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SPECTRAL APPROACH TO METASTABILITY OF NON-REVERSIBLE COMPLEX PROCESSES

by

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Declarations

I confirm that this thesis is my own work and the use of all material from other sources has been properly and fully acknowledged. This work has not been submitted for any other degree.

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Contents

Chapter 1

Introduction

In chemistry, conformations refer to the shapes a molecule takes from rotation about its bonds. Different conformations of the same molecule can yield totally different properties. In order to understand the functions or ability of a molecule, knowledge of the dynamical behavior the molecule has as it changes between its different conformations is necessary. Typically, conformation changes are rare events. A molecule usually remains in one conformation for a long period of time before converting to another conformation. This poses a challenge when the observation of the molecular dynamics is done by computer simulation. Although higher computer power nowadays has become available, the long time spans required by direct simulation to characterize the conformation changes are still not economical. In applications like drug design, the conformational changes often occur in microseconds, whereas the time step of direct simulation is of femtoseconds. This time span discrepancy hence makes the direct molecular simulation impractical.

Several techniques were introduced in recent years to address these timescale problems. In Deuflhard et al. (1999), the authors demonstrated that chemical conformations related to a Hamiltonian dynamical system can be interpreted as *metastable* or as *almost invariant sets* in the phase space. In 1996, Dellnitz et al. proposed that such almost invariant sets can be identified via the *dominant* eigenvectors of the *transfer operator* associated with discrete perturbed dynamical systems (see Dellnitz and Junge (2004)). This transfer operator approach was later applied to the system of discrete time reversible Markov chains in continuous space by Schütte et al. (1999) and has been successfully used to identify the metastable sets in large biomolecular systems by Schütte (1998).

Langevin dynamics and Extended detailed balance

Motivated by the aforementioned works, we aim to extend these concepts to another class of systems, the so-called Langevin dynamics. Langevin dynamics

is one of the most common models used to describe the dynamics of molecular systems. The equations of the process read

$$\begin{aligned} \mathrm{d}q_t &= p_t \mathrm{d}t \\ \mathrm{d}p_t &= -\nabla V(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}W_t, \end{aligned} \tag{1.0.1}$$

where q and p are position and momentum of the system, respectively, V is a potential energy function, and W is a standard Wiener process. The inverse temperature β and the friction coefficient γ are assumed to be fixed. What differentiates Langevin dynamics from other types of dynamics considered in the previous studies is the fact that Langevin dynamics is not reversible; hence the associated transfer operator is in general not a self-adjoint operator. This creates challenges in the analysis of the spectral properties. In particular, a non-self-adjoint operator can have complex eigenvalues, and even more the operator is not necessarily diagonalizable. Thus, the approach of identifying metastable sets via the dominant eigenvalues and eigenvectors seem inapplicable. However, it has been empirically observed that for small temperatures, the transfer operator related to the Langevin dynamics has real dominant eigenvalues. Moreover, the dominant eigenvectors are "almost" orthogonal and the dominant part of the transfer operator is "nearly" self-adjoint (see Huisinga (2001)). This motivates us to investigate the structure of Langevin dynamics. It turns out that the underlying process admits a form of generalized reversibility, the so-called *extended detailed balance* (EDB) condition (see Lelièvre et al. (2010, p.90)), which is more general than a detailed balance condition found in a reversible process. This means that the infinitesimal generator L of the process satisfies

$$\langle ALf, g\rangle_\mu = \langle Af, Lg\rangle_\mu, \quad f, g \in L^2(\mu), \tag{1.0.2}$$

where μ is the unique invariant measure of the process and where

$$(Af)(q,p) = f(q,-p)$$

is an involution on $L^2(\mu)$, i.e. $A^2 f = f$ for $f \in L^2(\mu)$. Here, the operator A is referred to as the momentum reversal. Note that for $A = Id$, (1.0.2) reduces to the usual detailed balance condition. Similarly, in terms of the transfer operator T_t at time t, which can formally be written as $T_t f = e^{tL} f$, we have

$$\langle AT_t f, g\rangle_\mu = \langle Af, T_t g\rangle_\mu .$$

If we define a Hermitian form $\langle\cdot,\cdot\rangle_{A,\mu}$ by

$$\langle f, g\rangle_{A,\mu} := \langle Af, g\rangle_\mu ,$$

then this equation reads as

$$\langle T_t f, g\rangle_{A,\mu} = \langle f, T_t g\rangle_{A,\mu} . \tag{1.0.3}$$

In general $\langle \cdot, \cdot \rangle_{A,\mu}$ is not a scalar product, but nevertheless this notation suggests that T_t may behave similarly to a self-adjoint operator. Equation (1.0.3) is actually the starting point of this thesis. Instead of analyzing Langevin dynamics directly, we will study more generally processes whose transfer operators satisfy the extended detailed balance condition in (1.0.3). Our goal is to analyze spectral properties of such transfer operators and how they can be used to characterize metastable partitions.

