METASTABILITY AND LOW LYING SPECTRA IN REVERSIBLE MARKOV CHAINS

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Abstract: We study a large class of reversible Markov chains with discrete state space and transition matrix P_N. We define the notion of a set of *metastable points* as a subset of the state space Γ_N such that (i) this set is reached from any point $x \in \Gamma_N$ without return to x with probability at least b_N, while (ii) for any two point x, y in the metastable set, the probability $T_{x,y}^{-1}$ to reach y from x without return to x is smaller than $a_N^{-1} \ll b_N$. Under some additional non-degeneracy assumption, we show that in such a situation:

(i) To each metastable point corresponds a metastable state, whose mean exit time can be computed precisely.

(ii) To each metastable point corresponds one simple eigenvalue of $1 - P_N$ which is essentially equal to the inverse mean exit time from this state. Moreover, these results imply very sharp uniform control of the deviation of the probability distribution of metastable exit times from the exponential distribution.

Keywords: Markov chains, metastability, eigenvalue problems, exponential distribution

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1. Introduction

In a recent paper [BEGK] we have presented rather sharp estimates on metastable transition times, both on the level of their mean values, their Laplace transforms, and their distribution, for a class of reversible Markov chains that may best be characterized as random walks in multi-well potentials, and that arise naturally in the context of Glauber dynamics for certain mean field models. These results allow for a very precise control of the behaviour of such processes over very long times.

In the present paper we continue our investigation of metastability in Markov chains focusing however on the connection between *metastability and spectral theory* while working in a more general abstract context. Relating metastability to spectral characteristics of the Markov generator or transition matrix is in fact a rather old topic. First mathematical results go back at least as far as Wentzell [W] and Freidlin and Wentzell [FW]. Freidlin and Wentzell relate the eigenvalues of the transition matrix of Markov processes with exponentially small transition probabilities to exit times from "cycles"; Wentzell has a similar result for the spectral gap in the case of certain diffusion processes. All these relations are on the level of logarithmic equivalence, i.e. of the form $\lim_{\epsilon\downarrow 0} \epsilon \ln(\lambda_i^\epsilon T_i^\epsilon) = 0$ where ϵ is the small parameter, and $\lambda_i^\epsilon, T_i^\epsilon$ are the eigenvalues, resp. exit times. For more recent results of this type, see [M,Sc]. Rather recently, Gaveau and Schulman [GS] (see also [BK] for an interesting discussion) have developed a more general program to give a spectral *definition* of metastability in a rather general setting of Markov chains with discrete state space. In their approach low lying eigenvalues are related to metastable time scales and the corresponding eigenfunctions are related to metastable states. This interesting approach still suffers, however, from rather imprecise relations between eigenvalues and time-scales, and eigenfunctions and states.

In this paper we will put these notions on a mathematically clean and precise basis for a wide class of Markov chains X_t with countable state space Γ_N[5], indexed by some large parameter N. Our starting point will be the definition of a *metastable set* of points each of which is supposed to be a representative of one *metastable state*, on a chosen time scale. It is important that our approach allows to consider the case where the cardinality of $\mathcal{M}_N$ depends on N. The key idea behind our definition will be that it ensures that the time it takes to visit the representative point once the process enters a "metastable state" is very short compared to the lifetime of the metastable state. Thus, observing the visits of the

[5] We expect that this approach can be extended with suitable modifications to processes with continuous state space. Work on this problem is in progress.

process at the metastable set suffices largely to trace the history of the process. We will then show that (under certain conditions ensuring the simplicity of the low-lying spectrum) the expected times of transitions from each such metastable point to "more stable" ones (this notion will be defined precisely later) are *precisely* equal to the inverse of one eigenvalue (i.e. $T_i = \lambda_i^{-1}(1 + o(1))$) and that the corresponding eigenfunction is essentially the indicator function of the *attractor* of the corresponding metastable point. This relation between times and eigenvalues can be considered as the analogue of a quantum mechanical "uncertainty principle". Moreover, we will give precise formulas expressing these metastable transition times in terms of escape probabilities and the invariant measure. Finally, we will derive uniform convergence results for the probability distribution of these times to the exponential distribution. Let us note that one main clue to the precise uncertainty principle is that we consider *transition times* between metastable points, rather than *exit times from domains*. In the existing literature, the problem of transitions between states involving the passage through some "saddle point" (or "bottle neck") is almost persistently avoided (for reasons that we have pointed out in the introduction of [BEGK]), except in one-dimensional situations where special methods can be used (as mentioned e.g. in the very recent paper [GM]). But the passage through the saddle point has a significant impact on the transition time which in general can be neglected only on the level of logarithmic equivalence[6]. Our results here, together with those in [BEGK], appear to be the first that systematically control these effects.

Let us now introduce our setting. We consider a discrete time[7] and specify our Markov chains by their transition matrix P_N whose elements $p_N(x, y)$, $x, y \in \Gamma_N$ denote the one-step transition probabilities of the chain. In this paper we focus on the case where the chain is *reversible*[8] with respect to some probability measure $\mathbb{Q}_N$ on Γ_N. We will always be interested in the case where the cardinality of Γ_N is finite but tends to infinity as $N \uparrow \infty$. Intuitively, metastability corresponds to a situation where the state space Γ_N can be decomposed into a number of disjoint components each containing a state such that the time to reach one of these states from anywhere is much smaller than the time it takes to travel between any two of these states. We will now make this notion precise. Recall from [BEGK] the notation τ_I^x for the first instance the chain starting in x at time 0 reaches the set $I \subset \Gamma_N$,

$$\tau_I^x \equiv \inf\left\{t > 0 : X_t \in I \middle| X_0 = x\right\} \tag{1.1}$$

[6] E.g. the lack of precision in the relation $T_M = \mathcal{O}(1/(1-(1-\lambda)^t))$ in [GS] is partly due to this fact.
[7] There is no difficulty in applying our results to continuous time chains by using suitable embeddings.
[8] The case of irreversible Markov chains will be studied in a forthcoming publication [EK].

Definition 1.1: *A set $\mathcal{M}_N \subset \Gamma_N$ will be called a set of* metastable points *if it satisfies the following assumptions. For finite positive constants a_N, b_N such that, for some sequence $\varepsilon_N \downarrow 0$, $a_N^{-1} \leq \varepsilon_N b_N$ it holds that*

(i) For all $z \in \Gamma_N$,

$$\mathbb{P}\left[\tau^z_{\mathcal{M}_N} \leq \tau^z_z\right] \geq b_N \tag{1.2}$$

(ii) For any $x \neq y \in \mathcal{M}_N$,

$$\mathbb{P}\left[\tau^x_y < \tau^x_x\right] \leq a_N^{-1} \tag{1.3}$$

We associate with each $x \in \mathcal{M}_N$ its *local valley*

$$A(x) \equiv \left\{ z \in \Gamma_N : \mathbb{P}\left[\tau^z_x = \tau^z_{\mathcal{M}_N}\right] = \sup_{y \in \mathcal{M}_N} \mathbb{P}\left[\tau^z_y = \tau^z_{\mathcal{M}_N}\right] \right\} \tag{1.4}$$

We will set

$$R_x \equiv \frac{\mathbb{Q}_N(x)}{\mathbb{Q}_N(A(x))} \tag{1.5}$$

and

$$\begin{aligned} r_N &\equiv \max_{x \in \mathcal{M}_N} R_x \leq 1 \\ c_N^{-1} &\equiv \min_{x \in \mathcal{M}_N} R_x > 0 \end{aligned} \tag{1.6}$$

Note that the sets $A(x)$ are not necessarily disjoint. We will however show later that the set of points that belong to more than one local valley has very small mass under $\mathbb{Q}_N$. The above conditions do not fix $\mathcal{M}_N$ uniquely. It will be reasonable to choose $\mathcal{M}_N$ always such that for all $x \in \mathcal{M}_N$,

$$\mathbb{Q}_N(x) = \sup_{z \in A(x)} \mathbb{Q}_N(z) \tag{1.7}$$

The quantities $\mathbb{P}\left[\tau^x_I \leq \tau^x_x\right]$, $I \subset \mathcal{M}_N$ furnish crucial characteristics of the chain. We will therefore introduce some special notation for them: for $I \subset \mathcal{M}_N$ and $x \in \mathcal{M}_N \backslash I$, set

$$T_{x,I} \equiv \left(\mathbb{P}[\tau^x_I \leq \tau^x_x]\right)^{-1} \tag{1.8}$$

and

$$T_I \equiv \sup_{x \in \mathcal{M}_N \backslash I} T_{x,I} \tag{1.9}$$

Note that these quantities depend on N, even though this is suppressed in the notation.

For simplicity we will consider in this paper only chains that satisfy an additional assumption of *non-degeneracy*:

Definition 1.2: *We say that the family of Markov chains is* generic *on the level of the set $\mathcal{M}_N$, if there exists a sequence $\epsilon_N \downarrow 0$, such that*

(i) For all pairs $x, y \in \mathcal{M}_N$, and any set $I \subset \mathcal{M}_N \backslash \{x, y\}$ either $T_{x,I} \leq \epsilon_N T_{y,I}$ or $T_{y,I} \leq \epsilon_N T_{x,I}$.

(ii) There exists $m_1 \in \mathcal{M}_N$, s.t. for all $x \in \mathcal{M}_N \backslash m_1$, $\mathbb{Q}_N(x) \leq \epsilon_N \mathbb{Q}_N(m_1)$.

We can now state our main results. We do this in a slightly simplified form; more precise statements, containing explicit estimates of the error terms, will be formulated in the later sections.

Theorem 1.3: *Consider a discrete time Markov chain with state space Γ_N, transition matrix P_N, and metastable set $\mathcal{M}_N$ (as defined in Definition 1.1). Assume that the chain is generic on the level $\mathcal{M}_N$ in the sense of Definition 2.1. Assume further that $r_N \varepsilon_N |\Gamma_N||\mathcal{M}_N| \downarrow 0$, and $r_N c_N \epsilon_N \downarrow 0$, as $N \uparrow \infty$. For every $x \in \mathcal{M}_N$ set $\mathcal{M}_N(x) \equiv \{y \in \mathcal{M}_N : \mathbb{Q}_N(y) > \mathbb{Q}_N(x)\}$, define the* metastable exit time *$t_x \equiv \tau^x_{\mathcal{M}_N(x)}$. Then*

(i) For any $x \in \mathcal{M}_N$,

$$\mathbb{E}\, t_x = R_x^{-1} T_{x,\mathcal{M}_N(x)}(1 + o(1)) \tag{1.10}$$

(ii) For any $x \in \mathcal{M}_N$, there exists an eigenvalue λ_x of $1 - P_N$ that satisfies

$$\lambda_x = \frac{1}{\mathbb{E}\, t_x}(1 + o(1)) \tag{1.11}$$

Moreover, there exists a constant $c > 0$ such that for all N

$$\sigma(1 - P_N) \backslash \cup_{x \in \mathcal{M}_N} \lambda_x \subset (c b_N |\Gamma_N|^{-1}, 1] \tag{1.12}$$

(here $\sigma(1 - P_N)$ denotes the spectrum of $1 - P_N$).

(iii) If ϕ_x denotes the right-eigenvector of P_N corresponding to the eigenvalue λ_x, normalized so that $\phi_x(x) = 1$, then

$$\phi_x(y) = \begin{cases} \mathbb{P}[\tau^y_x < \tau^y_{\mathcal{M}_N(x)}](1 + o(1)), & \text{if} \quad \mathbb{P}[\tau^y_x < \tau^y_{\mathcal{M}_N(x)}] \geq \epsilon_N \\ O(\epsilon_N), & \text{otherwise} \end{cases} \tag{1.13}$$

(iv) For any $x \in \mathcal{M}_N$, for all $t > 0$,

$$\mathbb{P}[t_x > t \mathbb{E}\, t_x] = e^{-t(1+o(1))}(1 + o(1)) \tag{1.14}$$

Remark: We will see that $\mathbb{P}[\tau_x^y < \tau_{\mathcal{M}_N(x)}^y]$ is extremely close to one for all $y \in A(x)$, with the possible exception of some points for which $\mathbb{Q}_N(y) \ll \mathbb{Q}_N(x)$. Therefore, the corresponding (normalized) left eigenvectors $\psi_x(y) \equiv \frac{\mathbb{Q}_N(y)\phi_x(y)}{\sum_{z\in\Gamma_N}\mathbb{Q}_N(y)\phi_x(y)}$ are to very good approximation equal to the invariant measure conditioned on the valley $A(x)$. As the invariant measure $\mathbb{Q}_N$ conditioned on $A(x)$ can be reasonably identified with a metastable state, this establishes in a precise way the relation between eigenvectors and metastable distributions. Brought to a point, our theorem then says that the left eigenfunctions of $1 - P_N$ are the metastable states, the corresponding eigenvalues the mean lifetime of these states which can be computed in terms of exit probabilities via (1.10), and that the lifetime of a metastable state is exponentially distributed.

Remark: Theorem 1.3 actually holds under slightly weaker hypothesis than those stated in Definition 1.2. Namely, as will become clear in the proof given in Section 5, the non-degeneracy of the quantities $T_{x,I}$ is needed only for certain sets I. On the other hand, if these weaker conditions fail, the theorem will no longer be true in this simple form. Namely. in a situation where certain subsets $\mathcal{S}_i \subset \mathcal{M}_N$ are such that for all $x \in \mathcal{S}_i$, $T_{x,I}$ (for certain relevant sets I, see Section 5) differ only by constant factors, the eigenvalues and eigenfunctions corresponding to this set will have to be computed specially through a finite dimensional, non-trivial diagonalisation problem. While this can in principle be done on the basis of the methods presented here, we prefer to stay within the context of the more transparent generic situation for the purposes of this paper. Even more interesting situations crating genuinely new effect occur when degenerate subsets of states whose cardinality tends to infinity with N are present. While these fall beyond the scope of the present paper, the tools provided here and in [BEGK] can still of use, as is shown in [BBG].

Let us comment on the general motivation behind the formulation of Theorem 1.3. The theorem allows, in a very general setting, to reduce all relevant quantities governing the metastable behaviour of a Markov chain to the computation of the key parameters, $T_{x,y}$ and R_x, $x, y \in \mathcal{M}_N$. The first point to observe is that these quantities are in many situations rather easy to control with good precision. In fact, control of R_x requires only knowledge of the invariant measure. Moreover, the "escape probabilities", $T_{x,y}^{-1}$, are related by a factor $\mathbb{Q}_N(x)$ to the *Newtonian capacity* of the point y relative to x and thus satisfy a *variational principle* that allows to express them in terms of certain constraint minima of the Dirichlet form of the Markov chain in question. In [BEGK] we have shown how this well-known fact

(see e.g. [Li], Section 6) can be used to give very sharp estimates on these quantities for the discrete diffusion processes studied there. Similar ideas may be used in a wide variety of situations (for another example, see [BBG]); we remind the reader that the same variational representation is at the basis of the "electric network" method [BS]. Let us mention that our general obsession with sharp results is motivated mainly by applications to *disordered* models there the transition matrix P_N is itself a random variable. Fluctuation effects on the long-time behaviour provoked by the disorder can then only be analysed if sharp estimates on the relevant quantities are available. For examples see [BEGK, BBG].

In fact, in the setting of [BEGK], i.e. a random walk on $(\mathbb{Z}/N)^d \cap \Lambda$ with reversible measure $\mathbb{Q}_N(x) = \exp(-NF_N(x))$, where F_N is "close" to some smooth function F with finite number of local minima satisfying some additional genericity requirements, and the natural choice for $\mathcal{M}_N$ being the set of local minima of F_N, the key quantities of Theorem 1.3 were estimated as

$$b_N \geq cN^{-1/2} \tag{1.15}$$

$$\begin{aligned} r_N &\leq cN^{-d/2} \\ c_N &\leq CN^{d/2} \end{aligned} \tag{1.16}$$

$$T_{x,y} = e^{\mathcal{O}(1)} N^{-(d-2)/2} e^{N[F_N(z^*(x,y)) - F_N(x)]} \tag{1.17}$$

where $z^*(x,y)$ is the position of the saddle point between x and y. Moreover, under the genericity assumption of [BEGK],

$$\epsilon_N \leq e^{-N^\alpha} \tag{1.18}$$

for some $\alpha > 0$. The reader will check that Theorem 1.3, together with the precisions detailed in the later sections, provides very sharp estimates on the low-lying eigenvalues of $1 - P_N$ and considerably sharpens the estimates on the distribution function of the metastable transition times given in [BEGK].

Let us note that Theorem 1.3 allows to get results under much milder regularity assumptions on the functions F_N then were assumed in [BEGK]; in particular, it is clear that one can deal with situations where an unbounded number of "shallow" local minima is present. Most of such minima can simply be ignored in the definition of the metastable set $\mathcal{M}_N$ which then will take into account only sufficiently deep minima. This is an important point in many applications, e.g. to spin glass like models (but also molecular dynamics, as discussed below), where the number of local minima is expected to be very large (e.g. $\exp(aN)$), while the metastable behaviour is dominated by much fewer "valleys". For a discussion from a physics point of view, see e.g. [BK].

A second motivation for Theorem 1.3 is given by recent work of Schütte et al. [S,SFHD]. There, a numerical method for the analysis of metastable conformational states of macromolecules is proposed that relies on the numerical investigation of the Gibbs distribution for the molecular equilibrium state via a Markovian molecular dynamics (on a discretized state space). The key idea of the approach is to replace the time-consuming full simulation of the chain by a numerical computation of the low-lying spectrum and the corresponding eigenfunctions, and to deduce from here results on the metastable states and their life times. Our theorem allows to rigorously justify these deductions in a quantitative way in a setting that is sufficiently general to incorporate their situations.

