\lambda_i)$ and thus is invertible. \diamond

We now return to the proof of Theorem 7.7. First we divide the row x of the matrix $\mathcal{E}(\lambda)$ by $\|h_x\|_2$ and multiply by $\mu(x)$, and then divide the columns by $\|h_z\|_2$, to obtain a symmetric matrix $\mathcal{G}(\lambda)$ with identical determinant that can be written as

$$\mathcal{G}(\lambda) = \mathcal{K} - \lambda\mathbb{I} - \lambda B(\lambda) \quad (7.55)$$

where

$$B(\lambda)_{zx} = \frac{\sum_y \mu(y) h_z(y) h_x(y) (\mathbb{1}_{x \neq y} + \psi_x^\lambda(y)/h_x(y))}{\|h_z\|_2 \|h_x\|_2} \quad (7.56)$$

Note that $\mathcal{G}(\lambda)$ is symmetric. We must estimate the operator norm of $B(\lambda)$. We will use the corresponding standard estimator $(\sum_{x,z \in \mathcal{M}} B_{zx}^2)^{1/2}$.

We first deal with the off-diagonal elements that have no additional λ or other small factor in front of them.

Lemma 7.9: *There is a constant $C < \infty$ such that*

$$\max_{x \neq z \in \mathcal{M}} \frac{\sum_{y \in \Gamma} \mu(y) h_x(y) h_z(y)}{\|h_x\|_2 \|h_z\|_2} \leq C a^{-1} \max_{m \in \mathcal{M}} \mu(m)^{-1} \text{cap}(m, \mathcal{M} \setminus m) \leq \rho(\epsilon) \quad (7.57)$$

Proof: Note first by the estimate (5.40) the equilibrium potentials $h_x(y)$ are essentially equal to one on $A(x)$. Namely,

$$1 \geq h_x(y) \geq 1 - \frac{\text{cap}(y, \mathcal{M} \setminus x)}{\text{cap}(y, x)} \quad (7.58)$$

By Corollary 6.4, $\text{cap}(y, \mathcal{M} \setminus x) \leq 2\text{cap}(x, \mathcal{M}_x)$, or $\mu(y) \leq 3\|\mathcal{M}\|a^{-1}\text{cap}(x, \mathcal{M}_x)$.

Thus

$$\begin{aligned} \sum_{y \in A(x)} \mu(y) h_x(y)^2 &\geq \sum_{\substack{y \in A(x) \\ \mu(y) \geq 3\|\mathcal{M}\|a^{-1}\text{cap}(x, \mathcal{M}_x)}} \left(1 - \frac{\text{cap}(x, \mathcal{M} \setminus x)}{\text{cap}(y, x)}\right)^2 \\ &\geq \sum_{\substack{y \in A(x) \\ \mu(y) \geq 3\|\mathcal{M}\|a^{-1}\text{cap}(x, \mathcal{M}_x)}} \mu(y) - \sum_{y \in A(x)} 2 \frac{\mu(y)}{\text{cap}(y, x)} \text{cap}(x, \mathcal{M} \setminus x) \\ &= \mu(A(x)) \left(1 - 3\|A(x)\|\|\mathcal{M}\|a^{-1} \frac{\text{cap}(x, \mathcal{M} \setminus x)}{\mu(A(x))}\right) \\ &\geq \mu(A(x)) (1 - O(\rho)) \end{aligned} \quad (7.59)$$

Thus the denominator in (7.57) is bounded from below by

$$\sqrt{\sum_{y \in A(x)} \mu(y) h_x^2(y) \sum_{y \in A(z)} \mu(y) h_z^2(y)} \geq \sqrt{\mu(A(x))\mu(A(z))} (1 - O(\rho)) \quad (7.60)$$

To bound the numerators, we will use Lemma 6.6 in the special situation when $J = \mathcal{M} \setminus x$.

Lemma 7.10: *For any $x \neq z \in \mathcal{M}$,*

$$\sum_{y \in \Gamma} \mu(y) h_x(y) h_z(y) \leq C \rho \sqrt{\mu(x)\mu(z)} \quad (7.61)$$

Proof: By (ii) of Lemma 6.7, if $y \in A(m)$, then

(i) If $m = z$, either

$$\mu(y) \leq \frac{3}{2}\mu(x)a^{-1}|\mathcal{M}|\frac{\text{cap}(m,x)}{\mu(x)} \quad (7.62)$$

or

$$\mu(y)h_x(y)h_z(y) \leq \frac{3}{2}\mu(x)a^{-1}|\mathcal{M}|\frac{\text{cap}(m,x)}{\mu(x)} \quad (7.63)$$

(ii) If $m = x$,

$$\mu(y) \leq \frac{3}{2}\mu(z)a^{-1}|\mathcal{M}|\frac{\text{cap}(m,z)}{\mu(z)} \quad (7.64)$$

or

$$\mu(y)h_x(y)h_z(y) \leq \frac{3}{2}\mu(z)a^{-1}|\mathcal{M}|\frac{\text{cap}(m,z)}{\mu(z)} \quad (7.65)$$

(iii) Let $m \notin \{x, z\}$, and assume w.r.g. that $\text{cap}(m, x) \geq \text{cap}(m, z)$. Then, if $\text{cap}(m, y) > 3\text{cap}(m, z)$, already

$$\mu(y)\sqrt{h_x(y)h_z(y)} \leq \frac{3}{2}\sqrt{\mu(x)\mu(z)}a^{-1}|\mathcal{M}|\sqrt{\frac{\text{cap}(m,x)\text{cap}(m,z)}{\mu(x)\mu(z)}} \quad (7.66)$$

while otherwise

$$\mu(y) \leq 3\mu(y)\frac{\text{cap}(m,z)}{\text{cap}(y,m)} \leq 3a^{-1}|\mathcal{M}|\sqrt{\text{cap}(m,z)\text{cap}(m,x)} \quad (7.67)$$

Summing over y yields e.g. in case (i)

$$\begin{aligned} \sum_{y \in A(m)} \mu(y)h_x(y)h_y(y) &\leq C |\{y \in A(m) : \mu(y) \geq 32a^{-1}|\mathcal{M}|\text{cap}(m,x)\}| \\ &\quad \times a^{-1}|\mathcal{M}|\text{cap}(m,x) \end{aligned} \quad (7.68)$$

and in case (ii) the same expression with x replaced by z . The case (iii) is concluded in the same way.