Markov chains, metastability and perturbation analysis

In general, molecular dynamics are modeled with Markov processes describing the transitions between states. For simplicity, we restrict ourselves to consider discrete-time Markov chains on a finite state space S. The benefit of discussing the finite case is that it directly connects to numerical discretization or simulation. For instance, after discretization, the Langevin dynamics yields a finite dimensional Markov chain. Our main assumptions to the Markov chains under consideration are that there exists a unique invariant measure μ and that the transfer operators $T \equiv T_t$ at any time t satisfy the extended detailed balance condition (1.0.3) with respect to some involution A. In this very general setting, we want to find metastable partitions of the state space S. Loosely speaking, a disjoint *full* partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ of S, i.e. $\bigcup_{k=1}^{m} S_k = S$, is metastable, if the process stays most of the time in the sets S_i, while transitioning between the sets only rarely. In all generality, finding metastable partitions is difficult. In principle, assuming that there are only finitely many states or configurations we could try all possibilities and looking for the "best" partition. However, as our models typically involve huge numbers of molecules, the brute-force method can be impossible. A better approach is to use the properties of the Markov chain for finding good partitions. There are two main ideas involved in finding such metastable partitions in this thesis. The first one is to use spectral properties of the transfer operator. The second main idea is to use perturbation analysis of linear operators which we motivate now shortly.

Intuitively, a partition with respect to a Markov chain with transition matrix P is metastable if, after a possible reordering, P (and thus also the associated transfer operator) is almost block-diagonal while the Markov chain is still ergodic in the sense that there is a positive probability to move between the blocks. In particular, a true block-diagonal transition matrix is not metastable because then the Markov chain is not irreducible. On the other hand, such a matrix is simple enough to allow for an easy analysis of its spectral properties. In order to benefit from this, we assume that the Markov chain that we begin with is "close" to another Markov chain with block-diagonal transition matrix P_0 (and transfer operator T_0). We then hope that properties of P (or T) can be deduced from properties of P_0 (or T_0). This is actually a common approach in the stability analysis of physical systems where we often assume that there exists an ideal system for which the analysis is simple, while the actual observed system is close enough to show interesting properties which might otherwise not

be accessible. In practice, this approach is justified since the dynamical systems that we consider depend fundamentally on the temperature of the system. The temperature can then be interpreted as a perturbation parameter, leading to a simple system when approaching a specific temperature.

Main results

Apart from providing a number of interesting properties of transfer operators satisfying extended detailed balance, we have two main results. The first one is Theorem 3.19 which essentially provides a mathematical justification for the empirical observation that the dominant eigenvalues of Langevin dynamics (and more generally Markov chains whose transfer operators satisfy extended detailed balance) are real valued. This is further generalized in the concept of weak reversibility (Theorem 3.25) which is however difficult to apply in practice. The second main result is an algorithm, along with mathematical justifications and numerical simulations, for finding metastable partitions in the case of Markov chains whose transfer operators satisfy extended detailed balance. We make explicitly use of the involution A and outperform other approaches for finding metastable partitions which apply to non-reversible processes.

Overview

This thesis has three main chapters. In Chapter 2 we provide the necessary background on Markov chains, transfer operators and perturbation analysis. Instead of giving full account of these subjects, which are all interesting on their own, we sum up in a concise way the facts that we need. In Chapter 3 we introduce two notions of generalized reversibility, namely the aforementioned extended detailed balance and an even more general concept which is called *weak reversibility*. Along with introducing the concepts, we also describe their consequences with respect to the spectral properties of the transfer operators. Finally, in Chapter 4 we discuss in detail the concept of metastability, how it can be characterized in terms of spectral properties of the transfer operators and how this can be used to formulate an algorithm for finding metastable partitions. Together with theoretical justifications for the obtained algorithm, we also provide numerical verifications.