The remainder of this article is organized as follows. In Section 2 we recall some basic notions, and more importantly, show that the knowledge of $T_{x,y}$ for all $x, y \in \mathcal{M}_N$ is enough to estimate more general transition probabilities. As a byproduct, we will show the existence of a natural "valley-structure" on the state space, and the existence of a natural (asymptotic) ultra-metric on the set $\mathcal{M}_N$. In Section 3 we show how to estimate mean transition times. The key result will be Theorem 3.5 which will imply the first assertion of Theorem 1.3. In Section 4 we begin our investigation of the relation between spectra and transition times. The key result there is a characterization of parts of the spectrum of $(1 - P_N)$ in terms of the roots of some non-linear equation involving certain Laplace transforms of transitions times, as well as a representation of the corresponding eigenvectors in terms of such Laplace transforms. This together with some analysis of the properties of these Laplace transforms and an upper bound, using a Donsker-Varadhan [DV] argument, will give sharp two-sided estimates on the first eigenvalue of general Dirichlet operators in terms of mean exit times. These estimates will furnish a crucial input for Section 5 where we will prove that the low-lying eigenvalues of $1 - P_N$ are very close to the principal eigenvalues of certain Dirichlet operators $(1 - P_N)^{\Sigma_j}$, with suitably constructed exclusion sets Σ_j. This will prove the second assertion of Theorem 1.3. In the course of the proof we will also provide rather precise estimates on the corresponding eigenfunction. In the last Section we use the spectral information obtained before to derive, using Laplace inversion formulas, very sharp estimates on the probability distributions of transition times. These will in particular imply the last assertion of Theorem 1.3.

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2. Some notation and elementary facts.

In this section we collect some useful notations and a number of more or less simple facts that we will come back to repeatedly.

The most common notion we will use are the stopping times τ_I^x defined in (1.1). To avoid having to distinguish cases where $x \in I$, it will sometimes be convenient to use the alternative quantities

$$\sigma_I^x \equiv \min\{t \geq 0 \,:\, X_t \in I \,|\, X_0 = x\} \tag{2.1}$$

that take the value 0 if $x \in I$.

Our analysis is largely based on the study of Laplace transforms of transition times. For $I \subset \Gamma_N$ we denote by $(P_N)^I$ the Dirichlet operator

$$(P_N)^I \equiv \mathbb{1}_{I^c} P_N \,:\, \mathbb{1}_{I^c}\mathbb{R}^{\Gamma_N} \to \mathbb{1}_{I^c}\mathbb{R}^{\Gamma_N}, \qquad I^c \equiv \Gamma_N \backslash I \tag{2.2}$$

Since our Markov chains are reversible with respect to the measure $\mathbb{Q}_N$, the matrix $(P_N)^I$ is a symmetric operator on $\mathbb{1}_{I^c}\ell^2(\Gamma_N, \mathbb{Q}_N)$ and thus

$$||(P_N)^I|| = \max\{|\lambda| \,|\, \lambda \in \sigma((P_N)^I)\} \tag{2.3}$$

where $||\cdot||$ denotes the operator norm induced by $\mathbb{1}_{I^c}\ell^2(\Gamma_N, \mathbb{Q}_N)$. For a point $x \in \Gamma_N$, subsets $I, J \subset \Gamma_N$ and $u \in \mathbb{C}$, $\Re(u) < -\log||(P_N)^{I\cup J}||$, we define

$$G_{I,J}^x(u) \equiv \mathbb{E}\big[e^{u\tau_I^x}\mathbb{1}_{\tau_I^x \leq \tau_J^x}\big] = \sum_{t=1}^{\infty} e^{ut}\mathbb{P}[\tau_I^x = t \leq \tau_J^x] \tag{2.4}$$

and

$$K_{I,J}^x(u) \equiv \mathbb{E}\big[e^{u\sigma_I^x}\mathbb{1}_{\sigma_I^x \leq \sigma_J^x}\big] = \begin{cases} G_{I,J}^x(u) & \text{for} \quad x \notin I \cup J, \\ 1 & \text{for} \quad x \in I, \\ 0 & \text{for} \quad x \in J\backslash I \end{cases} \tag{2.5}$$

The Perron-Frobenius theorem applied to the positive matrix $(P_N)^I$ implies that $G_{I,J}^x(u)$ and $K_{I,J}^x(u)$ converge locally uniformly on their domain of definition, more precisely

$$-\log||(P_N)^I|| = \sup\{u \in \mathbb{R} \,|\, K_{I,I}^x(u) \text{ exists for all } x \notin I\} \tag{2.6}$$

We now collect a number of useful standard results that follow trivially from the strong Markov property and/or reversibility, for easy reference.

From the strong Markov property one gets:

Lemma 2.1: *Fix $I, J, L \subset \Gamma_N$. Then for all $\Re(u) < -\log||(P_N)^{I\cup J}||$*

$$G^x_{I,J}(u) = G^x_{I\setminus L, J\cup L}(u) + \sum_{y\in L} G^x_{y,I\cup J\cup L}(u) K^y_{I,J}(u), \qquad x \in \Gamma_N \tag{2.7}$$

In the following we will adopt the (slightly awkward) notation $P_N F^x \equiv \sum_{z\in\Gamma_N} P_N(x,z)F^z$ The following are useful specializations of the foregoing result which we state without proof:

Corollary 2.2: *Fix $I, J \subset \Gamma_N$. Then for $x \in \Gamma_N$*

$$e^u P_N K^x_{I,J}(u) = G^x_{I,J}(u), \qquad x \in \Gamma_N \tag{2.8}$$

and

$$(1 - e^u P_N)\partial_u K^x_{I,J}(u) = G^x_{I,J}(u), \qquad x \notin I \cup J \tag{2.9}$$

where ∂_u denotes differentiation w.r.t. u.

The following *renewal equation* will be used heavily:

Corollary 2.3: *Let $I \subset \Gamma_N$. Then for all $x \notin I \cup y$ and $\Re(u) < -\log||(P_N)^{I\cup y}||$*

$$G^x_{y,I}(u) = \frac{G^x_{y,I\cup x}(u)}{1 - G^x_{x,I\cup y}(u)} \tag{2.10}$$

finally, from reversibility of the chain one has

Lemma 2.4: *Fix $x, y \in \Gamma_N$ and $I \subset \Gamma_N$. Then*

$$\mathbb{Q}_N(x) G^x_{y,I\cup x} = \mathbb{Q}_N(y) G^y_{x,I\cup y} \tag{2.11}$$

The next few Lemmata imply the existence of a nested valley structure and that the knowledge of the quantities $T_{x,y}$ and the invariant measure are enough to control all transition probabilities with sufficient precision. The main result is an approximate ultra-metric triangle inequality. Let us define (the capacity of x relative to y) $E(x,y) = \mathbb{Q}_N(x) T^{-1}_{x,y}$. We will show that

Lemma 2.5: *Assume that $y, m \in \Gamma_N$ and $J \subset \Gamma_N \setminus y \setminus m$ such that for $0 < \delta < \frac{1}{2}$, $E(m,J) \le \delta E(m,y)$. Then*

$$\frac{1-2\delta}{1-\delta} \le \frac{E(m,J)}{E(y,J)} \le \frac{1}{1-\delta} \tag{2.12}$$

Proof: We first prove the upper bound. We write

$$\mathbb{P}[\tau_J^m < \tau_m^m] = \sum_{x \in J} \frac{\mathbb{Q}_N(x)}{\mathbb{Q}_N(m)} \mathbb{P}[\tau_m^x < \tau_J^x] \tag{2.13}$$

Now

$$\mathbb{P}[\tau_m^x < \tau_J^x] = \mathbb{P}[\tau_m^x < \tau_J^x, \tau_y^x < \tau_J^x] + \mathbb{P}[\tau_m^x < \tau_{J\cup y}^x] \frac{\mathbb{P}[\tau_J^m < \tau_{y\cup m}^m]}{\mathbb{P}[\tau_{J\cup y}^m < \tau_m^m]} \tag{2.14}$$

Now by assumption,

$$\frac{\mathbb{P}[\tau_J^m < \tau_{y\cup m}^m]}{\mathbb{P}[\tau_{J\cup y}^m < \tau_m^m]} \leq \frac{\mathbb{P}[\tau_J^m < \tau_m^m]}{\mathbb{P}[\tau_y^m < \tau_m^m]} \leq \delta \tag{2.15}$$

Inserting (2.15) into (2.14) we arrive at

$$\mathbb{P}[\tau_m^x < \tau_J^x] \leq \mathbb{P}[\tau_y^x < \tau_J^x, \tau_m^x < \tau_J^x] + \delta \mathbb{P}[\tau_m^x < \tau_{J\cup y}^x] \leq \mathbb{P}[\tau_y^x < \tau_J^x] + \delta \mathbb{P}[\tau_m^x < \tau_J^x] \tag{2.16}$$

Inserting this inequality into (2.13) implies

$$\mathbb{P}[\tau_J^m < \tau_m^m] \leq (1-\delta)^{-1} \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(m)} \mathbb{P}[\tau_J^y < \tau_y^y] \tag{2.17}$$

We now turn to the lower bound. We first show that the assumption implies

$$\mathbb{P}[\tau_J^y < \tau_m^y] < \delta(1-\delta)^{-1} \tag{2.18}$$

Namely,

$$\mathbb{P}[\tau_J^m < \tau_m^m] \geq \mathbb{P}[\tau_y^m < \tau_J^m < \tau_m^m] = \mathbb{P}[\tau_y^m < \tau_{J\cup m}^m] \mathbb{P}[\tau_J^y < \tau_m^y] \tag{2.19}$$

But

$$\begin{aligned} \mathbb{P}[\tau_y^m < \tau_{J\cup m}^m] =& \mathbb{P}[\tau_y^m < \tau_m^m] - \mathbb{P}[\tau_J^m < \tau_y^m < \tau_m^m] \\ &\geq \mathbb{P}[\tau_y^m < \tau_m^m] - \mathbb{P}[\tau_J^m < \tau_m^m] \\ &\geq \mathbb{P}[\tau_y^m < \tau_m^m](1-\delta) \end{aligned} \tag{2.20}$$

where the last inequality follows from the assumption. Thus

$$\mathbb{P}[\tau_J^m < \tau_m^m] \geq \mathbb{P}[\tau_y^m < \tau_m^m] \mathbb{P}[\tau_J^y < \tau_m^y](1-\delta) \tag{2.21}$$

Solving this inequality for $\mathbb{P}[\tau_J^y < \tau_m^y]$, the assumption yields (2.18).

We continue as in the proof of the upper bound and write for $x \in J$, using (2.18),

$$\begin{aligned} \mathbb{P}[\tau_y^x < \tau_J^x] &= \mathbb{P}[\tau_y^x < \tau_J^x, \tau_m^x < \tau_J^x] + \mathbb{P}[\tau_y^x < \tau_{J\cup m}^x] \mathbb{P}[\tau_J^y < \tau_m^y] \\ &\leq \mathbb{P}[\tau_m^x < \tau_J^x] + \mathbb{P}[\tau_y^x < \tau_J^x] \delta(1-\delta)^{-1} \end{aligned} \tag{2.22}$$

proving

$$\mathbb{P}[\tau_y^x < \tau_J^x] \leq \mathbb{P}[\tau_m^x < \tau_J^x] \frac{1-\delta}{1-2\delta} \tag{2.23}$$

Inserting (2.23) into (2.13) for $m \equiv y$ and, using once more (2.13) in the resulting estimate, we obtain

$$\mathbb{P}[\tau_J^y < \tau_y^y] \leq \frac{1-\delta}{1-2\delta} \frac{\mathbb{Q}_N(m)}{\mathbb{Q}_N(y)} \mathbb{P}[\tau_J^m < \tau_m^m] \tag{2.24}$$

which yields the lower bound in (2.12). $\diamondsuit$

Corollary 2.6: *Assume that $x, y, z \in \mathcal{M}_N$. Then*

$$E(x,y) \geq \frac{1}{3} \min\left(E(x,z), E(z,y)\right) \tag{2.25}$$

Proof: By contradiction. Assume that $E(x,y) < \frac{1}{3}\min\left(E(x,z), E(z,y)\right)$. Then $E(x,y) < \frac{1}{3}E(x,z)$, and so by Lemma 2.5,

$$\frac{1}{2} \leq \frac{E(x,y)}{E(z,y)} \leq \frac{3}{2} \tag{2.26}$$

and in particular $E(y,z) \leq 2E(x,y)$, in contradiction with the assumption. $\diamondsuit$

If we set

$$e(x,y) \equiv \begin{cases} -\ln E(x,y), & \text{if} \quad x \neq y \\ 0, & \text{if} \quad x = y \end{cases} \tag{2.27}$$

then Lemma 2.5 implies that e furnishes an "almost" ultra-metric, i.e. it holds that $e(x,y) \leq \max(e(x,z), e(z,y)) + \ln 3$ which will turn out to be a useful tool later. We mention that in the case of discrete diffusions in potentials, the quantities $e(x,y)$ are essentially N times the heights of the essential saddles between points x and y.

The appearance of a natural ultra-metric structure on the set of metastable states under our minimal assumptions is interesting in itself.

A simple corollary of Lemma 2.5 shows that the notion of elementary valleys, $A(m)$, is reasonable in the sense that "few" points may belong to more than one valley.

Lemma 2.7: *Assume that $x, m \in \mathcal{M}_N$ and $y \in \Gamma_N$. Then*

$$\mathbb{P}[\tau_m^y < \tau_y^y] \geq \epsilon \quad \textit{and} \quad \mathbb{P}[\tau_x^y < \tau_y^y] \geq \epsilon \tag{2.28}$$

implies that

$$\mathbb{Q}_N(y) \leq 2\epsilon^{-1} \mathbb{Q}_N(m) \mathbb{P}[\tau_x^m < \tau_m^m] \tag{2.29}$$

We leave the easy proof to the reader.

3. Mean transition times

In this chapter we will prove various estimates of conditioned transition times $\mathbb{E}[\tau_I^x \,|\tau_I^x \leq \tau_J^x]$, where $I \cup J \subset \mathcal{M}_N$. The control obtained is crucial for the investigation of the low lying spectrum in Chapters 4 and 5. In the particular setting of the paper [BEGK], essentially the same types of estimates have been proven. Apart from re-proving these in the more abstract setting we consider here, we also present entirely different proofs that avoid the inductive structure of the proofs given in [BEGK]. Instead, it uses heavily a representation formula for the Green's function (which first appeared in Section 3, Eq. (3.12) of [BEGK][9]). While the new proofs are maybe less intuitive from a probabilistic point of view, they are considerably simpler.

Theorem 3.1: *Fix a nonempty, irreducible, proper subset $\Omega \subset \Gamma_N$. Let $(1-P_N)^{\Omega^c}$ denote the Dirichlet operator with zero boundary conditions at Ω^c. Then the Green's function defined as $G_N^{\Omega^c}(x,y) \equiv ((1-P_N)^{\Omega^c})^{-1}\mathbb{1}_y(x)$, $x,y \in \Omega$, is given by*

$$G_N^{\Omega^c}(x,y) = \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(x)} \frac{\mathbb{P}[\sigma_x^y < \tau_{\Omega^c}^y]}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]} \qquad (x,y \in \Omega) \tag{3.1}$$

Proof: This theorem follows essentially from the proof of Eq. (3.12) of [BEGK]. Using e.g. the maximum principle, it follows that $(1-P_N)^{\Omega^c}$ is invertible. From (2.8) we obtain, using (2.5),

$$(1-P_N)^{\Omega^c} K_{x,\Omega^c}^y(0) = \mathbb{1}_x(y) G_{\Omega^c,x}^x(0) \qquad (x,y \in \Omega) \tag{3.2}$$

This function serves as a fundamental solution and we compute for $x,y \in \Omega$, using the symmetry of $(1-P_N)^{\Omega^c}$,

$$\begin{aligned} \mathbb{Q}_N(x) G_{\Omega^c,x}^x(0) G_N^{\Omega^c}(x,y) =& \langle (1-P_N)^{\Omega^c} K_{x,\Omega^c}^{(\cdot)}(0), G_N^{\Omega^c}(\cdot,y)\rangle_{\mathbb{Q}_N} \\ =& \langle K_{x,\Omega^c}^{(\cdot)}(0), (1-P_N)^{\Omega^c} G_N^{\Omega^c}(\cdot,y)\rangle_{\mathbb{Q}_N} \\ =& \mathbb{Q}_N(y) K_{x,\Omega^c}^y(0) \end{aligned} \tag{3.3}$$

This proves (3.1).$\diamondsuit$

Remark: Observe that (3.1) still makes sense for $x \in \Omega$ and $y \in \partial\Omega$, where we define the boundary ∂I of a set $I \subset \Gamma_N$ to be

$$\partial I \equiv \{x \in I^c \,|\, \exists y \in I \,:\, P_N(y,x) > 0\} \tag{3.4}$$

[9] More recently, the same formula was rederived by Gaveau and Moreau [GM] also for the non-reversible case.

For such x and y reversibility (2.11) and the renewal relation (2.10) for $u \equiv 0$ and $I \equiv \Omega^c$ imply

$$G_N^{\Omega^c}(x,y) = \mathbb{P}[\tau_y^x = \tau_{\Omega^c}^x] \qquad (x \in \Omega, y \in \partial\Omega) \tag{3.5}$$

Based on Theorem 3.1 we can derive an alternative representation of a particular h-transform of the Green's function with $h(y) = \mathbb{P}[\tau_I^y \leq \tau_J^y]$ that will prove useful in the sequel.