This implies the statement of the lemma. \diamond

Remark: Note that the estimates in the proof of Lemma 7.9 also imply that

$$\mu(A(x))(1 - O(\rho(\epsilon))) \leq \sum_y \mu(y)h_x(y)^2 \leq \mu(A(x))(1 + O(\rho(\epsilon))) \quad (7.69)$$

The remaining contribution to the matrix elements of $B(\lambda)$ are of order λ , and thus the crudest estimates will suffice:

Lemma 7.11: *If λ^0 denotes the principal eigenvalue of the operator L with Dirichlet boundary conditions in \mathcal{M} , then*

$$\begin{aligned} & \left| \sum_{y \in \Gamma} \mu(y) (h_z(y) \psi_x^\lambda(y)) \right| \\ & \leq \frac{\lambda}{(\lambda^0 - \lambda)} \|h_z\|_2 \|h_x\|_2 \end{aligned} \quad (7.70)$$

Proof: Recall that ψ_x^λ solves the Dirichlet problem (7.23). 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

$$\|\psi_x^\lambda\|_2^2 \leq \left(\frac{\lambda}{\lambda^0 - \lambda} \right)^2 \|h_x\|_2^2 \quad (7.71)$$

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

As a consequence of the preceding lemmata, we see that the matrix $B(\lambda)$ is indeed bounded in norm by

$$\|B(\lambda)\| \leq C\rho(\epsilon) + c \frac{\lambda}{\lambda^0 - \lambda} \quad (7.72)$$

The theorem follows from Lemma 7.8. \diamond

The computation of the eigenvalues of the capacity matrix is now in principle a finite, though in general not trivial problem. The main difficulty is of course the computation of the capacities and induction coefficients. Capacities can be estimated quite efficiently, as we will see in the next section, the off-diagonal terms however, pose in general a more serious problem, although in many practical cases exact symmetries may be very helpful (since after all, the sum of the off-diagonal terms is given by the diagonal ones). On the other hand, a particularly nice situation arises when no symmetries are present.

In fact we will prove the following theorem.

Proposition 7.12: *Assume that there exists $x \in \mathcal{M}$ such that for some $\delta \ll 1$*

$$\delta \frac{\text{cap}(x, \mathcal{M} \setminus x)}{\|h_x\|_2^2} \geq \max_{z \in \mathcal{M} \setminus x} \frac{\text{cap}(z, \mathcal{M} \setminus z)}{\|h_z\|_2^2} \quad (7.73)$$

Then the largest eigenvalue of L below λ_0 is given by

$$\lambda_x = \frac{\text{cap}(x, \mathcal{M} \setminus x)}{\|h_x\|_2^2} (1 + O(\delta)) \quad (7.74)$$

and all smaller eigenvalues of L satisfy

$$\lambda \leq C\sqrt{\delta}\lambda_x \quad (7.75)$$

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

Remark: This may look strange: we can compute the largest of the small eigenvalues, while we should think that we would be most interested in computing the smallest eigenvalues first. However, the logic is the same as that of our overall approach: we begin by controlling the large part of the spectrum to gain successively control over the smaller eigenvalues. So we must compute λ^0 first, then the largest of the remaining $|\mathcal{M}|$ eigenvalues, then we can compute the second largest, etc.

Proof: By the Cauchy-Schwartz inequality,

$$\Phi(h_x, h_z) = \left| \frac{1}{2} \sum_{y, y'} \mu(y') p(y', y) [h_x(y') - h_x(y)] [h_z(y') - h_z(y)] \right| \leq \sqrt{\text{cap}(x, \mathcal{M} \setminus x) \text{cap}(z, \mathcal{M} \setminus z)} \quad (7.76)$$

Thus

$$|\mathcal{K}_{zx}^2| \leq \mathcal{K}_{xx} \mathcal{K}_{zz} \quad (7.77)$$

Whence by assumption,

$$\|\check{\mathcal{K}}\| \leq \mathcal{K}_{xx} \sqrt{\delta|\mathcal{M}| + \delta^2|\mathcal{M}|^2} \quad (7.78)$$

Since obviously $\hat{\mathcal{K}}$ has one eigenvalue \mathcal{K}_{xx} with the obvious eigenvector and all other eigenvalues are zero, the announced result follows from perturbation theory. Let f_0 be the eigenvector of eigenvalue $\lambda \equiv \mathcal{K}_{xx}$, and write $v = f_0 + g$, where g is chosen orthogonal to f_0 , for the full eigenvector of \mathcal{K} . We have

$$(\hat{\mathcal{K}} + \check{\mathcal{K}})(f_0 + g) = \lambda(f_0 + g) \quad (7.79)$$

Since $\hat{\mathcal{K}}g = 0$, it follows that

$$\mathcal{K}_{xx}f_0 + \check{\mathcal{K}}f_0 + \check{\mathcal{K}}g = \lambda(f_0 + g) \quad (7.80)$$

resp.

$$(\lambda - \check{\mathcal{K}})g = (\mathcal{K}_{xx} - \lambda + \check{\mathcal{K}})f_0 \quad (7.81)$$

Using our bounds on $\|\check{\mathcal{K}}\|$ and $|\lambda - \mathcal{K}_{xx}|$, it follows that

$$\|g\|_2 \leq \frac{\mathcal{K}_{xx} \sqrt{\delta |\mathcal{M}| + \delta^2 |\mathcal{M}|^2}}{\mathcal{K}_{xx} (1 - C\sqrt{\delta})} = C\sqrt{\delta} \quad (7.82)$$

◇

Theorem 7.12 has the following simple corollary, that allows in many situations a complete characterization of the small eigenvalues of L .

Theorem 7.13: *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 , $\mathcal{M}_i \setminus \mathcal{M}_{i-1} = x_i$ is a single point, and that each \mathcal{M}_i satisfies the assumptions of Theorem 7.12. Then L has k eigenvalues*

$$\lambda_i = \frac{\text{cap}(x_i, \mathcal{M}_{i-1})}{\mu(A(x_i))} (1 + O(\delta)) \quad (7.83)$$

As a consequence,

$$\lambda_i = \frac{1}{\mathbb{E}_{x_i} \tau_{\mathcal{M}_{i-1}}} (1 + O(\delta)) \quad (7.84)$$

The corresponding normalized eigenfunction is given by

$$\psi_i(y) = \frac{h_{x_i, \mathcal{M}_{i-1}}(y)}{\|h_{x_i, \mathcal{M}_{i-1}}\|_2} + \sum_{j=1}^{i-1} O(\delta) \frac{h_{x_i, \mathcal{M}_{j-1}}(y)}{\|h_{x_i, \mathcal{M}_{j-1}}\|_2} \quad (7.85)$$

Proof: The idea behind this theorem is simple. Let the sets \mathcal{M}_i of the corollary be given by $\mathcal{M}_i = \{x_1, \dots, x_i\}$. 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 would arrive at the conclusion of the theorem. Thus, Theorem 7.13 will follow directly from the following