Chapter 2

Theoretical Background

2.1 Markov chains

As we are only concerned with discrete models, our main probabilistic objects of interest are Markov chains. We expect the reader to be familiar with basic concepts from probability theory such as the notions of a (discrete) probability space, conditional probabilities and random variables. Instead of giving a full mathematical treatment of Markov chains, we focus on the relevant facts important to us and on the intuition behind them. Interested readers can refer to many books on this topic for details (see for example Bremaud (2001); Meyn and Tweedie (2009); Stroock (2013); Klenke (2006)). Note that we restrict ourselves in this thesis to Markov chains with finite state spaces for simplicity.

In the following $(\Omega, \mathcal{F}, \mathbb{P})$ always denotes the underlying probability space. A *stochastic process in discrete time* is a family $X = (X_n)_{n\in\mathbb{N}_0}$ of random variables on $(\Omega, \mathcal{F}, \mathbb{P})$ taking their values in some measurable space $(S, \mathcal{S})$ which we call the *state space*. Elements in S are called *states*. The process X models the stochastic evolution between states in S, with X_n being the state at time n. An important example is the random walk $X_n = \sum_{k=0}^{n} Y_k$ with independent and identically distributed (iid) random variables Y_k taking values in $\{-1, 1\}$ with probabilities $p > 0$ and $1 - p$, respectively. The key property of such a random walk is the decomposition $X_{n+1} = X_n + Y_{n+1}$, i.e. X_{n+1} depends on the past only through the last state X_n and an independent random variable Y_{n+1}. This fact greatly simplifies the analysis of random walks and reduces complexity and memory requirements in implementations. Actually, the random walk is only one example of a bigger class of stochastic processes X for which the next state X_{n+1} depends only on X_n, but not on the other previous states $X_0, \ldots, X_{n-1}$.

Definition 2.1. A stochastic process in discrete time $X = (X_n)_{n\in\mathbb{N}_0}$ is a

(discrete-time) Markov chain if it has the *Markov property*, i.e. if

$$\mathbb{P}\left(X_{n+1} = y \,|X_n = x, X_{n-1} = x_{n-1}, \ldots, X_0 = x_0\right) \quad = \quad \mathbb{P}\left(X_{n+1} = y \,|X_n = x\right),$$

for all times n and states $x, y, x_0, \ldots, x_{n-1} \in S$. A Markov chain is said to be *time-homogeneous* if transitions do not depend on time, i.e. if

$$\mathbb{P}\left(X_{n+1} = y \,|X_n = x\right) = \cdots = \mathbb{P}\left(X_1 = y \,|X_0 = x\right).$$

In this case we can define a *transition function* $P : S \times S \to [0, 1]$ via

$$P\left(x, y\right) \quad = \quad \mathbb{P}\left(X_{n+1} = y \,|X_n = x\right), \tag{2.1.1}$$

and call $P(x, y)$ the *transition probability from x to y*.

The random walk from above is a Markov chain, because

$$\begin{aligned}
&\mathbb{P}\left(\, X_{n+1} = y| \, X_n = x, X_{n-1} = x_{n-1}, \ldots, X_0 = x_0\right) \\
&\quad = \mathbb{P}\left(Y_{n+1} = y - x\right) \\
&\quad = \mathbb{P}\left(Y_{n+1} = y - x \,|X_n = x\right) \\
&\quad = \mathbb{P}\left(X_{n+1} = y \,|X_n = x\right)
\end{aligned}$$

by independence. For such a system we assume that there exists some knowledge on the initial state through an *initial distribution* $\mu_0(\cdot) = \mathbb{P}(X_0 \in (\cdot))$. Starting from the (random) initial state, the evolution of the system is fully determined by the transition probabilities. In contrast to deterministic dynamics described by a system of differential equations, the evolution is, however, random and thus different for each realization of the Markov chain. Time-homogeneity is a further simplification, because it means that the transition functions does not depend on time. An important question is the long-time behavior of a Markov chain, i.e. which states can be reached after a long time and how long does it take to reach them. For us, Markov chains and their continuous-time counterparts, the Markov processes, are the prime tools for the mathematical description of molecular dynamics and for answering relevant questions. We will now discuss briefly the existence of Markov chains and a few simple but important properties which are useful for calculations. Finally, we will discuss their long-time behavior.