Proposition 3.2: *For every nontrivial partition $I \cup J = \Omega^c$ such that I and J are not empty and $I \backslash J$ communicates with Ω we have*

$$\mathbb{P}[\tau_I^x \leq \tau_J^x]^{-1} G_N^{\Omega^c}(x,y) \mathbb{P}[\tau_I^y \leq \tau_J^y] = \frac{\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_J^x]}{\mathbb{P}[\tau_{\Omega^c}^y < \tau_y^y]} \Delta_{\Omega^c}(x,y), \qquad x,y \in \Omega \tag{3.6}$$

where

$$\Delta_{\Omega^c}(x,y) \equiv \frac{\mathbb{P}[\tau_{\Omega^c}^y < \tau_y^y]\mathbb{P}[\sigma_{\Omega^c \cup y}^x < \tau_x^x]}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\sigma_{\Omega^c \cup x}^y < \tau_y^y]}, \qquad x,y \in \Omega \tag{3.7}$$

Furthermore,

$$\frac{1}{3} \leq \Delta_{\Omega^c}(x,y) \leq 3 \tag{3.8}$$

Proof: (3.6) is a straightforward calculation that uses the renewal equation (2.10), reversibility, and the strong Markov property. Indeed, by (3.1) the left-hand side of (3.6) equals

$$\frac{\mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_{\Omega^c}^y]\mathbb{P}[\tau_I^y \leq \tau_J^y]}{\mathbb{Q}_N(x)\mathbb{P}[\sigma_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_I^x \leq \tau_J^x]} \tag{3.9}$$

By the renewal equation, this equals

$$\frac{\mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_{\Omega^c \cup y}^y]\mathbb{P}[\tau_I^y \leq \tau_J^y]}{\mathbb{Q}_N(x)\mathbb{P}[\tau_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\sigma_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_I^x \leq \tau_J^x]} \tag{3.10}$$

which by reversibility turns into

$$\begin{aligned} &\frac{\mathbb{P}[\sigma_y^x < \tau_{\Omega^c \cup x}^x]\mathbb{P}[\tau_I^y \leq \tau_J^y]}{\mathbb{P}[\tau_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\sigma_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_I^x \leq \tau_J^x]} \\ &= \frac{\mathbb{P}[\sigma_y^x < \tau_{\Omega^c}^x]\mathbb{P}[\sigma_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\tau_x^y < \tau_{\Omega^c}^y]\mathbb{P}[\tau_I^y \leq \tau_J^y]}{\mathbb{P}[\tau_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\sigma_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_I^x \leq \tau_J^x]} \\ &= \frac{\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_J^x]\mathbb{P}[\sigma_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\tau_x^y < \tau_{\Omega^c}^y]}{\mathbb{P}[\tau_{\Omega^c \cup x}^y < \tau_y^y]\mathbb{P}[\sigma_{\Omega^c}^x < \tau_x^x]} \end{aligned} \tag{3.11}$$

where the last identity uses that by the strong Markov property

$$\mathbb{P}[\sigma_y^x < \tau_I^x, \tau_I^x \leq \tau_J^x] = \mathbb{P}[\sigma_y^x < \tau_I^x \leq \tau_J^x] = \mathbb{P}[\sigma_y^x < \tau_{I\cup J}^x]\mathbb{P}[\tau_I^y \leq \tau_J^x] \tag{3.12}$$

(3.11) immediately implies (3.6).

We now turn to the proof of the bound (3.8). Since $\Delta_{\Omega^c}(x,x) = 1$ it is enough to consider the case where $x \neq y$. Moreover, since $\Delta_{\Omega^c}(x,y) = \frac{1}{\Delta_{\Omega^c}(y,x)}$, an upper bound $\Delta_{\Omega^c}(x,y) \leq 3$ will immediately imply the claimed lower bound.

The basic input here is the observation that a path from y to Ω^c either visits a point x or it does not, yielding, together with the strong Markov property

$$\begin{aligned}\mathbb{P}[\tau_{\Omega^c}^y < \tau_y^y] =& \mathbb{P}[\tau_{\Omega^c}^y < \tau_{x\cup y}^y] + \mathbb{P}[\tau_x^y < \tau_{\Omega^c}^y < \tau_y^y] \\ &= \mathbb{P}[\tau_{\Omega^c}^y < \tau_{x\cup y}^y] + \mathbb{P}[\tau_x^y < \tau_{\Omega^c\cup y}^y]\mathbb{P}[\tau_{\Omega^c}^x < \tau_y^x]\end{aligned} \tag{3.13}$$

Using this identity for the first factor in the numerator of (3.7), we obtain that $\Delta_{\Omega^c}(x,y)$ can be written as $\Delta_{\Omega^c}(x,y) = (I) + (II)$ where

$$(I) = \frac{\mathbb{P}[\tau_{\Omega^c}^y < \tau_{x\cup y}^y]\mathbb{P}[\tau_{\Omega^c\cup y}^x < \tau_x^x]}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_{\Omega^c\cup x}^y < \tau_y^y]} = \frac{\mathbb{P}[\tau_{\Omega^c}^y < \tau_x^y]\mathbb{P}[\tau_{\Omega^c\cup y}^x < \tau_x^x]}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]} \tag{3.14}$$

The renewal equation was used in the second equality. Decompose the event in the second factor of the numerator and use (3.13) in the denominator. This yields

$$(I) = \frac{\mathbb{P}[\tau_{\Omega^c}^y < \tau_x^y]\left(\mathbb{P}[\tau_{\Omega^c}^x < \tau_{x\cup y}^x] + \mathbb{P}[\tau_y^x < \tau_{\Omega^c\cup x}^x]\right)}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_{x\cup y}^x] + \mathbb{P}[\tau_y^x < \tau_{\Omega^c\cup x}^x]\mathbb{P}[\tau_{\Omega^c}^y < \tau_x^y]} \leq \mathbb{P}[\tau_{\Omega^c}^y < \tau_x^y] + 1 \leq 2 \tag{3.15}$$

For (II) we get

$$(II) = \frac{\mathbb{P}[\tau_x^y < \tau_{\Omega^c\cup y}^y]\mathbb{P}[\tau_{\Omega^c}^x < \tau_{x\cup y}^x]\mathbb{P}[\tau_{\Omega^c\cup y}^x < \tau_x^x]}{\mathbb{P}[\tau_{\Omega^c\cup y}^x < \tau_x^x]\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_{\Omega^c\cup x}^y < \tau_y^y]} = \frac{\mathbb{P}[\tau_x^y < \tau_{\Omega^c\cup y}^y]\mathbb{P}[\tau_{\Omega^c}^x < \tau_{x\cup y}^x]}{\mathbb{P}[\tau_{\Omega^c}^x < \tau_x^x]\mathbb{P}[\tau_{\Omega^c\cup x}^y < \tau_y^y]} \leq 1 \tag{3.16}$$

The bounds (3.8) are now obvious. $\diamondsuit$

The representation (3.6) for the Green's function implies immediately a corresponding representation for the (conditioned) expectation of entrance times τ_I^x. To see this, recall from (2.9) for $u \equiv 0$ that

$$(1-P_N)^{I\cup J}\mathbb{E}\left[\sigma_I^y \mathbb{1}_{\{\sigma_I^y \leq \sigma_J^y\}}\right] = \mathbb{P}[\tau_I^y \leq \tau_J^y], \qquad y \notin I \cup J \tag{3.17}$$

This yields immediately the

Corollary 3.3: *Let $I, J \subset \Gamma_N$. Then for all $x \notin I \cup J$*

$$\begin{aligned}\mathbb{E}[\tau_I^x | \tau_I^x \leq \tau_J^x] &= \sum_{y \in (I \cup J)^c} \mathbb{P}[\tau_I^x \leq \tau_J^x]^{-1} G_N^{\Omega^c}(x,y) \mathbb{P}[\tau_I^y \leq \tau_J^y] \\ &= \sum_{y \in (I \cup J)^c} \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(x)} \frac{\mathbb{P}[\sigma_x^y < \tau_{I \cup J}^y]}{\mathbb{P}[\tau_{I \cup J}^x < \tau_x^x]} \frac{\mathbb{P}[\tau_I^y \leq \tau_J^y]}{\mathbb{P}[\tau_I^x \leq \tau_J^x]}\end{aligned} \tag{3.18}$$

A first consequence of the representation given above is

Corollary 3.4: *Fix $I \subset \mathcal{M}_N$. Then for all $x \in \Gamma_N$*

$$\mathbb{E}[\tau_I^x | \tau_I^x < \tau_{\mathcal{M}_N \setminus I}^x] \leq 3 b_N^{-1} |\Gamma_N| \tag{3.19}$$

In particular,

$$\mathbb{E}[\tau_{\mathcal{M}_N}^x] \leq 3 b_N^{-1} |\Gamma_N| \tag{3.20}$$

Proof: Using (3.7) in (3.19), we get that

$$\mathbb{E}[\tau_I^x | \tau_I^x < \tau_{\mathcal{M}_N \setminus I}^x] = \sum_{y \in \Gamma_N \setminus \mathcal{M}_N} \frac{\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_{\mathcal{M}_N \setminus I}^x]}{\mathbb{P}[\tau_{\mathcal{M}_N}^y < \tau_y^y]} \Delta_{\mathcal{M}_N}(x,y) \tag{3.21}$$

Using the lower bound (1.2) from Definition 1.1 together with the upper bound (3.8), we get

$$\mathbb{E}\left[\tau_I^x | \tau_I^x < \tau_{\mathcal{M}_N \setminus I}^x\right] \leq 3 b_N^{-1} \sum_{y \in \Gamma_N \setminus \mathcal{M}_N} \mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_{\mathcal{M}_N \setminus I}^x] \tag{3.22}$$

from which the claimed estimate follows by bounding the conditional probability by one[10]. The special case $I = \mathcal{M}_N$ follows in the same way, with the more explicit bound

$$\mathbb{E}\tau_{\mathcal{M}_N}^x \leq 3 b_N^{-1} \sum_{y \in \Gamma_N \setminus \mathcal{M}_N} \mathbb{P}[\sigma_y^x < \tau_{\mathcal{M}_N}^x] \tag{3.23}$$

This concludes the proof of the corollary.$\diamondsuit$

Theorem 3.1 allows to compute very easily the mean times of metastable transitions.

Theorem 3.5: *Assume that $J \subset \mathcal{M}_N$, $x \in \mathcal{M}_N$, and x, J satisfy the condition*

$$T_{x,J} = T_J \tag{3.24}$$

[10] It is obvious that in cases when $|\Gamma_N| = \infty$ this bound can in many cases be improved to yield a reasonable estimate. Details will however depend upon assumptions on the global geometry.

Then

$$\mathbb{E}\tau_J^x = \frac{\mathbb{Q}_N(A(x))}{\mathbb{Q}_N(x)\mathbb{P}[\tau_J^x < \tau_x^x]}\left(1 + \mathcal{O}(1)\left(\frac{R_x|\mathcal{M}_N||\Gamma_N|}{b_N a_N} + \epsilon_N R_x c_N\right)\right) \tag{3.25}$$

Proof: Specializing Corollary 3.3 to the case $J = \emptyset$, we get the representation

$$\mathbb{E}\tau_J^x = \frac{1}{\mathbb{Q}_N(x)\mathbb{P}[\tau_J^x < \tau_x^x]}\sum_{y \notin J}\mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_J^y] \tag{3.26}$$

We will decompose the sum into three pieces corresponding to the two sets

$$\begin{aligned}\Omega_1 \equiv & A(x)\\ \Omega_2 \equiv & \Gamma_N \backslash A(x) \backslash J\end{aligned} \tag{3.27}$$

The sum over Ω_1 gives the main contribution; the trivial upper bound

$$\sum_{y\in\Omega_1}\mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_J^y] \le \sum_{y\in\Omega_1}\mathbb{Q}_N(y) \tag{3.28}$$

is complemented by a lower bound that uses (we ignore the trivial case $x = y$ where $\mathbb{P}[\sigma_x^x < \tau_J^x] = 1$)

$$\mathbb{P}[\tau_x^y < \tau_J^y] = 1 - \mathbb{P}[\tau_J^y < \tau_x^y] \ge 1 - \frac{\mathbb{P}[\tau_J^y < \tau_y^y]}{\mathbb{P}[\tau_x^y < \tau_y^y]} \tag{3.29}$$

By Lemma 2.5, if $\mathbb{P}[\tau_J^x < \tau_x^x] \le \frac{1}{3}\mathbb{P}[\tau_y^x < \tau_x^x]$, then

$$\mathbb{P}[\tau_J^y < \tau_y^y] \le \frac{3}{2}\frac{\mathbb{Q}_N(x)}{\mathbb{Q}_N(y)}\mathbb{P}[\tau_J^x < \tau_x^x] \tag{3.30}$$

so that

$$\mathbb{Q}_N(y)\frac{\mathbb{P}[\tau_J^y < \tau_y^y]}{\mathbb{P}[\tau_x^y < \tau_y^y]} \le \frac{3}{2}\mathbb{Q}_N(x)\frac{|\mathcal{M}_N|}{b_N a_N} \tag{3.31}$$

On the other hand, if $\mathbb{P}[\tau_J^x < \tau_x^x] > \frac{1}{3}\mathbb{P}[\tau_y^x < \tau_x^x]$, then

$$\mathbb{Q}_N(y) \le 3\mathbb{Q}_N(x)\frac{\mathbb{P}[\tau_J^x < \tau_x^x]}{\mathbb{P}[\tau_x^y < \tau_y^y]} \le 3\mathbb{Q}_N(x)\frac{|\mathcal{M}_N|}{b_N a_N} \tag{3.32}$$

Thus

$$\begin{aligned}\sum_{y\in\Omega_1}\mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_J^y] &\ge \sum_{y\in\Omega_1}\mathbb{Q}_N(y) - 3|A(x)|\mathbb{Q}_N(x)\frac{|\mathcal{M}_N|}{b_N a_N}\\ &= \mathbb{Q}_N(A(x))\left(1 - 3|A(x)|R_x\frac{|\mathcal{M}_N|}{b_N a_N}\right)\end{aligned} \tag{3.33}$$

We now consider the remaining contributions. This is bounded by

$$\frac{1}{\mathbb{Q}_N(x)\mathbb{P}[\tau_J^x < \tau_x^x]} \sum_{m \in \mathcal{M}\setminus x} L_m \tag{3.34}$$

where

$$L_m \equiv \sum_{y \in A(m)\setminus J} L_m(y) \equiv \sum_{y \in A(m)\setminus J} \mathbb{Q}_N(y)\mathbb{P}[\sigma_x^y < \tau_J^y] \tag{3.35}$$

Assume first that y is such that

(CJ) $\mathbb{Q}_N(y)\mathbb{P}[\tau_J^y < \tau_y^y] \sim \mathbb{Q}_N(m)\mathbb{P}[\tau_J^m < \tau_m^m]$ and

(Cx) $\mathbb{Q}_N(y)\mathbb{P}[\tau_x^y < \tau_y^y] \sim \mathbb{Q}_N(m)\mathbb{P}[\tau_x^m < \tau_m^m]$ hold,

where we introduced the notation $a \sim b \Leftrightarrow \frac{1}{3} \le \frac{a}{b} \le 3$. Then

$$L_m(y) \le 9\mathbb{Q}_N(y)\frac{\mathbb{P}[\tau_x^m < \tau_m^m]}{\mathbb{P}[\tau_J^m < \tau_m^m]} \tag{3.36}$$

There are two cases:

(i) If $E(m,J) \le \frac{1}{3}E(m,x)$, then by Lemma 2.5, $\frac{\mathbb{Q}_N(m)\mathbb{P}[\tau_J^m < \tau_m^m]}{\mathbb{Q}_N(x)\mathbb{P}[\tau_J^x < \tau_x^x]} \le \frac{3}{2}$ or

$$\mathbb{Q}_N(m) \le \frac{3}{2}\mathbb{Q}_N(x)\frac{T_{m,J}}{T_{x,J}} \le \epsilon_N \frac{3}{2}\mathbb{Q}_N(x) \tag{3.37}$$

Hence

$$L_m(y) \le \mathbb{Q}_N(y) \le \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(m)}\epsilon_N \frac{3}{2} R_x \mathbb{Q}_N(A(x)) \tag{3.38}$$

(ii) If $E(m,J) > \frac{1}{3}E(m,x)$, then $E(x,J) \ge \frac{1}{3}E(m,x)$ or $\mathbb{Q}_N(x)\mathbb{P}[\tau_J^x < \tau_x^x] \ge \frac{1}{3}\mathbb{Q}_N(m)\mathbb{P}[\tau_x^m < \tau_m^m]$ so that

$$L_m(y) \le 27\frac{\mathbb{Q}_N(y)\mathbb{Q}_N(x)}{\mathbb{Q}_N(m)}\frac{T_{m,J}}{T_{x,J}} \le 27\epsilon_N R_x \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(m)}\mathbb{Q}_N(A(x)) \tag{3.39}$$

Finally we must consider the cases where (CJ) or (Cx) are violated.