Lemma 7.14: *Under the assumptions of Theorem 7.13, it is true that*

$$\lambda_{\mathcal{M}_\ell} = \lambda_{\ell+1} (1 + O(\delta)) \quad (7.86)$$

Moreover, the corresponding eigenfunction $\psi_{\mathcal{M}_\ell}$ is given by

$$\psi_{\mathcal{M}_\ell}(y) = \frac{h_{x_{\ell+1}, \mathcal{M}_\ell}(y)}{\|h_{x_{\ell+1}, \mathcal{M}_\ell}(y)\|_2} (1 + O(\lambda)) \quad (7.87)$$

Proof: The proof is very simple. We use the same strategy as for the computation of the usual eigenvalues, that is we search a solution of the eigenvalue problem

$$\begin{aligned} (L - \lambda)\psi_{\mathcal{M}_\ell}(x) &= 0, & x \in \Gamma \setminus \mathcal{M}_\ell \\ \psi_{\mathcal{M}_\ell}(x) &= 0, & x \in \Gamma \setminus \mathcal{M}_\ell \end{aligned} \quad (7.88)$$

among the solutions of the Dirichlet problem

$$\begin{aligned} (L - \lambda)f(x) &= 0, & x \in \Gamma \setminus \mathcal{M}_\ell \\ f(x) &= 0, & x \in \Gamma \setminus \mathcal{M}_\ell \\ f(x_{\ell+1}) &= 1 \end{aligned} \quad (7.89)$$

Of course we recognize that $f(x) = h_{x_{\ell+1}, \mathcal{M}_\ell}^\lambda(x)$, and the condition for λ to be an eigenvalue smaller than $\lambda_{\mathcal{M}_{\ell+1}}$ is simply

$$(L - \lambda)h_{x_{\ell+1}, \mathcal{M}_\ell}^\lambda(x_{\ell+1}) = 0 \quad (7.90)$$

But this can be written as

$$\text{cap}(x_{\ell+1}, \mathcal{M}_\ell) - \lambda \left(\|h_{x_{\ell+1}, \mathcal{M}_\ell}\|_2^2 + (h_{x_{\ell+1}, \mathcal{M}_\ell}, \psi_{x_{\ell+1}, \mathcal{M}_\ell}^\lambda)_\mu \right) = 0 \quad (7.91)$$

which gives in fact

$$\lambda = \frac{\text{cap}(x_{\ell+1}, \mathcal{M}_\ell)}{\|h_{x_{\ell+1}, \mathcal{M}_\ell}\|_2^2} (1 + O(\lambda/\lambda_{\mathcal{M}_{\ell+1}})) \quad (7.92)$$

which up to the error terms equals $\lambda_{\ell+1}$. The corresponding eigenfunction is simply (up to normalization) $h_{x_{\ell+1}, \mathcal{M}_\ell}^\lambda(x)$. Using Lemma 7.5 to compare h^λ with h , we arrive at the conclusion of the Lemma. \diamond

Remark: Of course we need not stop here. We can actually compute all the $k - \ell$ small eigenvalues of the Dirichlet operator $L^{\mathcal{M}_\ell}$ in exactly the same way we did for L itself, except that the values of ϕ_x for $x \in \mathcal{M}_\ell$ are now frozen to zero. It is not surprising that the outcome of this procedure will simply be that the $i - th$ eigenvalue of $L^{\mathcal{M}_\ell}$ is essentially equal to the $\ell + i$ th eigenvalue of L . Also, the eigenfunctions will be almost the same, except that the terms corresponding to $x \in \mathcal{M}_\ell$ are set to zero.

The theorem is now immediate except for the statement (7.84). To conclude, we need to show that $\text{cap}(x_{\ell+1}, \mathcal{M}_\ell) = \text{cap}(x_\ell, \mathcal{M}_{x_\ell})$. 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}_ℓ , then $\text{cap}(x, \mathcal{M}_\ell \setminus x) \sim \text{cap}(x_{\ell+1}, \mathcal{M}_\ell)$, while

$\|h_{x_{\ell+1}, \mathcal{M}_\ell}\|_2 \leq \|h_{x, \mathcal{M}_{\ell+1} \setminus x}\|_2$, contradicting the assumption in the construction of the set \mathcal{M}_ℓ . Thus $\text{cap}(x_{\ell+1}, \mathcal{M}_\ell) \geq \text{cap}(x_\ell, \mathcal{M}_{x_\ell})$.

Similarly, if there was any point $x \in \mathcal{M}_\ell$ for which $\text{cap}(x_{\ell+1}, \mathcal{M}_\ell) < \text{cap}(x_\ell, \mathcal{M}_{x_\ell})$, 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 $M\mathcal{M}_{\ell+1}$ 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} . \diamond

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 7.12 hold. Note that

$$\mathbb{P}_x[\tau_{\mathcal{M}_x} > t] = \sum_{x_1, \dots, x_t \notin \mathcal{M}_x} p(x, x_1) \prod_{i=1}^{t-1} p(x_i, x_{i+1}) = \sum_{y \notin \mathcal{M}_x} (P^{\mathcal{M}_x})_{xy}^t \quad (7.93)$$

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 $P^{\mathcal{M}_x}$. Then

$$(P^{\mathcal{M}_x})_{xy}^t = \sum_{y \notin \mathcal{M}_x} \left((P^{\mathcal{M}_x})^t \Pi \right)_{xy} + \sum_{y \notin \mathcal{M}_x} \left((P^{\mathcal{M}_x})^t \Pi^c \right)_{xy} \quad (7.94)$$

Using our estimate for the principal eigenfunction of $L^{\mathcal{M}_x}$ the first term in (7.94) equals

$$(1 - \lambda^{\mathcal{M}_x})^t \sum_{y \notin \mathcal{M}_x} \frac{h_{x, \mathcal{M}_x}(y)}{\|h_{x, \mathcal{M}_x}\|_2} (1 + o(\lambda^{\mathcal{M}_x})) \sim e^{-\lambda^{\mathcal{M}_x} t} \quad (7.95)$$

The remaining term is bounded in turn by

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

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

8. Computation of capacities.

We have seen so far that in metastable dynamics we can largely reduce the computation of key quantities to the computation of *capacities*. The usefulness of all this thus depends on how well we can compute capacities. While clearly the universality of our approach ends here, and model specific properties have to enter the game, it is rather surprising to what extent precise computations of capacities are possible in a multitude of specific systems. In the following I give some basic principles that work in many cases, but that are not fool-proof. I have mostly models in mind that are short range, in models with long range jumps things are a bit more involved.

8.1. General principles. The key to success is the variational representation of capacities through the Dirichlet principle, i.e. Eq. (3.17). The Dirichlet principle immediately yields two avenues towards bounds:

- Upper bounds via judiciously chosen test functions
- Lower bounds via monotonicity of the Dirichlet form in the transition probabilities via simplified processes.

These two principles are well-known and give rise to the so-called “Rayleigh’s short-cut rules” in the language of electric networks (see e.g. [DS] and references therein). In the context of metastable systems, the usefulness of these principle can be enhanced by an iterative method.