From now on, if not mentioned otherwise, we restrict our attention to discrete-time, time-homogeneous Markov chains associated with a finite state space S. For a finite state space, the transition probabilities $P(x, y)$ define a stochastic matrix P, i.e. all entries of P are non-negative and the row sums are one. We call P the *transition matrix* of X. In the following, P may be referred as a transition function or stochastic matrix. However, its usage should be clear from the context.

From its definition it is clear that a Markov chain defines a transition matrix. The reverse is also true; a transition matrix P and an *initial distribution* $\mu_0(\cdot) =$

$\mathbb{P}(X_0 \in (\cdot))$ completely characterize a Markov chain, as indicated in the next theorem.

Theorem 2.2. *For any stochastic matrix P and any probability distribution μ_0, there exists a Markov chain $(X_n)_{n\in\mathbb{N}_0}$ on $(\Omega, \mathcal{F}, \mathbb{P})$ (possibly on an extension) such that*

$$\mathbb{P}(X_{n+1} = y \,|X_n = x) \quad = \quad P(x,y), \qquad \mathbb{P}(X_0 = x_0) = \mu_0(x_0).$$

We are thus able to consider a fixed stochastic matrix P and analyze the resulting dynamics for different initial distributions μ_0. If the initial distribution μ is not clear from the context, we indicate it as $\mathbb{P}_\mu$. We identify P with a "generic" Markov chain X which is a well-defined stochastic process when an initial distribution is specified. The Markov property allows for simple calculations. For instance, the probability of some finite path $x_0, \ldots, x_n$ can be obtained using the definition of conditional expectations:

$$\begin{aligned}
&\mathbb{P}(X_n = x_n, \ldots, X_0 = x_0) \\
&= \mathbb{P}(X_n = x_n \,|X_{n-1} = x_{n-1}, \ldots, X_0 = x_0) \cdot \mathbb{P}(X_{n-1} = x_{n-1}, \ldots, X_0 = x_0) \\
&= \mathbb{P}(X_{n-1} = x_{n-1}, \ldots, X_0 = x_0) \cdot P(x_{n-1}, x_n) \\
&= \mathbb{P}(X_{n-2} = x_{n-2}, \ldots, X_0 = x_0) \cdot P(x_{n-2}, x_{n-1}) \cdot P(x_{n-1}, x_n) \\
&= \mu_0(x_0) \prod_{k=1}^{n} P(x_{k-1}, x_k). \qquad (2.1.2)
\end{aligned}$$

Similarly, we can easily compute the k-step transition probabilities

$$P^{(k)}(x,y) \quad = \quad \mathbb{P}(X_{n+k} = y \,|X_n = x).$$

Using again the Markov property we can deduce for $k = 2$

$$\begin{aligned}
P^{(2)}(x,y) &= \mathbb{P}(X_2 = y \,|X_0 = x) \\
&= \sum_{z\in S} \mathbb{P}(X_2 = y, X_1 = z \,|X_0 = x) \\
&= \sum_{z\in S} (\mathbb{P}(X_2 = y \,|X_1 = z, X_0 = x) \cdot \mathbb{P}(X_1 = z \,|X_0 = x)) \\
&= \sum_{z\in S} (\mathbb{P}(X_2 = y \,|X_1 = z) \cdot \mathbb{P}(X_1 = z \,|X_0 = x)) \\
&= \sum_{z\in S} (P(x,z)\, P(z,y)). \qquad (2.1.3)
\end{aligned}$$

For this, time-homogeneity is crucial. By induction, we obtain the *Chapman Kolmogorov* equations for $k, j \geq 0$

$$P^{(k+j)}(x,y) \quad = \quad \sum_{z\in S} P^{(k)}(x,z)\, P^{(j)}(z,y), \qquad (2.1.4)$$

where we define $P^{(0)}(x,y) = \delta_{xy}$. From (2.1.3) it follows that $P^{(2)} = P^2$ such that we can write (2.1.4) in terms of the transition matrix

$$\left(P^{k+j}\right)_{x,y} = \sum_z \left(P^k\right)_{x,z} \left(P^j\right)_{z,y},$$

where P^k is the k-th power of the transition matrix P.