(iii) Assume that (Cx) fails. Then by Lemma 2.5, $\mathbb{P}[\tau_x^m < \tau_m^m] \ge \frac{1}{3}\mathbb{P}[\tau_y^m < \tau_m^m]$ which implies that

$$\begin{aligned} L_m(y) \le \mathbb{Q}_N(y) &\le 3\mathbb{Q}_N(m)\frac{\mathbb{P}[\tau_x^m < \tau_m^m]}{\mathbb{P}[\tau_m^y < \tau_y^y]} \le 3\mathbb{Q}_N(m)\frac{\mathbb{P}[\tau_x^m < \tau_m^m]|\mathcal{M}_N|}{b_N} \\ &\le 3\mathbb{Q}_N(x)\frac{\mathbb{P}[\tau_m^x < \tau_x^x]|\mathcal{M}_N|}{b_N} \le \frac{3|\mathcal{M}_N|}{b_N a_N} R_x \mathbb{Q}_N(A(x)) \end{aligned} \tag{3.40}$$

(iv) Finally it remains the case where (CJ) fails but (Cx) holds. Then $\mathbb{P}[\tau_J^y < \tau_y^y] > \frac{1}{3}\mathbb{P}[\tau_m^y < \tau_y^y] \geq \frac{b_N}{3|\mathcal{M}_N|}$ and $\mathbb{Q}_N(y)\mathbb{P}[\tau_x^y < \tau_y^y] \leq \frac{3}{2}\mathbb{Q}_N(m)\mathbb{P}[\tau_x^m < \tau_m^m] = \frac{3}{2}\mathbb{Q}_N(x)\mathbb{P}[\tau_m^x < \tau_x^x]$. Thus $L_m(y)$ satisfies equally the bound (3.40).

Using these four bounds, summing over y one gets

$$L_m \leq 27\mathbb{Q}_N(A(x)) \max\left(\epsilon_N R_x R_m^{-1}, \frac{|\mathcal{M}_N||A(m)|}{b_N a_N} R_x\right) \tag{3.41}$$

Putting everything together, we arrive at the assertion of the theorem.$\diamondsuit$

Remark: As a trivial corollary from the proof of Theorem 3.5 one has

Corollary 3.6: *Let $x \in \mathcal{M}_N$ and $J \subset \mathcal{M}_N(x)$. Then the conclusions of Theorem 3.5 also hold.*

Finally, we can easily prove a general upper bound on any conditional expectation.

Theorem 3.7: *For any $x \in \Gamma_N$ and $I, J \subset \mathcal{M}_N$,*

$$\mathbb{E}[\tau_I^x | \tau_I^x \leq \tau_J^x] \leq C \sup_{m \in \mathcal{M}_N \setminus I \setminus J} (R_m \mathbb{P}[\tau_{I\cup J}^m < \tau_m^m])^{-1} \tag{3.42}$$

To prove this theorem the representation of the Green's function given in Proposition 2.2 is particularly convenient. It yields

$$\mathbb{E}[\tau_I^x | \tau_I^x \leq \tau_J^x] = \sum_{y \in \Gamma_N \setminus I \setminus J} \frac{\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_J^x]}{\mathbb{P}[\tau_{I\cup J}^y < \tau_y^y]} \Delta_{I\cup J}(x,y) \tag{3.43}$$

Note first that the terms with y such that $\mathbb{P}[\tau_{I\cup J}^y < \tau_y^y] \geq \delta b_N$ yield a contribution of no more than $|\Gamma_N|(\delta b_N)^{-1}$ which is negligible. To treat the remaining terms, we use that whenever $y \in A(m)$, Lemma 2.5 implies that $\mathbb{P}[\tau_{I\cup J}^y < \tau_y^y] \geq \frac{\mathbb{Q}_N(m)}{\mathbb{Q}_N(y)}\mathbb{P}[\tau_{I\cup J}^m < \tau_m^m]$. Thus

$$\begin{aligned} \mathbb{E}[\tau_I^x | \tau_I^x \leq \tau_J^x] &\leq \frac{3|\Gamma_N|}{\delta b_N} + \sum_{m \in \mathcal{M}_N \setminus I \setminus J} \sum_{y \in A(m)} 3 \frac{\mathbb{Q}_N(y)}{\mathbb{Q}_N(m)} \frac{\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_J^x]}{\mathbb{P}[\tau_{J\cup I}^m < \tau_m^m]} \\ &\leq \frac{3|\Gamma_N|}{\delta b_N} + \sum_{m \in \mathcal{M}_N \setminus I \setminus J} 3R_m^{-1} \frac{1}{\mathbb{P}[\tau_{J\cup I}^m < \tau_m^m]} \end{aligned} \tag{3.44}$$

from which the claim of the theorem follows by our general assumptions. Note that by very much the same arguments as used before, it is possible to prove that

$$\mathbb{P}[\sigma_y^x < \tau_I^x | \tau_I^x \leq \tau_J^x] \leq (1+\delta)\mathbb{P}[\sigma_m^x < \tau_I^x | \tau_I^x \leq \tau_J^x] \tag{3.45}$$

which allows to get the sharper estimate

$$\mathbb{E}\left[\tau_I^x | \tau_I^x \leq \tau_J^x\right] \leq \frac{3|\Gamma_N|}{\delta b_N} + \sum_{m \in \mathcal{M}_N \setminus I \setminus J} 3(1+\delta) R_m^{-1} \frac{\mathbb{P}[\sigma_m^x < \tau_I^x | \tau_I^x \leq \tau_J^x]}{\mathbb{P}[\tau_{J \cup I}^m < \tau_m^m]} \tag{3.46}$$

$\diamondsuit$

We conclude this section by stating some consequences of the two preceding theorems that will be useful later.

Lemma 3.8: *Let I, m satisfy the hypothesis of Theorem 3.5. Then*

$$\max_{x \notin I} \mathbb{E}[\tau_I^x] = \mathbb{E}[\tau_I^m]\big(1 + \mathcal{O}(T_{I \cup m}/T_I)\big) \tag{3.47}$$

Moreover, we have

$$\frac{\mathbb{E}[\tau_m^m, \tau_m^m < \tau_I^m]}{\mathbb{P}[\tau_I^m < \tau_m^m]} = \mathbb{E}[\tau_I^m]\big(1 - \mathcal{O}(T_{I \cup m}/T_I))\big) \tag{3.48}$$

In particular,

$$\mathbb{E}[\tau_m^m, \tau_m^m < \tau_I^m] = R_m^{-1}\left(1 + \mathcal{O}(T_{I \cup m}/T_I)\right) \tag{3.49}$$

Proof: Decomposing into the events where m is and is not visited before I, and, using the strong Markov property, one gets

$$\mathbb{E}[\tau_I^x] = \mathbb{P}[\tau_I^x < \tau_m^x]\mathbb{E}[\tau_I^x | \tau_I^x < \tau_m^x] + \mathbb{P}[\tau_m^x < \tau_I^x]\big(\mathbb{E}[\tau_m^x | \tau_m^x < \tau_I^x] + \mathbb{E}[\tau_I^m]\big) \tag{3.50}$$

Using Theorems 3.5 and 3.7, this implies (3.47) readily. In the same way, or by differentiating the renewal equation (2.10), one gets

$$\mathbb{E}[\tau_I^m] = \mathbb{E}[\tau_I^m | \tau_I^m < \tau_m^m] + \frac{\mathbb{E}[\tau_m^m, \tau_m^m = \tau_I^m]}{\mathbb{P}[\tau_I^m < \tau_m^m]} \tag{3.51}$$

Bounding the first summand on the right by Theorem 3.7 gives (3.48). Using Theorem 3.5 for the right hand side of (3.48) gives (3.49). $\diamondsuit$

4. Laplace transforms and spectra

In this section we present a characterization of the spectrum of the Dirichlet operator $(1-P_N)^I$, $I \subset \mathcal{M}_N$, in terms of Laplace transforms of transition times (defined in (2.4) and (2.5)). This connection forms the basis of the investigation of the low-lying spectrum that is presented in Section 5. To exploit this characterization we study the region of analyticity and boundedness of Laplace transforms. As a first consequence we then show that the principal eigenvalue for Dirichlet operators are with high precision equal to the inverse of expected transition times. A combination of these results then leads to the characterization of the low-lying spectrum given in the next section.

For any $J \subset \mathcal{M}_N$ we denote the principal eigenvalue of the Dirichlet-operator P_N^J by

$$\lambda_J \equiv \min \sigma((1-P_N)^J) \tag{4.1}$$

For $I, J \subset \mathcal{M}_N$ we define the matrix

$$\mathcal{G}_{I,J}(u) \equiv \left(\delta_{m',m} - G^{m'}_{m,I\cup J}(u)\right)_{m',m\in J\setminus I} \tag{4.2}$$

where $\delta_{x,y}$ is Kronecker's symbol. We then have

Lemma 4.1: *Fix subsets $I, J \subset \mathcal{M}_N$ such that $J\setminus I \neq \emptyset$ and a number $0 \leq \lambda \equiv 1-e^{-u} < \lambda_{I\cup J}$. Then*

$$\lambda \in \sigma((1-P_N)^I) \qquad \Longleftrightarrow \qquad \det \mathcal{G}_{I,J}(u) = 0 \tag{4.3}$$

Moreover, the map $\ker \mathcal{G}_{I,J}(u) \ni \vec{\phi} \mapsto \phi \in \mathbb{1}_{I^c}\mathbb{R}^{\Gamma_N}$ defined by

$$\phi(x) \equiv \sum_{m\in J\setminus I} \vec{\phi}_m K^x_{m,I\cup J}(u), \qquad x \in \Gamma_N \tag{4.4}$$

is an isomorphism onto the eigenspace corresponding to the eigenvalue λ.

Proof: Assume that ϕ is an eigenfunction with corresponding eigenvalue $\lambda < \lambda_{I\cup J}$. We have to prove that $\mathcal{G}_{I,J}(u)$ is singular. In view of (2.6) the condition $\lambda_{I\cup J} > \lambda$ implies that $\tilde{\phi}$ defined below is finite.

$$\tilde{\phi} \equiv \sum_{m\in J} \phi(m) K^x_{m,I\cup J}(u), \qquad x \in \Gamma_N \tag{4.5}$$

Furthermore, (2.8) and (2.5) imply for $x \in \Gamma_N$

$$e^u(1-P_N-(1-e^{-u}))\tilde{\phi}(x) = (1-e^uP_N)\tilde{\phi}(x) = \sum_{m'\in I\cup J} \delta_{m',x} \sum_{m\in J} \phi(m)\left(\delta_{m',m} - G^{m'}_{m,I\cup J}(u)\right) \tag{4.6}$$

Let $\Delta \equiv \phi - \tilde{\phi}$. We want to show $\Delta = 0$. Obviously, we have Δ vanishes on $I \cup J$ and $\tilde{\phi}$ on I. Combining (4.6) with the eigenvalue equation for ϕ and the choice of u, we obtain

$$\begin{aligned}(1-P_N)^{I\cup J}\Delta &= \mathbb{1}_{(I\cup J)^c}(1-P_N)^I\Delta = \mathbb{1}_{(I\cup J)^c}\left((1-P_N)^I\phi - (1-P_N)\tilde{\phi}\right)\\ &= \mathbb{1}_{(I\cup J)^c}(\lambda\phi - (1-e^{-u})\tilde{\phi}) = \lambda\Delta\end{aligned} \tag{4.7}$$

Since $\lambda \notin \sigma((1-P_N)^{I\cup J})$, we conclude $\Delta = 0$. Replacing $\tilde{\phi}$ by ϕ in (4.6) and, using $\lambda \equiv 1-e^{-u}$ again, gives

$$0 = \sum_{m'\in I\cup J} \delta_{m',x} \sum_{m\in J} \phi(m)\left(\delta_{m',m} - G^{m'}_{m,I\cup J}(u)\right), \qquad x \in I^c \tag{4.8}$$

Choosing $x \in J\backslash I$ yields that $(\phi(m))_{m\in J\backslash I} \in \ker \mathcal{G}_{I,J}(u)$ and the right-hand side of the equivalence in (4.3) follows. In particular, we have proven that the restriction map $\phi \mapsto (\phi(m))_{m\in J\backslash I}$ defined on the eigenspace corresponding to λ is the inverse of the map defined in (4.4).

For the converse implication we note that for $\lambda < \lambda_{I\cup J}$ the entries of the matrix $\mathcal{G}_{I,J}(u)$ are finite. We replace $(\phi(m))_{m\in J\backslash I}$ in (4.5) by the solution $\vec{\phi}$ of the linear system $\mathcal{G}_{I,J}(u)\vec{\phi} = 0$ and deduce from (4.6) and (4.8) that λ is an eigenvalue with eigenfunction $\tilde{\phi}$. $\diamondsuit$

As a first step we now derive a lower bound on these eigenvalues, using a Donsker-Varadhan [DV] like argument that we will later prove to be sharp.

Lemma 4.2: *For every nonempty subset $J\subset\mathcal{M}_N$ we have*

$$\lambda_J \max_{x\notin J} \mathbb{E}[\tau^x_J] \geq 1 \tag{4.9}$$

Proof: For $\phi \in \mathbb{R}^{\Gamma_N}$ we have for all $x, y \in \Gamma_N$ and $C > 0$

$$\phi(y)\phi(x) \leq \frac{1}{2}(\phi(x)^2 C + \phi(y)^2/C) \tag{4.10}$$

Thus choosing $C \equiv \psi(y)/\psi(x)$, where $\psi \in \mathbb{R}^{\Gamma_N}$ is such that $\psi(x) > 0$ for all $x \in \operatorname{supp}\phi$, we compute, using reversibility,

$$\begin{aligned}\langle P_N\phi,\phi\rangle_{\mathbb{Q}_N} \leq& \frac{1}{2}\sum_{x,y\in\Gamma_N} \mathbb{Q}_N(x)P_N(x,y)(\phi(x)^2(\psi(y)/\psi(x)) + \phi(y)^2(\psi(x)/\psi(y)))\\ =& \sum_{x,y\in\Gamma_N} \mathbb{Q}_N(x)\phi(x)^2\frac{P_N(x,y)\psi(y)}{\psi(x)} = \left\langle \phi\left(\frac{P_N\psi}{\psi}\right),\phi\right\rangle_{\mathbb{Q}_N}\end{aligned} \tag{4.11}$$

Let ϕ be an eigenfunction for the principal eigenvalue and set $\psi(x) \equiv \mathbb{E}[\sigma_J^x]$, $x \in \Gamma_N$. Invoking (2.9) for $u \equiv 0$ and $I \equiv J$ we get

$$\lambda_J ||\phi||^2_{\mathbb{Q}_N} \geq \langle \phi/\psi, \phi \rangle_{\mathbb{Q}_N} \tag{4.12}$$

which in turn gives the assertion. $\diamondsuit$

We now study the behavior of Laplace transforms slightly away from their first pole on the real axis.

Lemma 4.3: *Fix nonempty subsets $I, J \subset \mathcal{M}_N$. Let $G^x_{I,J}$ be the Laplace transform defined in (2.4). It follows that for some $c > 0$ and for $k = 0, 1$ uniformly in $0 \leq \Re(u), |\Im(u)| \leq c/(c_N T_{I \cup J})$ and $x \in \Gamma_N$*

$$\partial_u^k G^x_{I,J}(u) = (1 + \mathcal{O}(|u| c_N T_{I \cup J}))\, \partial_u^k G^x_{I,J}(0) \tag{4.13}$$

Proof: By (2.6), we know that $G^x_{I,J}(u)$, $x \in \Gamma_N$, are finite for all u such that $1 - e^{-\Re(u)} < \lambda_{I \cup J}$. Put

$$K_{u,v} \equiv K^{(\cdot)}_{I,J}(u) - K^{(\cdot)}_{I,J}(v) \tag{4.14}$$

(2.8) and (2.9) imply that for $k = 0, 1$,

$$(1 - P_N)^{I \cup J} (\partial_u \partial_v)^k K_{u,0} = (1 - e^{-u}) \partial_u^k K^{(\cdot)}_{I,J}(u) + \delta_{k,1} K_{u,0} \tag{4.15}$$

We first consider the case where $k = 0$. Using (3.6), we get from (4.15) for all $x \notin I \cup J$

$$\frac{G^x_{I,J}(u)}{G^x_{I,J}(0)} = 1 + (1 - e^{-u}) \sum_{y \notin I \cup J} \frac{\mathbb{P}[\sigma^x_y < \tau^x_I | \tau^x_I \leq \tau^x_J]}{\mathbb{P}[\tau_{I \cup J} < \tau^y_y]} \Delta_{I \cup J}(x, y) \frac{G^y_{I,J}(u)}{G^y_{I,J}(0)} \tag{4.16}$$

where $\Delta_{I \cup J}$ is defined in (3.7). Setting

$$M_{N,k}(u) \equiv \max_{x \notin I \cup J} \frac{|\partial_u^k G^x_{I,J}(u)|}{G^x_{I,J}(0)} \tag{4.17}$$

and, using that $\frac{\partial_u^k G^x_{I,J}(0)}{G^x_{I,J}(0)} = \mathbb{E}[\tau^x_I \,|\tau^x_I < \tau^x_J]$, we obtain from (4.16) that for $1 - e^{-\Re(u)} < \lambda_{I \cup J}$

$$1 - |1 - e^{-u}| M_{N,0}(u) M_{N,1}(0) \leq M_{N,0}(u) \leq 1 + |1 - e^{-u}| M_{N,0}(u) M_{N,1}(0) \tag{4.18}$$

But by Theorem 3.7 we have a uniform bound on $M_{N,1}(0)$, and this implies (4.13) for $x \notin I \cup J$.