The key idea of iteration is to get first of all control of the minimizer in the Dirichlet principle, i.e. the equilibrium potential. In metastable systems, when we are interested in computing e.g. the capacity $\text{cap}(B_x, B_y)$ where B_x, B_y represent two metastable sets, our first goal will always be to identify domains where $h_{B_x, B_y}(z)$ is close to zero or close to one. This is done with the help of the renewal estimate of Lemma 6.2. While with looks cyclic at first glance (we need to know the capacities in order to estimate the equilibrium potential, which we want to use in order to estimate capacities...) it yields a tool to enhance “poor” bounds in order to get good ones. Thus the first step in the program is to get a first estimate on capacities of the form $\text{cap}(z, B)$ for arbitrary z, B .

- (i) Choose a roughly ok looking test function for the upper bound.
- (ii) Dramatically simplify the state space of the process to obtain a system that can be solved exactly for the lower bound. In most examples, this leads to choosing a one-dimensional

or quasi-one-dimensional system.

(iii) Insert the resulting bounds in (4.4) to obtain bounds on $h_{B_x, B_y}(z)$.

Using this bound we can now identify the set

- $D_x \equiv \{z : h_{B_x, B_y}(z) < \delta\}$
- $D_y \equiv \{z : h_{B_x, B_y}(z) > 1 - \delta\}$

for $\delta \ll 0$ suitably chosen.

If the complement of the set $D_x \cup D_y$ contains no further metastable set, we define

- $I \equiv \{z \in (D_x \cup D_y)^c : \mu(z) < \rho \sup_{w \in (D_x \cup D_y)^c} \mu(w)\}$

for $\rho \ll 1$ conveniently chosen.

Let us denote by $\mathcal{S} \equiv (D_x \cup D_y \cup I)^c$.

The idea is that the set I will be irrelevant for the value of the capacity, no matter what value $h_{B_x, B_y}(z)$ takes where, and that the sets D_x and D_y give no contribution to the capacity to leading order. The only problem is thus to find the equilibrium potential, or a reasonably good approximation to it on the set \mathcal{S} . We return to this problem shortly. Of course this idea can only make sense if the sets D_x and D_y can be connected through \mathcal{S} . If that is not the case, we will have to analyse the set $(D_x \cup D_y)^c$ more carefully.

$(D_x \cup D_y)^c$ contains further metastable sets, say w , then it will be possible to identify domains D_w on which $h_{B_x, B_y}(z)$ takes on a constant values c_w (to be determined later). Note that this can be done again with the help of the renewal bounds; The starting point (in the discrete case) is of course the observation that

$$\begin{aligned} h_{B_x, B_y}(z) &= \mathbb{P}_z[\tau_{B_x} < \tau_{B_y}] = \mathbb{P}_z[\tau_{B_x} < \tau_{B_y}, \tau_w < \tau_{B_x}] + \mathbb{P}_z[\tau_{B_x} < \tau_{B_y}, \tau_w \geq \tau_{B_x}] \\ &\leq \mathbb{P}_z[\tau_w < \tau_{B_x \cup B_y}] \mathbb{P}_w[\tau_{B_x} < \tau_{B_y}] + \delta \\ &= \mathbb{P}_z[\tau_w < \tau_{B_x \cup B_y}] c_w + \delta \end{aligned} \tag{8.1}$$

The problem, to be solved with the help of (4.4) and the a priori bounds on capacities is thus to determine the set of points for which $\mathbb{P}_z[\tau_w < \tau_{B_x \cup B_y}] > 1 - \delta$.

Once with is done, we proceed as in the former case, but increasing the set $D_x \cup D_y$ in their definition of I to $D \equiv D_x \cup D_y \cup D_{w_1} \cup \dots \cup D_{w_k}$ if k such sets can be identified. It should now be the case that the set $D_x \cup D_y \cup D_{w_1} \cup \dots \cup D_{w_k} \cup \mathcal{S}$ is connected. The remaining

problem consists then in the determination of the equilibrium potential on the set \mathcal{S} and of the values c_{w_i} .

At this stage we can then obtain upper and lower bounds in terms of variational problems that involve only the sets \mathcal{S} ; to what extent these problems then can be solved depends on the problem at hand.

Upper bound. To obtain the upper bound, we choose a test-function h^+ with the properties that

$$\begin{aligned} h^+(z) &= 1, & z \in D_x \\ h^+(z) &= 0, & z \in D_y \\ h^+(z) &= c_{w_i}, & z \in D_{w_i} \end{aligned} \tag{8.2}$$

where the constants c_{w_i} are determined only later. On I , the function h^+ can be chosen essentially arbitrarily, while on \mathcal{S} , we chose h^+ such that it optimizes the restriction of the Dirichlet form to \mathcal{S} with boundary conditions implied by (8.2) on $\partial\mathcal{S} \cap \partial D$. Finally, the constants c_{w_i} are determined by minimizing the result as a function of these constants.

Lower bound. For the lower bound, we use that if h^* denotes the true minimizer, then

$$\Phi(h^*) \geq \Phi_{\mathcal{S}}(h^*) \tag{8.3}$$

where $\Phi_{\mathcal{S}}$ is the restriction of the Dirichlet form to the subset \mathcal{S} , i.e.

$$\Phi_{\mathcal{S}}(h) = \frac{1}{2} \sum_{\substack{x \vee y \in \mathcal{S} \\ x \wedge y \in \mathcal{S} \cup D}} \mu(x)p(x,y)[h(x) - h(y)]^2 \tag{8.4}$$

Finally we minorize $\Phi_{\mathcal{S}}(h^*)$ by taking the infimum over all h on \mathcal{S} , with boundary conditions imposed by what we know a priori about the equilibrium potential. In particular we know that these boundary conditions are close to constants on the different components of D . Of course we do not really know the constants c_{w_i} , but taking the infimum over these, we surely are on the safe side.

Thus, if we can show that the minimizers in the lower bound differ little from the minimizers with constant boundary conditions, we get upper and lower bounds that coincide up to small error terms. Of course in general, it may remain difficult to actually compute these minimizers. However, the problem is greatly reduced in complexity with respect to the original problem, and in many instances this problem can be solved quite explicitly (see [BEGK1, BM]).

Example 1. Markov chains with exponentially small transition probabilities.

We will now consider an class of examples where the program outlined above works very nicely. These are (reversible) Markov chains on a finite state space with exponentially small transition probabilities. This example was studied in [BM].