Evolution of distribution

For a physical system, one of the key questions is how an initial state or distribution is propagated through time. In particular, we want to understand how different initial distributions influence the evolution of the system. Mathematically, we capture this through the linear operator $\mathcal{P} : \mathcal{X} \to \mathcal{X}$,

$$(\mathcal{P}\mu)(y) = \sum_{x \in S} P(x,y)\,\mu(x), \tag{2.1.5}$$

where $\mathcal{X}$ is the set of all functions on S. For a finite state space S with N elements, we can identify $\mathcal{X}$ with $\mathbb{C}^N$ such that a measure μ on S can also be understood as a vector in $\mathbb{R}_+^N$. In this way we see that $\mathcal{P}\mu = \mu^\top P$ is just a matrix vector product. Moreover, we have for all $y \in S$

$$\begin{aligned}(\mathcal{P}\mu)(y) &= \sum_{x \in S} \mathbb{P}(X_1 = y \,|X_0 = x)\,\mathbb{P}(X_0 = x) \\ &= \mathbb{P}(X_1 = y). \end{aligned} \tag{2.1.6}$$

We thus call $\mathcal{P}$ a *propagator* since it propagates distributions in time, i.e. $\mu^\top P$ is just the distribution of the Markov chain at time $n = 1$. If we define $\mu_n(x) = \mathbb{P}(X_n = x)$ for $x \in S$, then we obtain in a similar manner by (2.1.4) that

$$\mu_n = \mathcal{P}\mu_{n-1} = \mathcal{P}^2\mu_{n-2} = \cdots = \mathcal{P}^n\mu_0 \tag{2.1.7}$$

or $\mu_n^\top = \mu_0^\top P^n$. Therefore, the propagator $\mathcal{P}$, together with the initial distribution, indicates how the Markov chain will be distributed in the succeeding time steps.

For physical systems it is often desirable to find states of equilibrium. Clearly, according to (2.1.7) we can consider μ to be an "equilibrium distribution" of $\mathcal{P}$, if $\mu_n = \mu$ for all n. We therefore define the following:

Definition 2.3. We say that the Markov chain X with transition matrix P has an *invariant measure* μ, if μ is a probability measure and satisfies $\mu^\top P = \mu^\top$, i.e. for all $y \in S$

$$(\mathcal{P}\mu)(y) = \sum_{x \in S} P(x,y)\,\mu(x) = \mu(y). \tag{2.1.8}$$

Hence, we see that if μ is an invariant measure of a Markov chain X, then the

X_n have the same distribution for all $n \in \mathbb{N}$. In fact, it is easy to see that in this case the process X is *stationary*, i.e. the finite dimensional distributions of X are shift-invariant, which can formally be written as

$$(X_{t_1}, \ldots, X_{t_n}) \stackrel{d}{=} (X_{t_1+s}, \ldots, X_{t_n+s}) \tag{2.1.9}$$

for all $t_1, \ldots, t_n, s \in \mathbb{N}_0$. For applications, it is of high interest to find invariant measures, because they describe the dynamics of X for long times. For example, the ergodic theorem (see for example Bremaud (2001, Theorem 4.1)) tells us that for *ergodic* Markov chains (see Definition 2.6) long time averages can be calculated as space averages with respect to the invariant measure, i.e. for functions f with $\sum_{x \in S} |f(x)|\mu(x) < \infty$ we have

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f\left(X_k\right) \to \sum_{x \in S} f\left(x\right) \mu(x). \tag{2.1.10}$$

If we choose $f = \mathbf{1}_A$ for some set A, then we can therefore approximate the *sojourn times* of X, i.e. the time the Markov chain spends in a set A, which is highly useful in applications.

Irreducibility and Aperiodicity

It is intuitively clear that invariance of a measure depends on which states can and which states cannot be reached eventually, that is when $n \to \infty$. For instance, a probability measure μ cannot be invariant if the process can get stuck at some state, i.e. there is an absorbing state y which satisfies $P(y, y) = 1$. To see this, suppose μ is an invariant measure, then μ would satisfy for any other state $x \neq y$ with $\mu(x) > 0$ and $P(x, y) > 0$ that

$$\mu(y) = \sum_{x \in S} P(x, y)\mu(x) = \mu(y) + \sum_{x \neq y} P(x, y)\mu(x) > \mu(y),$$

which is a contradiction. Similarly, for μ to be invariant any state $x \in S$ from where we can start, i.e. with $\mu(x) > 0$, should always be "reachable" again after any time n, and any state from where we cannot start, i.e. with $\mu(x) = 0$, should never be reached at any time n. Otherwise, $\mu^\top P^n$ cannot be constant and we would have disconnected subsets of S where the process remains for infinite time. To formalize these notions we define the *return probabilities*

$$r_{xy} \quad := \quad \mathbb{P}\left(\exists n \in \mathbb{N} : X_n = y \,|X_0 = x\right)$$

which are the probabilities to ever reach $y \in S$ when starting in $x \in S$.