For $k = 1$ (4.15) gives

$$\frac{\partial_u G^x_{I,J}(u)}{G^x_{I,J}(0)} = \frac{\partial_u G^x_{I,J}(0)}{G^x_{I,J}(0)} + \sum_{y \notin I \cup J} \frac{\mathbb{P}[\sigma^x_y < \tau^x_I | \tau^x_I \leq \tau^x_J]}{\mathbb{P}[\tau_{I\cup J} < \tau^y_y]} \Delta_{I\cup J}(x,y) \left((1-e^{-u}) \frac{\partial_u G^y_{I,J}(u)}{G^y_{I,J}(0)} + \frac{G^y_{I,J}(u)}{G^y_{I,J}(0)} - 1 \right) \tag{4.19}$$

and the same arguments together with (4.13) for $k = 0$ show, for some $c > 0$ and all $0 \leq \Re(u), |\Im(u)| < cc^{-1} T^{-1}_{J\cup I}$, that

$$M_{N,1}(u) \leq M_{N,1}(0) \left(1 + \mathcal{O}(|u| c_N T_{I\cup J})\right) + |1 - e^{-u}| M_{N,1}(u) M_{N,1}(0) \tag{4.20}$$

In particular, we conclude that on the same set,

$$M_{N,1}(u) = \mathcal{O}(M_{N,1}(0)) = \mathcal{O}(c_N T_{I\cup J}) \tag{4.21}$$

Inserting this estimate into (4.19) (3.18) and (4.13) for $k = 0$ again gives for all $0 \leq \Re(u), |\Im(u)| < cc_N T_{I\cup J}$

$$\frac{\partial_u G^x_{I,J}(u)}{G^x_{I,J}(0)} = \left(1 + \mathcal{O}(|u| N e^{N d_{J\cup K}})\right) \frac{\partial_u G^x_{I,J}(0)}{G^x_{I,J}(0)}, \qquad x \notin I \cup J \tag{4.22}$$

which yields (4.13) for $k = 1$ and $x \notin I \cup J$.

The remaining part, namely $x \in I \cup J$, follows by first using (2.8), respectively (2.9), to express the quantities $\partial^k G^x_{I,J}$ in terms of $\partial^k G^y_{I,J}$ with $y \notin I \cup J$ and then applying the result obtained before. $\diamondsuit$

We now have all tools to establish a sharp relation between mean exit times and the principal eigenvalue λ_I of P^I_N. Set $u_I \equiv -\ln(1 - \lambda_I)$. We want to show that

$$G^m_{m,I}(u_I) = 1 \tag{4.23}$$

Indeed, this follows from Lemma 4.1 with $J = I \cup \{m\}$, $m \in \mathcal{M}_N$, if we can show that $\lambda_I < \lambda_{I\cup m}$. Now it is obvious by monotonicity that $\lambda_I \leq \lambda_{I\cup m}$. But if equality held, then by (2.6), $\lim_{u \uparrow u_I} G^m_{m,I}(u) = +\infty$; by continuity, it follows that there exists $u < u_I$ such that $G^m_{m,I}(u) = 1$, implying by Lemma 4.1 that $1 - e^{-u} < \lambda_I$ is an eigenvalue of P^I_N, contradicting the fact that λ_I is the smallest eigenvalue of P^I_N. We must conclude that $\lambda_I < \lambda_{I\cup m}$ and that (4.23) holds.

Theorem 4.4: *Fix a proper nonempty subset $I \subset \mathcal{M}_N$. Let $m \in \mathcal{M}_N \backslash I$ be the unique local minimum satisfying $T_I = T_{m,I}$. Then*

$$\lambda_I = \left(1 + \mathcal{O}(T_{I\cup m}/T_I)\right) \mathbb{E}[\tau^m_I]^{-1} \tag{4.24}$$

In particular,

$$\lambda_I = R_m T_I^{-1} \left(1 + \mathcal{O}(\epsilon_N |\Gamma_N| + |\Gamma_N|/(\epsilon_N a_N b_N))\right) \tag{4.25}$$

Proof: Using that for $x \geq 0$, $e^x > 1 + x$, for real and positive u,

$$G^m_{m,I}(u) = \mathbb{E}\left[e^{u\tau^m_m} \mathbb{1}_{\tau^m_m < \tau^m_I}\right] \geq \mathbb{P}[\tau^m_m < \tau^m_I] + u\mathbb{E}\left[\tau^m_m \mathbb{1}_{\tau^m_m < \tau^m_I}\right] \tag{4.26}$$

Using this in (4.23), we immediately obtain the upper bound

$$u_I \leq \frac{\mathbb{P}[\tau^m_I < \tau^m_m]}{\mathbb{E}\left[\tau^m_m \mathbb{1}_{\tau^m_m < \tau^m_I}\right]} \tag{4.27}$$

Using now Lemma 3.8 to bound the right hand side, gives the upper bound of (4.24). The lower bound is of course already contained in Lemma 4.2. $\diamondsuit$

The a priori control of the Laplace transforms given in Lemma 4.3 can be used to control denominators in the renewal relation (2.10) which will be important for the construction of the solution of the equation appearing in (4.3). We are interested in the behavior of $G^m_{m,I}$ near u_I.

Lemma 4.5: *Under the hypothesis of Theorem 4.4 there exists $c > 0$ such that for all $0 \leq \Re(u) < c/(c_N T_{I\cup m})$*

$$\begin{aligned} G^m_{m,I}(u) - 1 &= \mathbb{E}\left[\tau^m_m \mathbb{1}_{\tau^m_m < \tau^m_I}\right] \left(u - u_I + (u-u_I)^2 \mathcal{O}(c_N T_{I\cup m})\right) \\ &= (1 + \mathcal{O}(\epsilon_N)) R_m^{-1} \left(u - u_I + (u-u_I)^2 \mathcal{O}(c_N T_{I\cup m})\right) \end{aligned} \tag{4.28}$$

Proof: Performing a Taylor expansion at $u = u_I$ to second order of the Laplace transform on the left-hand side of (4.28) and recalling (4.23) we get

$$G^m_{m,I}(u) - 1 = \partial_u G^m_{m,I}(u_I) \left((u-u_I) - (u-u_I)^2 \mathcal{R}_I(u) \partial_u G^m_{m,I}(u_I)^{-1}\right) \tag{4.29}$$

where

$$\mathcal{R}_I(u) \equiv \int_0^1 s \ddot{G}^m_{m,I}((1-s)u_I + su) ds \tag{4.30}$$

(4.29) then follows from Cauchy's inequality combined with (4.13) and (4.25) which shows, for $c > 0$ small enough, $C < \infty$ large enough, and all u considered in the Theorem, that

$$\begin{aligned} |\ddot{G}^m_{m,I}(u)| \leq \ddot{G}^m_{m,I}\left(c/(c_N T_{I\cup m})\right) &\leq C c_N T_{I\cup m} \partial_u G^m_{m,I}\left(c/(c_N T_{I\cup m})\right) \\ &\leq C^2 c_N T_{I\cup m} \partial_u G^m_{m,I}(0) \end{aligned} \tag{4.31}$$

where we used Lemma 4.3. Using Lemma 3.8, the assertion of the lemma follows. $\diamondsuit$

5. Low lying eigenvalues

In the present section we prove the main new result of this paper. Namely, we establish a precise relation between the low-lying part of the spectrum of the operator $1 - P_N$ and the metastable exit times associated to the set $\mathcal{M}_N$. Together with the results of Section 2, this allows us to give sharp estimates on the entire low-lying spectrum in terms of the transition probabilities between points in $\mathcal{M}_N$ and the invariant measure.

As a matter of fact we will prove a somewhat more general result. Namely, instead of computing just the low-lying spectrum of $1 - P_N$, we will do so for any of the Dirichlet operators $(1 - P_N)^I$, with $I \subset \mathcal{M}_N$ (including the case $I = \emptyset$). In the sequel we will fix $I \subset \mathcal{M}_N$ with $I \neq \mathcal{M}_N$.

The strategy of our proof will be to show that to each of the points $m_i \in \mathcal{M}_N \backslash I$ corresponds exactly one eigenvalue λ_i^I of $(1 - P_N)^I$ and that this eigenvalue in turn is close to the principle eigenvalue of some Dirichlet operator $(1 - P_N)^{\Sigma_i}$, with $I \subset \Sigma_i \subset \mathcal{M}_N$. We will now show how to construct these sets Σ_i in such a way as to obtain an ordered sequence of eigenvalues.

We set the first exclusion set Σ_0 and the first effective depth T_1 to be

$$\Sigma_0 \equiv I \quad \text{and} \quad T_1 \equiv T_{\Sigma_0} \tag{5.1}$$

where T_K, $K \subset \mathcal{M}_N$, is defined in (1.9). If $I \neq \emptyset$, let m_1 be the unique point in $\mathcal{M}_N \backslash I$ such that

$$T_{m_1, I} = T_1 \tag{5.2}$$

If $I = \emptyset$, let m_1 be the unique element of $\mathcal{M}_N$ such that $\mathbb{Q}_N(m_1) = \max_{m \in \mathcal{M}_N} \mathbb{Q}_N(m)$.

For $j = 2, \ldots, j_0$, $j_0 \equiv |\mathcal{M}_N \backslash I|$, we define the corresponding quantities inductively by

$$\Sigma_{j-1} \equiv \Sigma_{j-2} \cup m_{j-1} \quad \text{and} \quad T_j \equiv T_{\Sigma_{j-1}} \tag{5.3}$$

and $m_j \in \mathcal{M}_N \backslash \Sigma_{j-1}$ is determined by the equation

$$T_N(m_j, \Sigma_{j-1}) = T_j \tag{5.4}$$

In order to avoid distinction as to whether or not $j = j_0$, it will be convenient to set $T_{j_0+1} \equiv b_N^{-1}$. Note that this construction and hence all the sets Σ_j depend on N. An important fact is that the sequence T_j is decreasing. To see this, note that by construction and the assumption of genericity

$$T_l = T_{m_l, \Sigma_{l-1}} \geq \epsilon_N^{-1} T_{m_{l+1}, \Sigma_{l-1}} \geq \epsilon_N^{-1} T_{m_{l+1}, \Sigma_l} = \epsilon_N^{-1} T_{l+1} \tag{5.5}$$

The basic heuristic picture behind this construction can be summarized as follows. To each $j = 1, \ldots, j_0$ associate a rank one operator obtained by projecting the Dirichlet operator $(1 - P_N)^{\Sigma_{j-1}}$ onto the eigenspace corresponding to its principal eigenvalue $\lambda_{\Sigma_{j-1}} \sim T_j^{-1}$. Note that our construction of Σ_j as an increasing sequence automatically guarantees that these eigenvalues will be in increasing order. The direct sum of these rank one operators acts approximately like $(1 - P_N)^I$ on the eigenspace corresponding to the exponentially small part of its spectrum. Hence the difference between both operators can be treated as a small perturbation.

Remark: We can now explain what the minimal non-degeneracy conditions are that are necessary for Theorem 1.3 to hold. Namely, what must be ensured is that the preceding construction of the sequence of sets is *unique*, and that the T_{Σ_j} are by a diverging factor ϵ_N^{-1} larger than all other T_{x,Σ_j}.

We are now ready to formulate the main theorem of this section. Let λ_j, $j = 1, \ldots, |\Gamma_N \backslash I|$, be the j-th eigenvalue of $(1 - P_N)^I$ written in increasing order and counted with multiplicity and pick a corresponding eigenfunction ϕ_j such that $(\phi_j)_j$ is an orthonormal basis of $\mathbb{1}_{I^c}\ell^2(\Gamma_N, \mathbb{Q}_N)$. We then have

Theorem 5.1: *Set $j_0 \equiv |\mathcal{M}_N \backslash I|$. There is $c > 0$ such that the Dirichlet operator $(1 - P_N)^I$ has precisely j_0 simple eigenvalues in the interval $[0, cb_N)|\Gamma_N|$, i.e.*

$$\sigma((1 - P_N)^I) \cap [0, cb_N|\Gamma_N|^{-1}) = \{\lambda_1, \ldots, \lambda_{j_0}\} \tag{5.6}$$

Define $\mathcal{T}_1 \equiv \infty$ and for $j = 2, \ldots, j_0$

$$\mathcal{T}_j \equiv \min_{1 \le k < j} T_{m_k, m_j}/T_j \ge \epsilon_N^{-1} \tag{5.7}$$

Then

$$\lambda_j = \left(1 + \mathcal{O}(\mathcal{T}_j^{-1} + T_{j+1}/T_j))\right) \lambda_{\Sigma_{j-1}} \tag{5.8}$$

where λ_K, $K \subset \mathcal{M}_N$, is defined in (4.1).

Moreover, the eigenfunction ϕ_j satisfies for $k = 1, \ldots, j-1$

$$\phi_j(m_k) = \phi_j(m_j)\mathcal{O}\left(R_{m_j} T_{m_k, m_j}/T_j\right) \tag{5.9}$$

Remark: Combining Theorem 5.1 with Theorem 4.4 and Theorem 3.5, we get immediately

Corollary 5.2: *With the notation of Theorem 5.1, for* $j = 1, \dots, j_0$ *that*

$$\begin{aligned} \lambda_j &= (1 + \mathcal{O}(\mathcal{T}_j + T_{j+1}/T_j))\, \mathbb{E}\left[\tau^{m_j}_{\Sigma_{j-1}}\right]^{-1} \\ &= \frac{1}{T_j} R_{m_j} \left(1 + \mathcal{O}\left(|\Gamma_N|(\epsilon_N + 1/(a_N b_N \epsilon_N))\right)\right) \end{aligned} \tag{5.10}$$

Note that Corollary 5.2 is a precise version of (ii) of Theorem 1.3. The estimate (5.9), together with the representation (4.4) and the estimates of the Laplace transforms in Lemma 4.3, gives a precise control of the eigenfunctions and implies in particular (iv) of Theorem 4.3.

The strategy of the proof will be to seek, for each $J \equiv \Sigma_j$, for a solution of the equation appearing in (4.3) with λ near the principle eigenvalue of the associated Dirichlet operator $(1 - P_N)^{\Sigma_{j-1}}$. We then show that these eigenvalues are simple and that no other small eigenvalues occur.

For the investigation of the structure of the equations written in (4.3) we have to take a closer look at the properties of the effective depths defined in (5.3). We introduce for all $m \in \mathcal{M}_N \backslash I$ the associated "metastable depth" with exclusion at I by

$$T_N(m) \equiv T_{m, \mathcal{M}_N(m)}, \quad \text{where} \quad \mathcal{M}_N(m) \equiv I \cup \{m' \in \mathcal{M}_N \,|\, \mathbb{Q}_N(m') > \mathbb{Q}_N(m)\} \tag{5.11}$$

Let us define for $j = 2, \dots, j_0$

$$\mathcal{E}_j \equiv \min_{1 \le l < j} T_{m_l, \Sigma_j \backslash m_l} \tag{5.12}$$

The following result relates our inductive definition to these geometrically more transparent objects and establishes some crucial properties:

Lemma 5.3: *Every effective depth is a metastable depth, more precisely for all* $j = 1, \dots, j_0$ *it follows*

$$T_j = T_N(m_j)(1 + \mathcal{O}(\epsilon_N |\mathcal{M}_N|)) \tag{5.13}$$

For $j = 2, \dots, j_0$ *we have*

$$\mathcal{T}_j \ge \mathcal{E}_j / T_j \ge \epsilon_N^{-1}. \tag{5.14}$$

Moreover, for $j, l = 1, \dots, j_0$, $l < j$, *we have*

$$T_{m_l, \Sigma_j \backslash m_l} = T_{\Sigma_j \backslash m_l}(1 + \mathcal{O}(\epsilon_N |\mathcal{M}_N|)) \tag{5.15}$$

Proof: Fix $l < j$. It will be convenient to decompose $\Sigma_j = \Sigma_{l-1} \cup m_l \cup \Sigma_j^+$, where $\Sigma_j^+ \equiv \Sigma_j \backslash \Sigma_l$. We will use heavily the (almost) ultra-metric $e(\cdot,\cdot)$ introduced in Section 2; for the purposes of the proof we can ignore the irrelevant errors in the ultra-metric inequalities (i.e. all equalities and inequalities relating the functions e in the course of the proof are understood up to error of at most $\ln 3$). Note that $\ln T_{x,J} = e(x,J) - f(x)$, where $f(x) \equiv -\ln \mathbb{Q}_N(x)$. In particular, $d_l \equiv \ln T_l = e(m_l, \Sigma_{l-1}) - f(m_l)$. As a first step we prove the following general fact that will be used several times:

Lemma 5.4: *Let m be such that $e(m, m_l) < e(m_l, \Sigma_{l-1})$. Then $f(m) \geq f(m_l) + |\ln \epsilon_N|$.*

Proof: Note that by ultra-metricity,

$$e(m, \Sigma_{l-1}) = \max\left(e(m, m_l), e(m_l, \Sigma_{l-1})\right) = e(m_l, \Sigma_{l-1}) \tag{5.16}$$

But since for any m,

$$e(m, \Sigma_{l-1}) - f(m) \leq d_l - |\ln \epsilon_N| = e(m_l, \Sigma_{l-1}) - f(m_l) - |\ln \epsilon_N| \tag{5.17}$$

which implies by (5.16) $f(m_l) \leq f(m) - |\ln \epsilon_N|$.$\diamondsuit$

Let us now start by proving (5.14). The first inequality is trivial. We distinguish the cases where $e(m_l, \Sigma_j^+)$ is larger or smaller than $e(m_l, \Sigma_{l-1})$.

(i) Let $e(m_l, \Sigma_j^+) \geq e(m_l, \Sigma_{l-1})$.
Since $e(m_l, \Sigma_j \backslash m_l) = \min\left(e(m_l, \Sigma_{l-1}), e(m_l, \Sigma_j^+)\right)$, this implies that $e(m_l, \Sigma_j \backslash m_l) = e(m_l, \Sigma_{l-1})$.