Let a function $H : \Gamma \rightarrow \mathbb{R}_+$ be given. We will think of Γ as a graph with edge set $E(\Gamma)$. We now consider transition probabilities

$$p(x, y) = \begin{cases} C e^{-\beta[H(y)-H(x)]_+}, & \text{if } (x, y) \in E(\Gamma) \\ 1 - \sum_{y:(x,y) \in E(\Gamma)} p(x, y), & \text{if } x = y \\ 0, & \text{else} \end{cases} \quad (8.5)$$

The invariant distribution of this process is

$$\mu_\beta(x) = \frac{e^{-\beta H(x)}}{\sum_{x \in \Gamma} e^{-\beta H(x)}} \quad (8.6)$$

Here we will think of β as a large parameter. As a consequence, transitions that would increase the value $H(x(t))$ are exponentially unlikely.

A relevant example of class is the *Stochastic Ising model*, where $\Gamma = \{-1, +1\}^\Lambda$, $\Lambda \subset \mathbb{Z}^d$, and

$$H(x) = H_\Lambda(x) = - \sum_{i,j \in \Lambda: \|i-j\|_2=1} x_i x_j - h \sum_{i \in \Lambda} x_i \quad (8.7)$$

In *Glauber dynamics*, the edges of the graph Γ are taken to be the pairs (x, y) where y can be obtained from x by changing exactly one of the components x_i by a factor -1 . In this example the graph Γ is simply connected. In *Kawasaki dynamics* edges are pairs (x, y) where y is obtained from x by exchanging the values of two coordinates i, j with $\|i - j\|_2 = 1$. This dynamics conserves the total magnetization $m = \sum_i x_i$. Thus the actual state space decomposes in invariant subspaces. In both cases, the parameter β is called the *inverse temperature*, and the Markov chains are supposed to model the dynamics of a magnetic system, resp. a lattice gas at low temperatures.

In the sequel we will assume to be in the situation of a Glauber dynamics. In particular, we assume that Γ is simply connected.

Let \mathcal{M} be the set of local minima of H . We would like to compute, for two points $x, y \in \mathcal{M}$, the capacity $\text{cap}(x, y)$ asymptotically for $\beta \uparrow \infty$. It is clear that the strategy to minimize the Dirichlet form with boundary conditions 0 in x and 1 in y must be to move the gradient

as close as possible to the regions where H is as large as possible. To do this, we need to introduce the notion of essential saddles.

We call a one-dimensional subgraph ω a *path*. If ω is any path with starting point in x and endpoint in y , it is obvious that any function h satisfying the boundary conditions 0 and 1 in x, y must change from 0 to 1 along any such path. For a given path, it would be nice to concentrate that change at the place where $H(\omega(t))$ is maximal; looking at the path for which this maximum is minimal indicates the lowest unavoidable height where some gradient needs to be put. Thus we define the *communication height* between x and y as

$$\widehat{H}(x, y) := \min_{\omega: x \rightarrow y} \max_{z \in \omega} H(z) \quad (8.8)$$

The set of all points that realize the mini-max in (8.8) is sometimes called the set of *essential saddles*, $\mathcal{S}(x, y)$. A particularly simple situation occurs when for each saddle point, one can find an optimal path from x to y that passes only through this particular saddle. We will for simplicity assume to be in this situation. Then it is clear topologically that there exists a separator Σ between x and y with the property that

- (i) any path ω from x to y intersects Σ , and for any point z in Σ there is a path ω from x to y whose intersection with Σ is z .
- (ii) $\min_{z \in \Sigma} H(z) = \widehat{H}(x, y)$. We will furthermore assume that the set $\mathcal{S}(x, y)$ is totally disconnected in Γ .

Clearly Σ separates the state space into subsets Γ_x and Γ_y such that $\Gamma_x \cup \Gamma_y \cup \Sigma = \Gamma$. The upper bound on the capacities can now be achieved by setting $h(z) = 0$, $z \in \Gamma_x$, $h(z) = 1$, $z \in \Gamma_y$, and optimizing over the remaining variables $h(z)$, $z \in \Sigma$. Unsurprisingly, the values of $h(z)$ in $\Sigma \setminus \mathcal{S}$ will be insignificant, and the problem decomposes typically into a finite number of variational problems that can be solved by hand exactly.

Finally, to get a lower bound, one reduces the state space to the subgraph consisting of

- (i) the connected components M_x and M_y of $\Gamma_x \cap \{z : H(z) < \widehat{H}(x, y)\}$ and $\Gamma_y \cup \{z : H(z) < \widehat{H}(x, y)\}$ that contains x and y , respectively.
- (ii) The set \mathcal{S} together with all edges that connect \mathcal{S} to M_x and M_y , and those connecting points in \mathcal{S} .

To prove that the two bounds obtained in this way are asymptotically the same, one only needs to prove that for $z \in M_x$, $h_{y,x}(z) \leq Ce^{-\beta a}$, for some $a > 0$. To do so, we use the

inequality

$$h_{y,x}(z) \leq \frac{\text{cap}(z,y)}{\text{cap}(z,x)} \quad (8.9)$$

The upper bound for the numerator is easily obtained through the upper bound on $\text{cap}(x,y)$ which we already have. The lower bound on the denominator is obtained by reducing the state space to a single path ω from z to y . Since the latter capacity can be computed explicitly, it follows easily that

$$\max_{z \in M_x} h_{y,x}(z) \leq C e^{-\beta(\widehat{H}(x,y) - \max_{z \in M_x} H(z))} \leq C e^{-\beta a} \quad (8.10)$$

for some $a > 0$. In the same way,

$$\inf_{z \in M_y} h_{y,x}(z) \geq C e^{-\beta(\widehat{H}(x,y) - \max_{z \in M_y} H(z))} \geq 1 - C e^{-\beta a} \quad (8.11)$$

Now, under the assumption that all saddle points are isolated and simple (in the sense that through each saddle point there exists a path ω from x to y such that the level $\widehat{H}(x,y)$ is attained only in this point), the lower bound takes the form

$$\text{capa}(x,y) \geq \inf_{h(z) \in [0,1], z \in \mathcal{S}(x,y)} \sum_{z \in \mathcal{S}(x,y)} \mu(z) \sum_{z' \in \mathcal{M}_x \cup \mathcal{M}_y} p(z,z') [h(z) - h(z')]^2 \quad (8.12)$$

Obviously, the solution of this variational problem is

$$h(z) = \frac{\sum_{z' \in \mathcal{M}_x \cup \mathcal{M}_y} p(z,z') h(z')}{\sum_{z' \in \mathcal{M}_x \cup \mathcal{M}_y} p(z,z')}, \quad z \in \mathcal{S}(x,y) \quad (8.13)$$

Obviously, $h(z)$ differs from the minimizer appearing in the upper bound only by a term that is smaller than $e^{-\beta a}$. Therefore, the upper and lower bounds are equal up to a term of order

$$\sum_{z \in \mathcal{S}(x,y)} \mu(z) e^{-\beta a} = e^{-\beta \widehat{H}(x,y)} e^{-\beta a} \quad (8.14)$$

which is by a factor of $e^{-\beta a}$ smaller than the principal contribution.