For any $m \in \mathbb{N}_0$ it holds

$$r_{xy} = \mathbb{P}\left(\bigcup_{n\in\mathbb{N}_0} \{X_n = y\} \middle| X_0 = x \right) \geq \mathbb{P}\left(X_m = y | X_0 = x \right) = P^{(m)}(x,y). \tag{2.1.11}$$

Note that $r_{xy} > 0$ and $r_{yz} > 0$ imply $r_{xz} > 0$, since by (2.1.11) there exist $k, l \in \mathbb{N}_0$ with $P^{(k)}(x,y) > 0, P^{(l)}(y,z) > 0$ such that by (2.1.4)

$$r_{xz} \geq P^{(k+l)}(x,z) \geq P^{(k)}(x,y) P^{(l)}(y,z) > 0.$$

Consequently, we can separate the state space into *classes* of states which are reachable when starting within the class and not reachable when starting outside the class. We then say that the Markov chain is *irreducible* if for all $x, y \in S$ we have $r_{xy} > 0$, because $r_{xy} = 0$ for some pair x, y implies that the state space S can be reduced into separate classes. Finally, because of (2.1.11) and because

$$r_{xy} = \mathbb{P}\left(\bigcup_{n\in\mathbb{N}_0} X_n = y \middle| X_0 = x \right) = \sum_{n\in\mathbb{N}_0} \mathbb{P}\left(X_n = y | X_0 = x \right) = \sum_{n\in\mathbb{N}_0} P^{(n)}(x,y),$$

we can equivalently say that X is irreducible if and only if for all $x, y \in S$ there exists $m \in \mathbb{N}_0$ such that $P^{(m)}(x,y) > 0$. This supports our above intuition that in an irreducible state space all states can be reached from each other.

Irreducibility is a strong property. For a finite state space S the assumption $r_{xx} > 0$ for every $x \in S$ already implies $r_{xx} = 1$, i.e. every state is reached infinitely many times (see Klenke (2006, Theorem 17.38)). On the other hand, for general countable state spaces S, irreducibility guarantees that an invariant measure, if it exists, is already unique (see Klenke (2006, Theorem 17.49)). The existence of an invariant measure μ is slightly more involved. However, for finite state spaces, the existence of an invariant measure can be stated as an eigenvalue problem, because (2.1.8) means that the transition matrix P has 1 as an eigenvalue with left eigenvector μ, i.e. $\mu^\top P = \mu$. Existence (and uniqueness) of μ follows then directly from the Perron-Frobenius Theorem (see Seneta (2006, Theorem 1.1)).

Theorem 2.4 (Perron-Frobenius)**.** *Let X be an irreducible Markov chain with transition matrix P on a finite state space S. Then we have:*

(i) $\lambda_1 = 1$ *is an eigenvalue of* P. λ_1 *is called the "Perron-Frobenius" eigenvalue of* P.

(ii) The left and right eigenspaces of P *associated with* λ_1 *are one-dimensional, i.e.* λ_1 *is a simple eigenvalue.*

(iii) There exists a positive left eigenvector μ*, i.e.* $\mu(x) > 0$ *for all* $x \in S$.

(iv) Any other eigenvalue λ *of* P *satisfies* $|\lambda| < 1$.

Uniqueness of μ follows since μ is a probability measure, i.e. it is normalized. From the discussion on irreducibility above we know that an irreducible Markov chain has at most one invariant measure. On the other hand, for a finite state space, we can therefore equivalently to Theorem 2.4 require the following.