Then, using (5.5) and genericity from Definition 1.2,

$$\begin{aligned} e(m_l, \Sigma_j \backslash m_l) - f(m_l) &= e(m_l, \Sigma_{l-1}) - f(m_l) = d_l \geq e(m_{j-1}, \Sigma_{l-1}) - f(m_{j-1}) \\ &\geq e(m_{j-1}\Sigma_{j-2}) - f(m_{j-2}) = d_{j-1} \geq d_j + |\ln \epsilon_N| \end{aligned} \tag{5.18}$$

Obviously, this gives (5.14) in this case.

(ii) Let $e(m_l, \Sigma_j^+) < e(m_l, \Sigma_{l-1})$.
In this case there must exist $m_k \in \Sigma_j^+$ such that $e(m_l, \Sigma_j \backslash m_l) = e(m_l, m_k)$, and hence $e(m_k, m_l) < e(m_l, \Sigma_{l-1})$. Thus we can use Lemma 5.4 for $m = m_k$. Together with the trivial inequality $e(m_k, m_l) \geq e(m_k, \Sigma_{k-1})$, it follows that

$$\begin{aligned} &e(m_l, \Sigma_j \backslash m_l) - f(m_l) = e(m_k, m_l) - f(m_l) \\ &\geq e(m_k, \Sigma_{k-1}) - f(m_k) + f(m_l) - f(m_k) \geq d_k + |\ln \epsilon_N| \geq d_j + |\ln \epsilon_N| \end{aligned} \tag{5.19}$$

This implies (5.14) in that case and concludes the proof of this inequality.

We now turn to the proof of (5.15). We want to proof that the maximum over $T_{m,\Sigma_j\setminus m_l}$ is realized for $m = m_l$. Note first that it is clear that the maximum cannot be realized for $m \in \Sigma_j\setminus m_l$ (since in that case $T_{m,\Sigma_j\setminus m_l} = 1$). Thus fix $m \notin \Sigma_j$. We distinguish the cases $e(m, m_l)$ less or larger than $e(m, \Sigma_j\setminus m_l)$.

(i) Assume $e(m, m_l) < e(m, \Sigma_j\setminus m_l)$.
The ultra-metric property of e then implies that $e(m_l, \Sigma_j\setminus m_l) = e(m, \Sigma_j\setminus m_l)$, and hence, using the argument from above, $f(m) > f(m_l) + |\ln \epsilon_N|$. Thus

$$e(m_l, \Sigma_j\setminus m_l) - f(m_l) = e(m, \Sigma_j\setminus m_l) - f(m) + f(m) - f(m_l) \geq e(m, \Sigma_j\setminus m_l) - f(m) + |\ln \epsilon_N| \tag{5.20}$$

which excludes that in this case m may realize the maximum. We turn to the next case.

(ii) Assume $e(m, m_l) \geq e(m, \Sigma_j\setminus m_l)$.
We have to distinguish the two sub-cases like in the proof of (5.14).

(ii.1) $e(m_l, \Sigma_j^+) \geq e(m_l, \Sigma_{l-1})$.
Here we note simply that by (5.18)

$$e(m_l, \Sigma_j\setminus m_l) = e(m_l, \Sigma_{l-1}) - f(m_l) = d_l > e(m, \Sigma_{l-1}) - f(m) \geq e(m, \Sigma_j\setminus m_l) - f(m) \tag{5.21}$$

which implies that m cannot be the maximizer.

(ii.2) $e(m_l, \Sigma_j^+) < e(m_l, \Sigma_{l-1})$.
This time we use (5.19) for some $m_k \in \Sigma_j^+$ and so

$$e(m_l, \Sigma_j\setminus m_l) - f(m_l) > d_k > e(m, \Sigma_{k-1}) - f(m) \geq e(m, \Sigma_j\setminus m_l) - f(m) \tag{5.22}$$

where in the last inequality we used that by assumption $e(m, m_l) > e(m, \Sigma_j\setminus m_l)$. Again (5.22) rules out m as maximizer, and since all cases are exhausted, we must conclude that (5.15) holds.

It remains to show that (5.13) holds. Now the crucial observation is that by Lemma 5.4,

$$\mathcal{M}_N(m_j) \cap \{m \in \mathcal{M}_N : e(m_j, m) < e(m_j, \Sigma_{j-1})\} = \emptyset \tag{5.23}$$

Thus, for all $m \in \mathcal{M}_N(m_j)$, $T_{m_j,m} \geq T_{m_j,\Sigma_{j-1}}$, which implies of course that

$$T_{m_j,\mathcal{M}(m_j)} \geq T_{m_j,\Sigma_{j-1}} \tag{5.24}$$

To show that the converse inequality also holds, it is obviously enough to show that the set

$$\{m|T_{m_j,m} \leq T_{m_j,\Sigma_{j-1}}\} \cap \mathcal{M}_N(m_j) \neq \emptyset \tag{5.25}$$

Assume the contrary, i.e. that for all $m \in \mathcal{M}(m_j)$ $T_{m_j,m} > T_{m_j,\Sigma_{j-1}}$. Now let $m \notin I$ be such a point. Then also $e(m_j,m) > e(m_j,\Sigma_{j-1})$, and so by ultra-metricity $e(m,\Sigma_{j-1}) = \max(e(m_j,m), e(m_j,\Sigma_{j-1})) > e(m_j,\Sigma_{j-1})$. But, since $f(m) \leq f(m_j)$, it follows that

$$T_{m,\Sigma_{j-1}} > T_{m_j,\Sigma_{j-1}} \tag{5.26}$$

in contradiction with the defining property of m_j. Thus (5.25) must hold, and so $T_{m_j,\mathcal{M}_N(m_j)} \leq T_{m_j,\Sigma_{j-1}}$. This concludes the proof of the Lemma.$\diamondsuit$

We now turn to the constructive part of the investigation of the low lying spectrum. Having in mind the heuristic picture described before Theorem 5.1 we are searching for solutions u of (4.3) for $J \equiv \Sigma_j$ near $u_{\Sigma_{j-1}} \equiv -\log(1-\lambda_{\Sigma_{j-1}})$. The procedure of finding u is as follows. The case $j=1$ was studied in Theorem 4.4. For $j = 2, \ldots, j_0$ we consider the matrices $\mathcal{G}_j = \mathcal{G}_{I,\Sigma_j}$ defined in (4.2), i.e.

$$\mathcal{G}_j \equiv \begin{pmatrix} \mathcal{K}_j & -\vec{g}_j \\ -(\vec{g}_j)^t & 1 - G^{m_j}_{m_j,\Sigma_j} \end{pmatrix} \equiv \begin{pmatrix} 1 - G^{m_1}_{m_1,\Sigma_j} & -G^{m_1}_{m_2,\Sigma_j} & \ldots & -G^{m_1}_{m_j,\Sigma_j} \\ -G^{m_2}_{m_1,\Sigma_j} & \ddots & & \vdots \\ \vdots & & & \\ & & & -G^{m_{j-1}}_{m_j,\Sigma_j} \\ -G^{m_j}_{m_1,\Sigma_j} & \ldots & -G^{m_j}_{m_{j-1},\Sigma_j} & 1 - G^{m_j}_{m_j,\Sigma_j} \end{pmatrix} \tag{5.27}$$

and define

$$\mathcal{N}_j \equiv \mathcal{D}_j - \mathcal{K}_j, \quad \text{where} \quad \mathcal{D}_j \equiv \text{diag}(1 - G^{m_l}_{m_l,\Sigma_j})_{1 \leq l < j} \tag{5.28}$$

Equipped with the structure of the effective depths written in Lemma 5.3 and the control of Laplace transforms of transition times obtained in the previous chapter one simply can write a Neumann series for $\mathbb{1} - \mathcal{D}_j(u)^{-1}\mathcal{N}_j(u)$ for u near $u_{\Sigma_{j-1}}$ proving the invertibility of $\mathcal{K}_j(u)$. We then compute

$$\det \mathcal{G}_j = \det \begin{pmatrix} \mathcal{K}_j & 0 \\ -(\vec{g}_j)^t & G_j \end{pmatrix} = G_j \det \mathcal{K}_j \tag{5.29}$$

where

$$G_j \equiv 1 - G^{m_j}_{m_j,\Sigma_j} - (\vec{g}_j)^t \mathcal{K}_j^{-1} \vec{g}_j \tag{5.30}$$

This follows by simply adding the column vector

$$\begin{pmatrix} \mathcal{K}_j \\ -(\vec{g}_j)^t \end{pmatrix} \mathcal{K}_j^{-1} \vec{g}_j$$

(which clearly is a linear combination of the first $j-1$ columns of $\mathcal{G}_j$) to the last column in $\mathcal{G}_j$, and the fact that this operation leaves the determinant unchanged. From this representation we construct solutions $\tilde{u}_j$ near $u_{\Sigma_{j-1}}$ of (4.3). We begin with

Lemma 5.5: *For all $j = 2, \dots, j_0$ there are constants $c > 0$, $C < \infty$ such that for all $C' < \infty$ and all*

$$CR_{m_j}\mathcal{E}_j^{-1} < \Re(u) < cc_N^{-1}T_{j+1}^{-1}, \qquad |\Im(u)| < c/(c_N T_{j+1}) \tag{5.31}$$

the inverse of $\mathcal{K}_j(u)$ exists. The l-th component of $\mathcal{K}_j(u)^{-1}\vec{g}_j(u)$ restricted to the real axis is strictly monotone increasing and, uniformly in u,

$$(\mathcal{K}_j(u)^{-1}\vec{g}_j(u))_l = \mathcal{O}(1)|\Sigma_j||u|^{-1}R_{m_l}T_{m_l,m_j}^{-1} \qquad (l = 1, \dots, j-1) \tag{5.32}$$

Moreover, we obtain

$$\lambda \equiv 1 - e^{-u} \in \sigma((1-P_N)^I) \qquad \Longleftrightarrow \qquad G_j(u) = 0 \tag{5.33}$$

where $G_j(u)$ is defined in (5.30).

Remark: Let us mention that the bound on $\Im(u)$ in (5.31) is not optimal and chosen just for the sake of convenience. The optimal bounds with respect to our control can easily be derived but they are of no particular relevance for the following analysis.

Proof: Fix $j = 2, \dots, j_0$. Formally we obtain

$$\mathcal{K}_j(u)^{-1} = \left(\mathbb{1} - \mathcal{D}_(u)^{-1}\mathcal{N}_j(u)\right)^{-1}\mathcal{D}_j(u)^{-1} = \sum_{s=0}^{\infty}(\mathcal{D}_j(u)^{-1}\mathcal{N}_j(u))^s\mathcal{D}_j(u)^{-1} \tag{5.34}$$

To use these formal calculations and to extract the decay estimate in (5.32) we must estimate the summands in (5.34). To do this we use a straightforward random walk representation for the matrix elements

$$\left(\mathcal{D}_j(u)^{-1}\mathcal{N}_j(u))^s\mathcal{D}_j(u)\right)_{l,k}^{-1} = \sum_{\substack{\omega: m_l \to m_k \\ |\omega| = s}} \prod_{t=1}^{|\omega|} \frac{G_{\omega_t,\Sigma_j}^{\omega_{t-1}}(u)}{1 - G_{\omega_{t-1},\Sigma_j}^{\omega_{t-1}}(u)}(1 - G_{m_k,\Sigma_j}^{m_k}(u))^{-1}, \quad 1 \le l,k < j \tag{5.35}$$

where $\omega : m_l \to m_k$ denotes a sequence $\omega = (\omega_0, \dots, \omega_{|\omega|})$ such that $\omega_0 = m_k$, $\omega_{|\omega|} = m_k$, $\omega_t \in \Sigma_j \backslash (I \cup J)$ and $\omega_{t-1} \neq \omega_t$ for all $t = 1, \dots, |\omega|$. Assuming that the series in (5.34) converges, (5.35) gives the convenient representation

$$(\mathcal{K}_j(u)^{-1}\vec{g}_j(u))_l = \sum_{\omega : m_l \to m_j} \prod_{t=1}^{|\omega|} \frac{G^{\omega_{t-1}}_{\omega_t, \Sigma_j}(u)}{1 - G^{\omega_{t-1}}_{\omega_{t-1}, \Sigma_j}(u)} \tag{5.36}$$

where the sum is now over all walks of arbitrary length. We will now show that this sum over random walks does indeed converge under our hypothesis.

By virtue of (5.15) we may apply (4.28) for $m \equiv m_l$ and $I \equiv \Sigma_j \backslash m_l$ and conclude that there are $c > 0$ and $C < \infty$ such that for all $C' < \infty$ and all $u \in \mathbb{C}$ satisfying (5.31)

$$\begin{aligned} G^{m_l}_{m_l, \Sigma_j}(u) - 1 &= (1 + \mathcal{O}(\epsilon_N)) R^{-1}_{m_l} \left(u - u_{\Sigma_j \backslash m_l}\right) \left(1 + (u - u_{\Sigma_j \backslash m_l}) \mathcal{O}(c_N T_{\Sigma_j})\right) \\ &= (1 + \mathcal{O}(\epsilon_N + 2c)) u R^{-1}_{m_l} \end{aligned} \tag{5.37}$$

where we used that $u_{\Sigma_j \backslash m_l} \leq c_N \mathcal{E}_j$. In addition, shrinking possibly $c > 0$ in (5.31), (4.13) implies that for all $k, l = 1, \dots, j$, $k \neq l$

$$G^{m_l}_{m_k, \Sigma_j}(u) = (1 + \mathcal{O}(|u| c_N T_{j+1}))\, G^{m_l}_{m_k, \Sigma_j}(0) \leq \mathcal{O}(1) \mathbb{P}[\tau^{m_l}_{m_k} \leq \tau^{m_l}_{\Sigma_j}] \tag{5.38}$$

Using these two bounds, (5.36) yields

$$(\mathcal{K}_j(u)^{-1}\vec{g}_j(u))_l \leq \sum_{\omega : m_l \to m_j} \prod_{t=1}^{|\omega|} \mathcal{O}(1) R_{\omega_{t-1}} \mathbb{P}[\tau^{\omega_{t-1}}_{\omega_t} \leq \tau^{\omega_{t-1}}_{\Sigma_j}] |u|^{-1} \tag{5.39}$$

To bound the product of probabilities, the following Lemma is useful:

Lemma 5.6: *Let $\omega_0, \omega_1, \omega_2, \omega_k \in \Sigma_j$ such that $\omega_i \neq \omega_{i+1}$, for all i and $\omega_0 \neq \omega_k$. Then*

$$\prod_{t=1}^{k} \mathbb{P}[\tau^{\omega_{t-1}}_{\omega_t} \leq \tau^{\omega_{t-1}}_{\Sigma_j}] \leq \mathbb{P}[\tau^{\omega_0}_{\omega_k} \leq \tau^{\omega_0}_{(\Sigma_j \backslash \omega_1 \backslash \dots \backslash \omega_k) \cup \omega_0}] (\mathcal{E}_j)^{k-1} \tag{5.40}$$

Proof: The proof is by induction over k. For $k = 1$ the claim is trivial. Assume that it for $k = l$. We will show that it holds for $k = l + 1$. Let $s \equiv \max\{0 \leq t \leq l \,|\, \omega_t = \omega_0\}$. Note that by induction hypothesis and definition of s,

$$\prod_{t=s+1}^{l+1} \mathbb{P}[\tau^{\omega_{t-1}}_{\omega_t} \leq \tau^{\omega_{t-1}}_{\Sigma_j}] \leq \mathbb{P}[\tau^{\omega_s}_{\omega_l} \leq \tau^{\omega_s}_{\Sigma_j \backslash \omega_{s+1} \backslash \dots \backslash \omega_l}] \mathbb{P}[\tau^{\omega_l}_{\omega_{l+1}} \leq \tau^{\omega_l}_{\Sigma_j}] (\mathcal{E}_j)^{l-s-1} \tag{5.41}$$

Now

$$\begin{aligned}\mathbb{P}[\tau^{\omega_s}_{\omega_{l+1}} \leq \tau^{\omega_s}_{\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_{l+1}}] &\geq \mathbb{P}[\tau^{\omega_s}_{\omega_{l+1}} \leq \tau^{\omega_s}_{\Sigma_j\setminus\omega_{s+1}\ldots\setminus\omega_{l+1}}, \tau^{\omega_s}_{\omega_l} < \tau^{\omega_s}_{\omega_{l+1}}] \\ &= \mathbb{P}[\tau^{\omega_s}_{\omega_l} \leq \tau^{\omega_s}_{\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l}]\mathbb{P}[\tau^{\omega_l}_{\omega_{l+1}} < \tau^{\omega_l}_{\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_{l+1}}] \\ &= \mathbb{P}[\tau^{\omega_s}_{\omega_l} \leq \tau^{\omega_s}_{\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l}]\frac{\mathbb{P}[\tau^{\omega_l}_{\omega_{l+1}} < \tau^{\omega_l}_{(\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_{l-1})\cup\omega_{l+1}}]}{\mathbb{P}[\tau^{\omega_l}_{(\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l)\cup\omega_{l+1}} < \tau^{\omega_l}_{\omega_l}]} \\ &\geq \mathbb{P}[\tau^{\omega_s}_{\omega_l} \leq \tau^{\omega_s}_{\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l}]\frac{\mathbb{P}[\tau^{\omega_l}_{\omega_{l+1}} \leq \tau^{\omega_l}_{\Sigma_j}]}{\mathbb{P}[\tau^{\omega_l}_{(\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l)\cup\omega_{l+1}} < \tau^{\omega_l}_{\omega_l}]}\end{aligned} \tag{5.42}$$