Let us note that the situation considered above holds in the case of the stochastic Ising model with Glauber dynamics. Proving this fact requires some rather complicated analysis of the function $H(\sigma)$. For more details see the paper [BM]. In the case of Kawasaki dynamics, the situation is quite more complicated. In that case, saddle point form “plateaus” and the associated variational problems are more complicated. Still, one can reduce the problem to the analysis of problems involving just the simple random walk on certain domains of \mathbb{Z}^d .

Example 2: Discrete diffusions in $d > 1$. A second example are random walks in a potential landscape that generalize our example from Chapter 4 to dimensions greater than one. These examples, that also emerge in the dynamics of certain mean-field spin systems, was the original motivation of our work on metastability and was studied in [BEGK1].

We take our state space Γ as a (subset of the) d -dimensional “lattice” of spacing ϵ , that is we take $\Gamma = \Gamma_\epsilon \subset (\epsilon\mathbb{Z})^d$, and transition probabilities

$$p(x, y) = \begin{cases} \frac{1}{2d} e^{-[F(y)-F(x)]_+}, & \text{if } \|y - x\|_2 = \epsilon, \\ 1 - \sum_{k=1}^d (p(x, x + \epsilon e_\mu) - p(x, x - \epsilon e_\mu)), & \text{if } x = y, \\ 0, & \text{else} \end{cases} \quad (8.15)$$

where $F = F_\epsilon$ is a smooth function bounded from below satisfying $\sum_{x \in \Gamma} \exp(-F(x)/\epsilon) = 1$. This chain has invariant measure

$$\mu(x) = \exp(-F(x)/\epsilon) \quad (8.16)$$

with $f(x)$ a smooth function on G with a finite number of local minima in G .

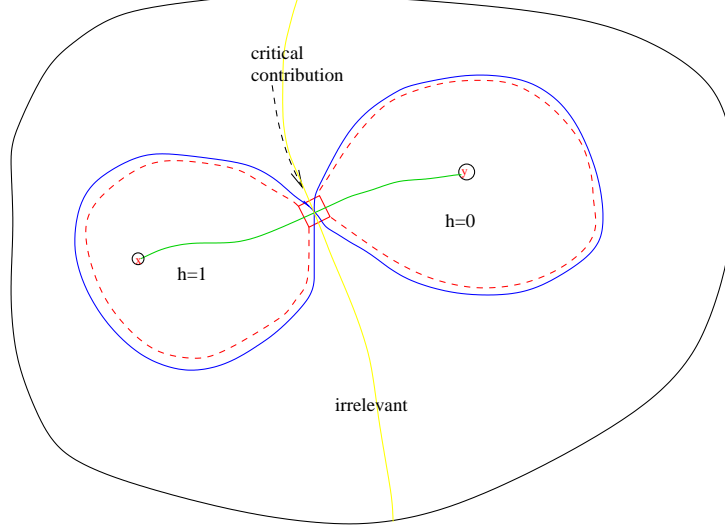
Given two local minima of F , the reasoning towards the computation of the capacity $\text{cap}(x, y)$ is essentially the same as in the preceding example. The only difference here is that since now elementary transition probabilities are not close to zero for steps in any direction, in particular in the vicinity of critical points, it will not be true that the equilibrium potential will be close to zero resp. one already one step below the “saddle points” \mathcal{S} . Of course we have seen this also already in the one-dimensional case.

Let us for simplicity consider the situation where we have two local minima at x and y and a single saddle point z^* between them. We also assume to be in the generic situation when the matrix of second derivatives of the function F at z^* has no zero-eigenvalue. We will make the further simplifying assumption that the eigenvectors of this matrix are parallel to the lattice directions³. We call the lattice direction corresponding to the unique negative eigenvalue of this matrix the 1-direction.

(i) The upper bound. From the explicit computations in the one-dimensional case we may expect that the equilibrium potential $h_{x,y}(z)$ behaves roughly like $1 - \exp(-F(z)/\epsilon)$ within the level set $F(z) < F(z^*)$ containing x , and $\exp(-F(z)/\epsilon)$ in the one containing y . Let us take a strip, Σ , of width $C\sqrt{\epsilon}|\ln \epsilon|$ around the stable manifold of z^* (for simplicity assume that

³The results remain true without this assumptions, but the proofs become considerably more complicated in the general case.

there are no further critical points), which we will further more rectify in such a way that it becomes rectangular and fitting to the lattice at least up to a distance $C'\sqrt{\epsilon}|\ln \epsilon|$ of z^* . We denote this small rectangular region by D . The complement of Σ decomposes into the two sets M_x and M_y . The point is then that within $\Sigma \setminus D$, the invariant measure is smaller than $\epsilon^c \exp(-F(z^*)/\epsilon)$ for some positive c if C and C' are chosen appropriately.



Then we choose our ansatz for the upper bound as follows

$$h^+(z) = \begin{cases} 1, & \text{if } z \in M_x \\ 0, & \text{if } z \in M_y \end{cases} \quad (8.17)$$

For z in D , $h^+(z)$ is chosen to be a function of z_1 only, e.g. $h^+(z) = f(z_1)$ where f is chosen in an optimal way. Moreover, in $\Sigma \setminus D$, $h^+(z)$ may be set to anything.

Inserting this ansatz into the Dirichlet form, we see that

$$\text{cap}(x, y) \leq \inf_f \frac{1}{2} \sum_{z \in M} \mu(z) \sum \pm p(z, z \pm \epsilon e_1) [f(z_1) - f(z_1 \pm \epsilon)]^2 + O\left(\epsilon^c e^{-F(z^*)/\epsilon}\right) \quad (8.18)$$

Now within D , we can Taylor expand

$$\begin{aligned} \mu(z) &= \exp\left(-F(z^*)/\epsilon + |\lambda_1|(z_1^* - z_1)^2/2\epsilon - \lambda_2(z_2^* - z_2)^2/2\epsilon - \dots - \lambda_d(z_d^* - z_d)^2/2\epsilon + O(\epsilon^{1/2}|\ln \epsilon|^3)\right) \end{aligned} \quad (8.19)$$