Corollary 2.5. *Let X be a Markov chain with unique invariant measure μ on a finite state space S. Then all results from Theorem 2.4 apply to the transition matrix P of X.*

Finally, another important property of many Markov chains with invariant measure μ is that they "forget" their initial distribution in the sense that $\mathcal{P}^n\nu \to \mu$ as $n \to \infty$ for any initial distribution ν. (see Theorem 2.7). This property is also useful when we want to approximate μ (just like (2.1.10)) and can be used for instance to define Markov chains for a given distribution μ from which we want to sample via a Markov chain Monte Carlo method (see Section 4.4.4). For this convergence it turns that it not only matters *if* we reach the state y after the state x, but also *when*. To be precise, let $N(x,y) = \{n \in \mathbb{N} : P^{(n)}(x,y) > 0\}$ for $x, y \in S$ and define

$$d(x) \quad := \quad gcd(N(x,x))$$

to be the *period* of x. If $d(x) > 1$, then irreducibility of X is not sufficient for the convergence of $\mathcal{P}^n\nu$ in general. For example, consider $S = \{e_1, e_2\}$ and

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Clearly, P is a stochastic matrix and the associated Markov chain is irreducible, with $\mu = (1/2, 1/2)^\top$ being the invariant measure. However, $P^2 = I = P^{2n}$, but $P^{2n+1} = P$ such that for example $\nu^\top P^n$ fails to converge for $\nu = (1,0)^\top$. In this case we have $d(e_1) = d(e_2) = 2$. It turns out that if we restrict to *aperiodic* Markov chains, i.e. $d(x) = 1$ for all $x \in S$, which are also irreducible then we indeed obtain the desired convergence. As these are exactly the Markov chains for which the ergodic theorem applies, we define:

Definition 2.6. An irreducible and aperiodic Markov chain on a finite state space is called *ergodic*.

In this work we focus mostly on ergodic Markov chains. Summing up this section, in this case we have the following fundamental result on the existence of an invariant measure and on the convergence of Markov chains.

Theorem 2.7. *An ergodic Markov chain has a unique invariant measure μ. For any distribution ν we have $\mathcal{P}^n\nu \to \mu$ as $n \to \infty$. In particular,*

$$\mu(y) \quad = \quad \lim_{n\to\infty} P^{(n)}(x,y), \quad \forall x, y \in S.$$

2.2 Transfer operator and the detailed balance condition

We have already defined the propagator in (2.1.5) which propagates distributions through time. Assume now that μ is an invariant measure of a Markov chain X with transition matrix P such that $\mu(x) > 0$ for all $x \in S$, and define another linear operator $T : \mathcal{X} \to \mathcal{X}$ which propagates densities with respect to μ:

$$(Tv)(y) = \frac{1}{\mu(y)} \sum_{x \in S} P(x,y)\, v(x)\, \mu(x), \quad y \in S. \tag{2.2.1}$$

We call T the *transfer operator*. We will analyze the dynamics of X mostly through the spectral properties of T. For later purposes, it is convenient to collect a few simple results on the spectrum of T here. For a measure μ define the *weighted scalar product* $\langle \cdot, \cdot \rangle_\mu$ by

$$\langle u, v \rangle_\mu = \sum_{x \in S} u(x)\, v(x)\, \mu(x), \quad u, v \in \mathcal{X}.$$

We say that a stochastic matrix is irreducible, if the corresponding Markov chain is irreducible. Then we have the following:

Proposition 2.8. *Let X be a Markov chain with invariant measure $\mu > 0$ on a finite state space S with transfer operator T. Then we have:*

(i) $v \in \mathcal{X}$ is an eigenvector of T for the eigenvalue 1 if and only if $v\mu$, i.e. $v\mu(x) = v(x)\,\mu(x)$, is a left eigenvector of P for the eigenvalue 1.

(ii) The adjoint of T with respect to $\langle \cdot, \cdot \rangle_\mu$ is given by

$$(T^* u)(x) = \sum_{y \in S} P(x,y)\, u(y), \quad x \in S.$$

(iii) The map

$$M : \mathcal{M} \to \mathcal{M},\ P \mapsto \tilde{T}_{x,y} = P_{y,x} \frac{\mu(y)}{\mu(x)}, \quad x, y \in S$$

is a bijection, where $\mathcal{M}$ is the set of all irreducible stochastic matrices, corresponding to an irreducible Markov chain with unique invariant measure μ. In particular, if X is irreducible, then the transition matrix P and its unique invariant measure μ can be recovered from the matrix representation $\tilde{T}$ of transfer operator T via M.

Proof. (i) Follows immediately by plugging in.