Now the denominator on the right is,

$$\mathbb{P}[\tau^{\omega_l}_{(\Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_l)\cup\omega_{l+1}} < \tau^{\omega_l}_{\omega_l}] \leq \mathbb{P}[\tau^{\omega_l}_{\Sigma_j\setminus\omega_l} < \tau^{\omega_l}_{\omega_l}] \leq \mathcal{E}_j \tag{5.43}$$

by (5.15). Thus, using the obvious bound

$$\prod_{t=1}^{s}\mathbb{P}[\tau^{\omega_{t-1}}_{\omega_t} \leq \tau^{\omega_{t-1}}_{\Sigma_j}] \leq (\mathcal{E}_j)^s \tag{5.44}$$

and once more that $\omega_0 \in \Sigma_j\setminus\omega_{s+1}\setminus\ldots\setminus\omega_{l+1}$, (5.42) inserted into (5.41) yields the claim for $k = l+1$ which concludes the proof. $\diamondsuit$

Using Lemma 5.6 in (5.38) and the trivial bound $R_{\omega_t} \leq 1$, we get

$$\begin{aligned}(\mathcal{K}_j(u)^{-1}\vec{g}_j(u))_l &\leq \mathbb{P}[\tau^{m_l}_{m_j} < \tau^{m_l}_{m_l}] \sum_{\omega:m_l\to m_j}\frac{CR_{m_l}}{|u|}\left(\frac{C\mathcal{E}_j}{|u|}\right)^{|\omega|-1} \\ &\leq \mathbb{P}[\tau^{m_l}_{m_j} < \tau^{m_l}_{m_l}] \sum_{k=1}^{\infty}\frac{CR_{m_l}}{|u|}\left(\frac{C|\Sigma_j|\mathcal{E}_j}{|u|}\right)^{k-1} \\ &\leq \mathbb{P}[\tau^{m_l}_{m_j} < \tau^{m_l}_{m_l}] \frac{CR_{m_l}|u|^{-1}}{1-C|\Sigma_j|\mathcal{E}_j|u|^{-1}}\end{aligned} \tag{5.45}$$

If $C|\Sigma_j|\mathcal{E}|u|^{-1}$ is say smaller than $1/2$, the estimate (5.32) follows immediately. (5.33) then is a direct consequence of (4.3) and (5.29), since by (5.32) the determinant of $\mathcal{K}_j(u)$ cannot vanish in the domain of u-values considered. $\diamondsuit$

Remark: Defining

$$\mathcal{D}_I \equiv \mathrm{diag}(1-G^{m_l}_{m_l,\mathcal{M}_N})_{1\leq l\leq j_0}, \qquad \mathcal{N}_I \equiv \mathcal{D}_I - \mathcal{G}_{I,\mathcal{M}_N} \quad \text{and} \quad (\vec{f}_I)^t \equiv (G^{m_k}_{I,\mathcal{M}_N})_{1\leq k\leq j_0} \tag{5.46}$$

where $\mathcal{G}_{I,\mathcal{M}_N}$ is defined in (4.2), a slight modification of the proof above shows that for $c>0$ small enough and all $\Re(u) < cb_N^{-1}$ such that

$$\alpha_I \equiv \min_{m\in\mathcal{M}_N\setminus I}|G^m_{m,\mathcal{M}_N}(u)-1| > (1/c)c_N^{-1}\max_{m\in\mathcal{M}_N\setminus I}T^{-1}_{m,\mathcal{M}_N\setminus m} \tag{5.47}$$

one can write an absolutely convergent Neumann series for $\left(\mathbb{1} - \mathcal{D}_I^{-1}(u)\mathcal{N}_I(u)\right)^{-1}$. Furthermore, as a consequence of a random walk expansion similar to (5.45) we obtain the bound

$$(\mathcal{G}_{I,\mathcal{M}_N}(u)^{-1}\vec{f}_I(u))_l = \mathcal{O}(\alpha_I^{-1}c_N^{-1}T_{m_l,I}) \tag{5.48}$$

This estimate is needed for the proof of Lemma 5.5. We are searching for solutions u near $u_{\Sigma_{j-1}}$ of the equation appearing in (5.33). The case $j = 1$ is already treated in Theorem 4.4. Fix $j = 2, \dots, j_0$. We want to apply Lagrange's Theorem to this equation (see [WW]) which tells us the following: Fix a point $a \in \mathbb{C}$ and an analytic function Ψ defined on a domain containing the point a. Assume that there is a contour in the domain surrounding a such that on this contour the estimate $|\Psi(\zeta)| < |\zeta - a|$ holds. Then the equation

$$\zeta = a + \Psi(\zeta) \tag{5.49}$$

has a unique solution in the interior of the contour. Furthermore, the solution can be expanded in the form

$$\zeta = a + \sum_{n=1}^{\infty}(n!)^{-1}\partial_\zeta^{n-1}\Psi(a)^n \tag{5.50}$$

We are in a position to prove

Proposition 5.7: *For $j = 1, \dots, j_0$ there is a simple eigenvalue $\tilde{\lambda}_j = 1 - e^{-\tilde{u}_j} < \lambda_{\Sigma_j}$ such that (5.8), (5.10) hold if we replace λ_j by $\tilde{\lambda}_j$. Let $\tilde{\phi}_j$ be a corresponding eigenfunction. Then (5.9) holds if we replace ϕ_j by $\tilde{\phi}_j$.*

Proof: By means of Theorem 4.4 and (4.4) we may assume that $j = 2, \dots, j_0$. The equation in (5.33) can be written as

$$G_{m_j,\Sigma_j}^{m_j}(u) - 1 + \Phi_j(\zeta) = 0 \tag{5.51}$$

where we have set $\zeta \equiv u\mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]$ and

$$\Phi_j(\zeta) \equiv \sum_{l=1}^{j-1} G_{m_l,\Sigma_j}^{m_j}(u)(\mathcal{K}_j(u)^{-1}\vec{g}_j(u))_l \tag{5.52}$$

Fix constants $c > 0$, $C < \infty$ and let us denote by U_j the strip of all $\zeta \in \mathbb{C}$ such that

$$T_j/\mathcal{E}_j < \Re(\zeta) < cT_j/T_{j+1}, \qquad |\Im(\zeta)| < cT_j/(T_{j+1}r_N c_N) \tag{5.53}$$

Putting $\zeta_{\Sigma_{j-1}} \equiv u_{\Sigma_{j-1}}\mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]$ it follows $\zeta_{\Sigma_{j-1}} = 1 + \mathcal{O}(\epsilon_N)$ from (4.26) and (4.25) and we may apply (4.28) for $c > 0$ small enough and all $\zeta \in U_j$ to obtain

$$G_{m_j,\Sigma_j}^{m_j}(u) - 1 = \mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]^{-1}(1 + \mathcal{O}(\epsilon_N))R_{m_j}^{-1}\left(\zeta - \zeta_{\Sigma_{j-1}} + (\zeta - \zeta_{\Sigma_{j-1}})^2 R_j(\zeta)\right) \tag{5.54}$$

where $\mathcal{R}_j(\zeta) \equiv \mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]^{-1}\mathcal{R}_{\Sigma_{j-1}}(u)$ is defined in (4.30). By (5.54) it follows that (5.51) is equivalent to

$$\zeta = \zeta_{\Sigma_{j-1}} + \Psi_j(\zeta) \tag{5.55}$$

for some function Ψ_j satisfying

$$\Psi_j(\zeta) = \mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}](1+\mathcal{O}(\epsilon_N))R_{m_j}^{-1}\Phi_j(\zeta) + (\zeta-\zeta_{\Sigma_{j-1}})^2\mathcal{R}_j(\zeta) \tag{5.56}$$

Using (3.25) in combination with (5.4), it follows

$$\mathcal{R}_j(\zeta) = \mathcal{O}(T_{j+1}/T_j) \tag{5.57}$$

Using (5.32) and the estimate (5.38), as well as (3.25), we see that for some $c>0$, $C<\infty$ for all $|\zeta-\zeta_{\Sigma_{j-1}}| \le 1$

$$\mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]\mathbb{E}\left[\tau_{m_j}^{m_j}\mathbb{1}_{\tau_{m_j}^{m_j}<\tau_{\Sigma_j}^{m_j}}\right]\Phi_j(\zeta) = \sum_{l=1}^{j-1}\mathcal{O}\left(c_N^2T_j^2T_{m_l,m_j}^{-1}T_{m_j,m_l}^{-1}\right) \le \mathcal{O}(c_N^2\mathcal{T}_j^{-1}) \tag{5.58}$$

By means of (5.57) and (5.58) it follows for $|\zeta-\zeta_{\Sigma_{j-1}}| \le 1$

$$\Psi_j(\zeta) = \mathcal{O}(\mathcal{T}_j^{-1} + T_{j+1}/T_j) \tag{5.59}$$

Since $\mathcal{T}_j \ge \mathcal{E}_j$, by (5.14) and Definition 1.2, we may apply Lagrange's Theorem to (5.55) giving the existence of a solution $\tilde{\zeta}_j = \tilde{u}_j\mathbb{E}[\tau_{\Sigma_{j-1}}^{m_j}]$ of (5.51) satisfying $|\tilde{\zeta}_j - \zeta_{\Sigma_{j-1}}| < 1$. We rewrite (5.55) in the form

$$\tilde{\zeta}_j = \zeta_{\Sigma_{j-1}} + \mathcal{O}(\mathcal{T}_j^{-1} + T_{j+1}/T_j) \tag{5.60}$$

By (5.33) $\tilde{\lambda}_j \equiv 1-e^{\tilde{u}_j}$ defines an eigenvalue. Since from the invertibility of $\mathcal{K}_j(\tilde{u}_j)$ it follows that the kernel of $\mathcal{G}_j(\tilde{u}_j)$ is at most one-dimensional, (4.4) implies that $\tilde{\lambda}_j$ is simple. Using (4.24) and (4.25) for $I \equiv \Sigma_{j-1}$, we derive from (5.60) that (5.10) and (5.8) hold, if we replace λ_j by $\tilde{\lambda}_j$. Moreover, using $\tilde{u}_j < u_{\Sigma_j}$ from (4.4), we conclude that

$$(\tilde{\phi}_j(m_l))_{1\le l<j} = \tilde{\phi}_j(m_j)\mathcal{K}_j(\tilde{u}_j)^{-1}\vec{g}_j(\tilde{u}_j) \tag{5.61}$$

Hence from (5.32) and $\tilde{u}_j = e^{\mathcal{O}(1)}u_{\Sigma_{j-1}}$ we obtain that (5.9) is satisfied if we replace ϕ_j by $\tilde{\phi}_j$. $\diamondsuit$

Now it is very easy to finish the

Proof of 5.1: Proposition 5.7 tells us that $\lambda_k \leq \tilde{\lambda}_k$ for $k = 1, \ldots, j_0$. Assume now that there is $k = 2, \ldots, j_0$ such that $\lambda_k < \tilde{\lambda}_k$. Let $k = 2, \ldots, j_0$ be minimal with this property. Since $\tilde{\lambda}_{k-1} = \lambda_{k-1}$ is simple, we have $\tilde{\lambda}_{k-1} < \lambda_k$. Lemma 5.5 in combination with (5.30) now tells us that for $j = 1, \ldots, j_0$ some constants $c > 0$, $C < \infty$ and all $Cc_N^{-1}\mathcal{E}_j^{-1} < u < cc_N^{-1}T_{j+1}^{-1}$ the function $G_j(u)$ is strictly monotone decreasing, i.e. has at most one zero. Hence from (5.33) for $j \equiv k-1$ and $G_{k-1}(\tilde{u}_{k-1}) = 0$ we deduce that $u_k \geq cc_N^{-1}T_k^{-1}$. But since we already know that $u_k \leq Cc_N^{-1}T_k^{-1}$ for some C, it then follows from (5.33) for $j \equiv k$ that $G_k(u_k) = 0$ implying the contradiction $\lambda_k = \tilde{\lambda}_k$.

Since λ_{j_0} is simple, (5.33) for $j \equiv j_0$ and $G_{j_0}(u_{j_0}) = 0$ implies $\lambda_{j_0+1} > cb_N$, where c denotes the constant appearing in (5.31).

The remaining assertions of Theorem 5.1 then follow from Proposition 5.7. $\diamondsuit$

6. The distribution function

The objective of this chapter is to show how the structure of the low lying spectrum implies a precise control of the distribution function of the times τ_I^m, in cases where Theorem 3.5 applies, i.e. $I \subset \mathcal{M}_N$, $I, \mathcal{M}_N \backslash I \neq \emptyset$, and $m_1 \in \mathcal{M}_N \backslash I$, $T_I = T_{m_1,I}$. It is already known that the normalized distribution function converges weakly to the exponential distribution (see [BEGK] for the sharpest estimates beyond weak convergence in the most general case).

The proof of these results proceeds by inverting the Laplace transforms $G_I^m(u)$, making use of the information about the analytic structure of these functions that is contained in the spectral decomposition of the low lying spectrum of $(1 - P_N)^I$ obtained in the previous section.

Let us denote by $\mathcal{L}_N$ the Laplace transform of the complementary distribution function, i.e.

$$\mathcal{L}_N(u) \equiv \mathcal{L}_{N,I}^{m_1}(u) \equiv \sum_{t=0}^{\infty} e^{ut}\mathbb{P}[\tau_I^{m_1} > t] \qquad (\Re(u) < u_I), \tag{6.1}$$

where u_I is defined in (4.26). The Perron-Frobenius Theorem gives $\lim(1/t)\log\mathbb{P}[\tau_I^{m_1} > t] = -u_I$. Hence the Laplace transform defined above is locally uniformly exponentially convergent. In order to obtain the continuation of $\mathcal{L}_N$ to the whole plane we perform a partial summation in the sum on the right-hand side of (6.1) and get

$$\mathcal{L}_N(u) = \frac{G_{I,I}^{m_1}(u) - 1}{e^u - 1}. \tag{6.2}$$

Invoking (2.8) a straightforward computation for $\lambda \equiv 1 - e^{-u}$ shows that

$$G^x_{I,I}(u) = ((1-P_N)^I - \lambda)^{-1}(\mathbb{1}_{I^c} P_N \mathbb{1}_I)(x) \qquad (x \notin I), \tag{6.3}$$

Hence $\mathcal{L}_N$ is a meromorphic function with poles in $u \in \{u_1, \ldots, u_{|\Gamma_N \setminus I|}\}$, where we recall the definition of the eigenvalues $\lambda_j = 1 - e^{-u_j}$ for $j = 1, \ldots, |\Gamma_N \setminus I|$ prior to Theorem 5.1. Since $\mathcal{L}_N$ is 2π-periodic in the imaginary direction, a short computation yields

$$\mathbb{P}[\tau_I^{m_1} > t] = \frac{1}{2\pi i} \int_{-i\pi}^{i\pi} e^{-tu} \mathcal{L}_N(u) du. \tag{6.4}$$

Deforming the contour in (6.4) gives for $u_{j_0} < \alpha < u_{j_0+1}$ and $U_\alpha \equiv (0, \alpha) \times (-\pi, \pi)$

$$\mathbb{P}[\tau_I^{m_1} > t] = \frac{1}{2\pi i} \int_{\alpha-i\pi}^{\alpha+i\pi} e^{-tu} \mathcal{L}_N(u) du - \sum_{u_j \in U_\alpha} e^{-tu_j} \operatorname{res}_{u_j} \mathcal{L}_N, \tag{6.5}$$

where $\operatorname{res}_u \mathcal{L}_N$ denotes the residue of $\mathcal{L}_N$ at u. Here we have used that periodicity of $\mathcal{L}_N$ shows that the integrals over $[\alpha + i\pi, i\pi]$ and $[-i\pi, \alpha - i\pi]$ cancel and that the poles u_j, $j = 1, \ldots, j_0$, are simple.

Our main result can be formulated as follows:

Theorem 6.1: *Let $j_0 \equiv |\mathcal{M}_N \setminus I|$. There is $c > 0$ such that for some $c > 0$,*

$$\mathbb{P}[\tau_I^{m_1} > t] = -\sum_{j=1}^{j_0} e^{-tu_j} \operatorname{res}_{u_j} \mathcal{L}_N + e^{-tcb_N^{-1}|\Gamma_N|} (2\pi i)^{-1} \int_{-i\pi}^{i\pi} e^{-tu} \mathcal{L}_N(u) du, \tag{6.6}$$

where $u_j = -\ln(1-\lambda_j)$ and λ_j are the eigenvalues of $(1-P_N)^I$ that are estimated in Theorem 5.1. Moreover, the residues satisfy

$$\operatorname{res}_{u_1} \mathcal{L}_N = -1 + \mathcal{O}\left(R_{m_1} c_N T_2 / T_1\right), \qquad \operatorname{res}_{u_j} \mathcal{L}_N = \mathcal{O}\left(R_{m_1} c_N T_j / T_1\right) \qquad (j = 2, \ldots, j_0) \tag{6.7}$$

while the remainder integral on the right-hand side of (6.6) is bounded by

$$(2\pi i)^{-1} \int_{-i\pi}^{i\pi} e^{-tu} \mathcal{L}_N(u) du = \mathcal{O}\left(c_N^{-1} b_N^{-2} |\Gamma_N|^2 / T_1\right). \tag{6.8}$$

Remark: Recalling (3.25) and Theorem 5.1, one sees that Theorem 6.1 implies that the distribution of $t_I^{m_1}$ is to a remarkable precision a pure exponential. In particular, one has the

Corollary 6.2: *Uniformly in* $t \in \mathbb{E}[\tau_I^{m_1}]^{-1}\mathbb{N}$

$$\mathbb{P}[\tau_I^{m_1} > t\mathbb{E}[\tau_I^{m_1}]] = (1 + \mathcal{O}(R_{m_1} c_N T_2/T_1))\, e^{-t\left(1+\mathcal{O}(R_{m_1} c_N T_2/T_1)\right)}. \tag{6.9}$$

We start with the computation of the residue of the Laplace transform at u_1.