We see that we can fully neglect the correction term in the exponent, since this gives only a multiplicative error of order $1 + O(\epsilon^{1/2}|\ln \epsilon|^3)$. The principle term in (8.18) can then be

written (up to this error) as

$$\begin{aligned} & \inf_f \frac{1}{2} \exp(-F(z^*)/\epsilon) \sum_{z_2, \dots, z_d} \exp(-\lambda_2(z_2^* - z_2^2)^2/2\epsilon - \dots - \lambda_d(z_d^* - z_d^d)^2/2\epsilon) \\ & \times \sum_{z_1} \exp(+|\lambda_1|(z_1^* - z_1^1)^2/2\epsilon) p(z_1, z_1 \pm \epsilon e_1) [f(z_1) - f(z_1 \pm \epsilon)]^2 \end{aligned} \quad (8.20)$$

where we used that under Metropolis dynamics the transition rates $p(z, z \pm \epsilon e_1)$ turn out to depend also only on z_1 . But now the infimum in all terms of the sum over z_2, \dots, z_d is reached for the same function f , which is simply the one realizing the infimum of the corresponding one-dimensional variational problem. Thus

$$\begin{aligned} \text{cap}(x, y) & \leq \exp(-F(z^*)) \sum_{z_2, \dots, z_d} \exp(-\lambda_2(z_2^* - z_2^2)^2/2\epsilon - \dots - \lambda_d(z_d^* - z_d^d)^2/2\epsilon) \\ & \times \text{cap}^0(-C\epsilon^{1/2}|\ln \epsilon|, C\epsilon^{1/2}|\ln \epsilon|) (1 + O(e^c, \sqrt{\epsilon}|\ln \epsilon|)) \end{aligned} \quad (8.21)$$

where by a simple transformation $f(z_i) \rightarrow e^{-|\lambda_1|(z_1^* - z_1^1)^2/2\epsilon} f(z_1)$,

$$\begin{aligned} & \text{cap}^0(-C\epsilon^{1/2}|\ln \epsilon|, C\epsilon^{1/2}|\ln \epsilon|) \\ & \equiv \inf_{f: f((z_1^* - C\epsilon^{1/2}|\ln \epsilon|)=1, f((z_1^* + C\epsilon^{1/2}|\ln \epsilon|)=0} \frac{1}{2} \sum_{z_1} \exp(-|\lambda_1|(z_1^* - z_1^1)^2/2\epsilon) \\ & p(z_1, z_1 \pm \epsilon e_1) [f(z_1) - f(z_1 \pm \epsilon)]^2 \end{aligned} \quad (8.22)$$

This problem is now easily solved and yields

$$\text{cap}^0(-C\epsilon^{1/2}|\ln \epsilon|, C\epsilon^{1/2}|\ln \epsilon|) \sim \frac{1}{d} \sqrt{\frac{|\lambda_1|\epsilon}{2\pi}} \quad (8.23)$$

Finally, estimating the remaining Gaussian sums, we get that

$$\text{cap}(x, y) \geq e^{-F(z^*)/\epsilon} \frac{1}{d} \sqrt{|\lambda_1|} 2\pi \sqrt{\frac{2\pi\epsilon}{\det \nabla^2 F(z^*)}} (1 + O(e^c, \sqrt{\epsilon}|\ln \epsilon|)) \quad (8.24)$$

(ii) To show that this upper bound gives the correct leading contribution, we use the monotonicity of the Dirichlet form to reduce the graph Γ to just the links in the one-direction within the set D . Then

$$\text{cap}(x, y) \geq \frac{1}{2} \sum_{z \in D} \sum_{\pm} \mu(z) (h_{x,y}(z) - h_{x,y}(z \pm \epsilon e_i))^2 \quad (8.25)$$

Clearly,

$$\begin{aligned} & \text{cap}(x, y) \\ & \geq \frac{1}{2} \sum_{z_2, \dots, z_d} \inf_{f_{z_\perp}: f_{z_\perp}(z_1^* - C\epsilon^{1/2}|\ln \epsilon|)=h_{x,y}, f_{z_\perp}(z_1^* + C\epsilon^{1/2}|\ln \epsilon|)=h_{x,y}} \frac{1}{2} \sum_{\pm} \mu(z) (-f_{z_\perp}(z_1) - f_{z_\perp}(z_1 \pm \epsilon))^2 \end{aligned} \quad (8.26)$$

Now we show, using the renewal argument and crude bounds on $h_{x,y}$ that at the boundaries of D towards x , resp. y , $h_{x,y}$ is close to one, resp. zero up to an error of order ϵ^c . It is easy to solve all the variational problems in (8.26), since they are again one-dimensional. We leave it as an exercise to show that the corresponding lower bound is essentially equal to the upper bound (8.25), so that we have indeed established the asymptotic estimate

$$\begin{aligned} & \text{cap}(x, y) \\ &= \frac{1}{2} \sum_{z_2, \dots, z_d} \inf_{f_{z_\perp}: f_{z_\perp}(z_1^* - C\epsilon^{1/2}|\ln \epsilon|) = h_{x,y}, f_{z_\perp}(z_1^* + C\epsilon^{1/2}|\ln \epsilon|) = h_{x,y}} \frac{1}{2} \sum_{\pm} \mu(z) (-f_{z_\perp}(z_1) - f_{z_\perp}(z_1 \pm \epsilon))^2 \\ & \quad \times (1 + O(e^c, \sqrt{\epsilon}|\ln \epsilon|)) \end{aligned} \tag{8.27}$$

This last estimate together with our general formulas for the mean transition times immediately implies the famous ‘‘Eyring-Kramers’’ formula

$$\mathbb{E}_x \tau_y = 2d \frac{2\pi}{|\lambda_1(z_i^*)|} \frac{\sqrt{|\det(\nabla^2 F(z^*))|}}{\sqrt{|\det(\nabla^2 F(x))|}} e^{[F(z^*) - F(x)]/\epsilon} \left(1 + O(\epsilon^{1/2}|\ln \epsilon|)\right) \tag{8.28}$$

to leading order.

A1. One-dimensional Laplace method.

In Section 4 we had to compute integrals of the form

$$\int_a^b e^{f(x)/\epsilon} dx \quad (10.1)$$

for small ϵ and real valued functions $f(x)$. The method commonly used to estimate such integrals is called *Laplace's method* or *saddle point method*, where the latter is more general and is applicable also in complex valued situations. I will give here a brief outline how this method can be used in simple cases to get *asymptotic* estimates in ϵ for such integrals.

We will assume that a and b are finite, and that f is k -times continuously differentiable in $[a, b]$. Note that these conditions can be considerably relaxed. Without loss of generality we assume that f has a unique global maximum at $x^* \in [a, b]$. We will assume that $x^* = b$. One should distinguish the cases where $f'(b) = 0$ and $f'(b) > 0$. I will for simplicity assume that b and therefore $f'(b)$ does not depend on ϵ , but it is not difficult to see that the method can also be adopted to situations (that may be of interest) where $b = B(\epsilon)$ depends on ϵ and e.g. $f'(b(\epsilon)) \downarrow 0$.

The Laplace method is based on three observations:

- (i) Depending on how fast $f(x)$ decays away from its maximum, the integral is dominated by the contribution from a neighborhood $[b - \delta, b]$, for suitably chosen $\delta = \delta(\epsilon) \downarrow 0$.
- (ii) Within $[b - \delta, b]$, we can expand $f(x)$ in a Taylor series to order $l < k$ where the remainder satisfies a uniform bound of order δ^{l+1} . Neglecting this term produces a multiplicative error of order $e^{C\delta^{l+1}/\epsilon}$ which will be negligible if δ is suitably chosen.
- (iii) The exponential function satisfies the bound

$$\left| e^y - \sum_{l=0}^n \frac{y^l}{l!} \right| \leq C_n |y|^{n+1} e^{|y|} \quad (10.2)$$

This can be used to remove terms in the exponent that are of higher than linear, resp. quadratic order. What remains are integrals of the form $\int_{b-\delta}^b e^{-c(b-x)/\epsilon} (b-x)^m dx$, resp. $\int_{b-\delta}^b e^{-d(b-x)^2/\epsilon} (b-x)^m dx$ and remainder terms that can be estimated by $C\delta^{l+1}$.

- (iv) The remaining integrals are written as e.g.

$$\int_{b-\delta}^b e^{-c(b-x)/\epsilon} (b-x)^m dx = \int_{-\infty}^0 e^{cx/\epsilon} x^l - \int_{-\infty}^{-\delta} e^{x/\epsilon} x^l \quad (10.3)$$

where the first term on the right is explicitly calculable, while the second can be made smaller than any desired power of ϵ if δ is chosen large enough (e.g. $\delta = \epsilon^{1-\alpha}$, for some $\alpha > 0$, in the case when $f'(d) > 0$, resp. $\delta = \epsilon^{1/2-\alpha}$ if the first derivative of f at b vanishes).

Let us carry through this procedure in the simplest case when $f'(b) > 0$ and when we only get the first correction of order ϵ to the principle result. First,

$$\int_a^{b-\delta} e^{f(x)/\epsilon} \leq e^{f(b)/\epsilon} e^{-f'(b)\delta/(2\epsilon)} (b-a) \leq e^{f(b)/\epsilon} e^{-C\epsilon^{-\alpha}} C \quad (10.4)$$

is smaller than any power of ϵ , for small ϵ . Now

$$\begin{aligned} \int_{b-\delta}^d e^{f(x)/\epsilon} &= \int_{b-\delta}^d e^{f(b)/\epsilon - f'(b)(b-x)/\epsilon + f''(b)(b-x)^2/(2\epsilon) + C(b-x)^3/\epsilon} dx \\ &= \int_{b-\delta}^d e^{f(b)/\epsilon - f'(b)(b-x)/\epsilon + f''(b)(b-x)^2/(2\epsilon)} dx \\ &\quad + \int_{b-\delta}^d e^{f(b)/\epsilon - f'(b)(b-x)/\epsilon + f''(b)(b-x)^2/(2\epsilon)} (e^{+C(b-x)^3/\epsilon} - 1) dx \end{aligned} \quad (10.5)$$

The second term is easily bounded by

$$C\delta^3 e^{f(b)/\epsilon} \leq C e^{f(b)/\epsilon} \epsilon^{3-3\alpha} \quad (10.6)$$

For the first integral we now write

$$e^{f''(b)(b-x)^2/(2\epsilon)} = 1 + f''(b)(b-x)^2/(2\epsilon) + \left(e^{f''(b)(b-x)^2/(2\epsilon)} - 1 - f''(b)(b-x)^2/(2\epsilon) \right) \quad (10.7)$$

But on the domain of integration, by

$$\left| e^{f''(b)(b-x)^2/(2\epsilon)} - 1 - f''(b)(b-x)^2/(2\epsilon) \right| \leq C \frac{\delta^4}{\epsilon^2} \leq C \epsilon^{2-4\alpha} \quad (10.8)$$

and so

$$\begin{aligned} &\left| \int_{b-\delta}^b e^{f(b)/\epsilon - f'(b)(b-x)/\epsilon} \left(e^{f''(b)(b-x)^2/(2\epsilon)} - 1 - f''(b)(b-x)^2/(2\epsilon) \right) \right| \\ &\leq e^{f(\beta)/\epsilon} C \epsilon^{2-4\alpha} \int_{b-\delta}^b e^{-f'(b)(b-x)/\epsilon} \\ &\leq e^{f(\beta)/\epsilon} C \epsilon^{2-4\alpha} \int_{-\infty}^0 e^{f'(b)x/\epsilon} \\ &= e^{f(\beta)/\epsilon} \frac{\epsilon}{f'(b)} C \epsilon^{2-4\alpha} \end{aligned} \quad (10.9)$$

What is left of our integral is

$$\begin{aligned}
& \int_{b-\delta}^b e^{f(b)/\epsilon - f'(b)(b-x)/\epsilon} \left(1 - \frac{f''(b)}{2\epsilon}(b-x)^2 \right) \\
&= e^{f(b)/\epsilon} \int_{-\infty}^0 e^{f'(b)x/\epsilon} \left(1 - \frac{f''(b)}{2\epsilon}x^2 \right) \\
&+ e^{f(b)/\epsilon} \int_{-\infty}^{-\delta} e^{f'(b)x/\epsilon} \left(1 - \frac{f''(b)}{2\epsilon}x^2 \right) \\
&= e^{f(b)/\epsilon} \left(\frac{\epsilon}{f'(b)} + \frac{2\epsilon^2 f''(b)}{2(f'(b))^2} \right) \\
&+ C e^{-f'(b)\epsilon^{-\alpha}}
\end{aligned} \tag{10.10}$$

Collecting all terms we find that

$$\int_a^b e^{f(x)/\epsilon} dx = e^{f(b)/\epsilon} \left(\frac{\epsilon}{f'(b)} + \frac{2\epsilon^2 f''(b)}{2(f'(b))^2} + C \left(\epsilon^{2-4\alpha} + e^{-C\epsilon^{-\alpha}} \right) \right) \tag{10.11}$$

It should now be clear how this computation has to be modified if $f'(b) = 0$, but $f''(b) < 0$, and how higher order corrections in ϵ can be computed.

The Laplace method can be used in a very similar manner to compute the corresponding finite sums, e.g. $\sum_{x=a+\epsilon}^b e^{f(x)/\epsilon}$. In the case then $f'(b) > 0$, the principal term then becomes the geometric series

$$e^{f(b)/\epsilon} \sum_{k=0}^{\infty} e^{-kf'(b)} = e^{f(b)/\epsilon} \frac{1}{1 - e^{-f'(b)}} \tag{10.12}$$

If $f'(b) = 0$, the remaining sum

$$\sum_{k=0}^{\infty} e^{-\epsilon k^2 f''(b)/2} \tag{10.13}$$

can be approximated by an integral with errors of order $\sqrt{\epsilon}$ only, i.e.

$$\epsilon \sum_{k=0}^{\infty} e^{-\epsilon k^2 f''(b)/2} = \int_{-\infty}^0 e^{-\epsilon^{-1} x^2 f''(b)/2} dx (1 + O(\sqrt{\epsilon})) \tag{10.14}$$

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