Lemma 6.3:

$$\mathrm{res}_{u_1} \mathcal{L}_N = -1 + \mathcal{O}(R_{m_1} c_N T_2/T_1). \tag{6.10}$$

Proof: From (4.23) for $m \equiv m_1$ and the renewal relation (2.10) and (6.2) follows

$$\mathrm{res}_{u_1} \mathcal{L}_N = \lim_{u\to u_1} \frac{G^{m_1}_{I,m_1}(u)}{e^u - 1} \frac{u - u_1}{G^{m_1}_{m_1,I}(u_1) - G^{m_1}_{m_1,I}(u)} = -\frac{1}{e^{u_1} - 1} \frac{G^{m_1}_{I,m_1}(u_1)}{\partial_u G^{m_1}_{m_1,I}(u_1)}. \tag{6.11}$$

Since $u_1 = e^{\mathcal{O}(1)} N^{-1} R_{m_1} T_1^{-1}$, (4.13) for $k = 0, 1$ gives for some $C < \infty$

$$\frac{G^{m_1}_{I,m_1}(u_1)}{\partial_u G^{m_1}_{m_1,I}(u_1)} = (1 + \mathcal{O}(R_{m_1} c_N T_2/T_2)) \frac{G^{m_1}_{I,m_1}(0)}{\partial_u G^{m_1}_{m_1,I}(0)}. \tag{6.12}$$

Hence (6.10) follows from (6.11) in combination with (5.10) and (3.48). $\diamondsuit$

In general we cannot prove lower bounds for the higher residues for the reason described in the remark after Theorem 5.1. However, we can show that they are very small:

Lemma 6.4:

$$\mathrm{res}_{u_j} \mathcal{L}_N = \mathcal{O}\left(T_j/T_1\right)) \qquad (j = 2, \dots, j_0). \tag{6.13}$$

Proof: For fixed $j = 0, \dots, j_0$ we compute, using (6.2) and (6.3),

$$\begin{aligned} \mathrm{res}_{u_j} \mathcal{L}_N &= \lim_{u\to u_j} \frac{1}{e^u - 1} \frac{u - u_j}{(1 - e^{-u_j}) - (1 - e^{-u})} \frac{\langle \mathbb{1}_{I^c} P_N \mathbb{1}_I, \phi_j\rangle_{\mathbb{Q}_N}}{(||\phi_j||_{\mathbb{Q}_N})^2} \phi_j(m_1) \\ &= -\frac{e^{u_j}}{e^{u_j} - 1} \frac{\langle \mathbb{1}_{I^c} P_N \mathbb{1}_I, \phi_j\rangle_{\mathbb{Q}_N}}{(||\phi_j||_{\mathbb{Q}_N})^2} \phi_j(m_1). \end{aligned} \tag{6.14}$$

We can assume that $\phi_j(m_j) = 1$. We can express $\phi_j(x)$, using the definition (4.4), Lemma 4.3, and Theorem 5.1 in the form

$$\begin{aligned} \phi_j(x) =& (1 + \mathcal{O}(\gamma)) K^x_{m_j,\Sigma_j}(0) + \sum_{l=1}^{j-1} \mathcal{O}(T_j/T_{m_l,m_j})(1 + \mathcal{O}(\gamma)) K^x_{m_l,\Sigma_j}(0) \\ =& (1 + \mathcal{O}(\gamma))\mathbb{P}[\sigma^x_{m_j} < \tau^x_{\Sigma_{j-1}}] + \mathcal{O}(\gamma). \end{aligned} \tag{6.15}$$

where $\gamma \equiv R_{m_j} \max(\mathcal{T}^{-1}, T_{j+1}/T_j)$. Using Lemma 2.7, one sees easily that this implies that for any $\epsilon > 0$,

$$(||\phi_j||_{\mathbb{Q}_N})^2 \geq (1 + \mathcal{O}(e^{-N\gamma}))\mathbb{Q}_N(\{x \in \Gamma_N \,|\, |x - m_j| < \varepsilon/2\}) \geq (1-\epsilon)\mathcal{Q}_N(A(m_j)) \tag{6.16}$$

We conclude from (4.4) that, for $J \equiv \Sigma_j$,

$$\begin{aligned} \langle \mathbb{1}_{I^c} P_N \mathbb{1}_I, \phi_j \rangle_{\mathbb{Q}_N} =& \sum_{k=1}^{j} \phi_j(m_k) \sum_{\substack{x \in \Gamma_N \\ y \in I}} \mathbb{Q}_N(x) P_N(x,y) K^x_{m_k,\Sigma_j}(u_j) \\ =& \sum_{k=1}^{j} \phi_j(m_k) \sum_{\substack{x \in \Gamma_N \\ y \in I}} \mathbb{Q}_N(y) P_N(y,x) K^x_{m_k,\Sigma_j}(u_j), \end{aligned} \tag{6.17}$$

where we have used the symmetry of P_N. Applying (2.8) and (2.11) to the right-hand side of (6.17) we get

$$\begin{aligned} \langle \mathbb{1}_{I^c} P_N \mathbb{1}_I, \phi_j \rangle_{\mathbb{Q}_N} =& \sum_{k=1}^{j} \phi_j(m_k) \sum_{y \in I} \mathbb{Q}_N(y) G^y_{m_k,\Sigma_j}(u_j) \\ =& \sum_{k=1}^{j} \phi_j(m_k) \mathbb{Q}_N(m_k) G^{m_k}_{I,\Sigma_j}(u_j). \end{aligned} \tag{6.18}$$

Using that $\phi_j(m_j) = 1$, we deduce from (5.9) and reversibility that

$$\mathbb{Q}_N(m_k)\phi_j(m_k) = \mathbb{Q}_N(m_j)\mathcal{O}(R_{m_j}^{-1} T_j / T_{m_j,m_k}) \tag{6.19}$$

Combining (6.19) with (5.38), (6.16), and, once more, (5.9) with $k \equiv 1$, gives

$$\begin{aligned} (||\phi_j||_{\mathbb{Q}_N})^{-2} \phi_j(m_1) \langle \mathbb{1}_{I^c} P_N \mathbb{1}_I, \phi_j \rangle_{\mathbb{Q}_N} =& \sum_{k=1}^{j} \mathcal{O}\left(R_{m_j} \frac{T_j^2}{T_{m_1,m_j} T_{m_j,m_k} T_{m_k,I}} \right) \\ =& \mathcal{O}\left(R_{m_j} \frac{T_j^2}{T_{m_1,m_j} T_{m_j,I}} \right), \end{aligned} \tag{6.20}$$

where we have used Lemma 5.6 for the sequences $\omega = (m_j, m_k, m)$ in the last equation. It is easy to verify that

$$\frac{T_j^2}{T_{m_1,m_j} T_{m_j,I}} \leq \frac{T_j}{T_{m_j, I \cup m_1} T_1}. \tag{6.21}$$

Inserting (6.20) and (6.21) into (6.14), using $u_j = R_{m_j} T_j^{-1}(1 + o(1))$ and $T_{m_j, I \cup m_1} \geq T_j$, we arrive at (6.13). $\diamondsuit$

The last ingredient for the proof of Theorem 6.1 consists in estimating of the remainder integral in (6.6). This essentially boils down to

Lemma 6.5: *There is $\delta > 0$ such that for all $\delta^{-1} R_{m_1} T_{j_0} < \alpha < \delta b_N |\Gamma_N|^{-1}$ and all $\lambda \equiv 1 - e^{-u}$ on the circle $|\lambda - 1| = e^{-\alpha}$ we have*

$$G^{m_1}_{I,I}(u) = \mathcal{O}(\alpha^{-1} c_N^{-1} T_1^{-1}). \tag{6.22}$$

Proof: From the strong Markov property (2.7) for $J \equiv I$ and $L \equiv \mathcal{M}_N \backslash I$ we obtain for $\Re(u) < u_{\mathcal{M}_N}$

$$K^x_{I,I}(u) = K^x_{I,\mathcal{M}_N}(u) + \sum_{l=1}^{j_0} K^{m_l}_{I,I}(u) K^x_{m_l,\mathcal{M}_N}(u) \qquad (x \in \Gamma_N). \tag{6.23}$$

Applying $(1 - P_N - \lambda)^I$ to both sides of the previous equation and evaluating the resulting equation at $x = m_k$, $k = 1, \ldots, j_0$, we conclude, as in (4.8), via (2.9) and (2.5) that

$$0 = -G^{m_k}_{I,\mathcal{M}_N}(u) + \sum_{l=1}^{j_0} G^{m_l}_{I,I}(u)(\delta_{lk} - G^{m_k}_{m_l,\mathcal{M}_N}(u)). \tag{6.24}$$

Thus the vector

$$\vec{\psi}_\lambda \equiv (G^{m_l}_{I,I}(u))_{1 \le l \le j_0} \tag{6.25}$$

solves the system of equations

$$\mathcal{G}_{I,\mathcal{M}_N}(u) \vec{\psi}_\lambda = \vec{f}_I(u), \tag{6.26}$$

where $\mathcal{G}_{I,\mathcal{M}_N}(u)$ and $\vec{f}_I(u)$ are defined in (4.2) and (5.46), respectively. In order to be able to apply (5.48) we claim that for some $\delta, c > 0$, for all $u = \alpha + iv$, $v \in [-\pi, \pi]$, and for all $m \in \mathcal{M}_N \backslash I$

$$|G^m_{m,\mathcal{M}_N}(u) - 1| \ge c\alpha. \tag{6.27}$$

We first observe that (2.2) shows that, for all $\Re(u') < u_{\mathcal{M}_N}$,

$$\mathbb{Q}_N(m)(G^m_{m,\mathcal{M}_N}(u) - 1) = -e^u \langle ((1 - P_N)^{\mathcal{M}_N \backslash m} - \lambda) K^{(\cdot)}_{m,\mathcal{M}_N}(u), K^{(\cdot)}_{m,\mathcal{M}_N}(u') \rangle_{\mathbb{Q}_N}, \tag{6.28}$$

where we have extended the inner product to $\mathbb{C}^{\Gamma_N}$ in the canonical way such that it is $\mathbb{C}$-linear in the second argument. For $|v \pm \pi| \le \pi/3$ we simply get from (6.28), for $u' \equiv u$ and some

$c > 0$, using that $\sigma((1-P_N)^{\mathcal{M}_N\setminus m})\subset(0,1)$,

$$\begin{aligned}
&|\mathbb{Q}_N(m)\,\mathrm{Re}(e^{-u}(G^m_{m,\mathcal{M}_N}(u)-1))|\\
&\quad=\left|\left\langle((1-P_N)^{\mathcal{M}_N\setminus m}-(1+e^{-\alpha}|\cos(v)|)K^{(\cdot)}_{m,\mathcal{M}_N}(u),K^{(\cdot)}_{m,\mathcal{M}_N}(u)\right\rangle_{\mathbb{Q}_N}\right|\\
&\quad\geq(1+ce^{-\alpha}-1)(||K^{(\cdot)}_{m,\mathcal{M}_N}(u)||_{\mathbb{Q}_N})^2\\
&\quad\geq ce^{-\alpha}\mathbb{Q}_N(m).
\end{aligned}\tag{6.29}$$

For $|v+\pi|>\pi/3$, $|v-\pi|>\pi/3$ and $|v|>\alpha$, we derive from (6.28) for $u'\equiv u$ and some $c>0$

$$\begin{aligned}
|\mathbb{Q}_N(m)\,\mathrm{Im}(e^{-u}(G^m_{m,\mathcal{M}_N}(u)-1))|&=|\sin(v)|e^{-\alpha}(||K^{(\cdot)}_{m,\mathcal{M}_N}(u)||_{\mathbb{Q}_N})^2\\
&\geq\mathbb{Q}_N(m)c\alpha e^{-\alpha}.
\end{aligned}\tag{6.30}$$

In the remaining case, namely where $|v|\leq\alpha$, we use (6.28) for $u'\equiv u_{\mathcal{M}_N\setminus m}$ and obtain via (4.4), for $I\equiv\mathcal{M}_N\setminus m$, $J\equiv m$, that

$$|\mathbb{Q}_N(m)e^{-u}(G^m_{m,\mathcal{M}_N}(u)-1)|=|\bar\lambda-\lambda_{\mathcal{M}_N\setminus m}|\,|\langle K^{(\cdot)}_{m,\mathcal{M}_N}(u),K^{(\cdot)}_{m,\mathcal{M}_N}(u_{\mathcal{M}_N\setminus m})\rangle_{\mathbb{Q}_N}|.\tag{6.31}$$

It follows from (4.13) for some $\delta>0$ uniformly in $x\in\Gamma_N$ and $|v|\leq\alpha$

$$K^x_{m,\mathcal{M}_N}(u)=(1+\delta\mathcal{O}(1))\,K^x_{m,\mathcal{M}_N}(u_{\mathcal{M}_N\setminus m}).\tag{6.32}$$

Since the minimum of the function $|\bar\lambda-\lambda_{\mathcal{M}_N\setminus m}|$ is attained at $\lambda=1-e^{-\alpha}$, we conclude from (6.31) and (6.32) in combination with (4.4) for $J\equiv m_1$ and (6.16) for some $c>0$ and all $|v|\leq\alpha$ that

$$\begin{aligned}
|\mathbb{Q}_N(m)e^{-u}(G^m_{m,\mathcal{M}_N}(u)-1)|&\geq c|\bar\lambda-\lambda_{\mathcal{M}_N\setminus m}|(||K^{(\cdot)}_{m,\mathcal{M}_N}(u_{\mathcal{M}_N\setminus m})||_{\mathbb{Q}_N})^2\\
&\geq c^2\mathbb{Q}_N(A(m))(1-e^{-\alpha}).
\end{aligned}\tag{6.33}$$

(6.33), (6.30) and (6.29) prove (6.27). Since by definition (5.3) and (5.14) it follows that

$$T_{j_0}=T_{m_{j_0},\mathcal{M}_N\setminus m_{j_0}}=\min_{m\in\mathcal{M}_N}T_{m,\mathcal{M}_N\setminus m}\geq b_N^{-1},\tag{6.34}$$

b_N is defined in Definition 1.1, combining (6.27) with (5.48) shows that the solution of (6.26) satisfies

$$\psi_\lambda(m_1)=(\vec\psi_\lambda)_1=\mathcal{O}\left(\alpha^{-1}c_N^{-1}/T_1\right).\tag{6.35}$$

Proof of Theorem 6.1: The proof of Theorem 6.1 now is reduced to the application of the Laplace inversion formula and estimation of the remainder integral. In view of (6.10) and (6.13) it remains to estimate the remainder integral on the right-hand side of (6.5). But

this is by means of (6.2) and (6.3) in combination with (6.22) for $\alpha \equiv cb_N|\Gamma_N|^{-1}$, $0 < c < \delta$, fairly easy. $\diamondsuit$

References

[BBG] G. Ben Arous, A. Bovier, and V. Gayrard, "Aging in the random energy model under Glauber dynamics", in preparation (2000).

[BEGK] A. Bovier, M.Eckhoff, V. Gayrard, and M. Klein, "Metastability in Stochastic Dynamics of Disordered Mean-Field Models", to appear in Probab. Theor. Rel. Fields (2000).

[BK] G. Biroli and J. Kurchan, "Metastable states in glassy systems", `http://www.xxx.lanl.gov/cond-mat/0005499` (2000).

[DS] P.G. Doyle and J.L. Snell, "Random walks and electrical networks", Carus Mathematical Monographs, 22, Mathematical Association of America, Washington, DC, 1984.

[DV] M.D. Donsker and S.R.S. Varadhan, "On the principal eigenvalue of second-order elliptic differential operators", Comm. Pure Appl. Math. **29**, 595-621 (1976).

[EK] M. Eckhoff and M. Klein, "Metastability and low lying spectra in non-reversible Markov chains", in preparation (2000).

[FW] M.I. Freidlin and A.D. Wentzell, "Random perturbations of dynamical systems", Springer, Berlin-Heidelberg-New York, 1984.

[GM] B. Gaveau and M. Moreau, "Metastable relaxation times and absorbtion probabilities for multidimensional stochastic systems", J. Phys. A: Math. Gen. **33**, 4837-4850 (2000).

[GS] B. Gaveau and L.S. Schulman, "Theory of nonequilibrium first-order phase transitions for stochastic dynamics", J. Math. Phys. **39**, 1517-1533 (1998

[Li] T.M. Liggett, "Interacting particle systems", Springer, Berlin, 1985.

[M] P. Mathieu, "Spectra, exit times and long times asymptotics in the zero white noise limit", Stoch. Stoch. Rep. **55**, 1-20 (1995).

[S] Ch. Schütte, "Conformational dynamics: modelling, theory, algorithm, and application to biomolecules", preprint SC 99-18, ZIB-Berlin (1999).

[SFHD] Ch. Schütte, A. Fischer, W. Huisinga, and P. Deuflhard, "A direct approach to conformational dynamics based on hybrid Monte Carlo", J. Comput. Phys. **151**, 146-168

(1999).

[Sc] E. Scoppola, "Renormalization and graph methods for Markov chains", Advances in dynamical systems and quantum physics (Capri, 1993), 260-281, World Sci. Publishing, River Edge, NJ, 1995.

[W] A.D. Wentzell, "On the asymptotic behaviour of the greatest eigenvalue of a second order elliptic differential operator with a small parameter in the higher derivatives", Soviet Math. Docl. **13**, 13-17 (1972).

[WW] E.T. Whittaker and G.N. Watson, "A course of Modern Analysis", Cambridge University Press, (1958).