(*ii*) For $u, v \in \mathcal{X}$

$$\begin{aligned}\langle u, Tv\rangle_\mu &= \sum_{x,y\in S} P(x,y)\, v(x)\, \mu(x)\, u(y) \\ &= \sum_{x\in S}\left(\sum_{y\in S} P(x,y)\, u(y)\right) v(x)\, \mu(x),\end{aligned}$$

which yields the statement.

(*iii*) We first show that M is well-defined. $\tilde{T} = M(P)$ is a stochastic matrix, since $\tilde{T}_{x,y} \geq 0$ and since μ is an invariant measure of P. We can write $\tilde{T} = D^{-1}P^\top D$, where D is a diagonal matrix with the vector μ on its diagonal. This implies that $\tilde{T}^n = D^{-1}\left(P^\top\right)^n D$. Since P is irreducible, $\tilde{T}$ is irreducible, i.e. $M(P) \in \mathcal{M}$, indeed. We show furthermore that M is bijective by giving explicitly its inverse. Let $\tilde{T} \in \mathcal{M}$. Since $\tilde{T}$ is irreducible, we can conclude by Theorem 2.4 that there exists a unique normalized left eigenvector $\tilde{\mu}$ of $\tilde{T}$ for the eigenvalue 1. We claim that

$$M^{-1}\left(\tilde{T}\right)(x,y) = \tilde{T}_{y,x}\frac{\tilde{\mu}(y)}{\tilde{\mu}(x)} := \tilde{P}_{x,y}.$$

Indeed,

$$\begin{aligned}M\left(\tilde{P}\right)(x,y) &= \tilde{P}_{y,x}\frac{\tilde{\mu}(y)}{\tilde{\mu}(x)} \\ &= \tilde{T}_{x,y}.\end{aligned}$$

The remaining statements are clear. □

The key idea is that properties of P are reflected in T and vice versa. The last property in the proposition, in particular, implies that P and μ can be recovered from T.

An important property of many physical or chemical processes is their reversibility. Mathematically, we say that a stochastic process $(X_n)_{n\in\mathbb{N}_0}$ is *reversible,* if the process and the reversed process coincide, i.e. if for all $n \in \mathbb{N}_0$ and all states $x_0, \ldots, x_n \in S$

$$\mathbb{P}(X_0 = x_0, \ldots, X_n = x_n) = \mathbb{P}(X_0 = x_n, \ldots, X_n = x_0).$$

For such a process we cannot distinguish if we see the chain going forward or backward in time. If X is a Markov chain with invariant measure μ, then it is easy to see by (2.1.9) and (2.1.2) that X is reversible if and only if it satisfies the *detailed balance condition*

$$\mu(x)\, P(x,y) = \mu(y)\, P(y,x), \quad x, y \in S. \tag{2.2.2}$$

The following theorem shows reversibility of the process directly corresponds to

the transfer operator T being self-adjoint with respect to $\langle \cdot, \cdot \rangle_\mu$. In combination with (2.2.2) it becomes then clear why we have the additional factor $1/\mu(y)$ in the definition of T in (2.2.1).

Theorem 2.9. *Let X be a reversible Markov chain with invariant measure μ. Then the corresponding transfer operator T is self-adjoint with respect to the scalar product $\langle \cdot, \cdot \rangle_\mu$, i.e.*

$$\langle u, Tv \rangle_\mu \quad = \quad \langle Tu, v \rangle_\mu .$$

2.3 Perturbation theory

In this work we model molecular dynamics with Markov chains which describe how we transition between states. We are interested in *metastable* partitions of the state space, where metastable means that the Markov chain moves in the long run most of the time within sets of the partition and jumps only rarely between sets. A popular approach for studying metastability is through the spectral properties of transfer operators of Markov chains. Intuitively, a partition with respect to a Markov chain with transition matrix P is metastable if, after a possible reordering, P is almost block-diagonal while the Markov chain is still ergodic in the sense of the last section, i.e. there is "enough" probability to move between the blocks. In particular, a true block-diagonal transition matrix is not metastable because then the Markov chain is not irreducible. On the other hand, such a matrix is simple enough to allow for an easy analysis of the spectral properties. In order to benefit from this, we assume that the Markov chain that we begin with is "close" to another Markov chain with block-diagonal transition matrix P_0. We then hope that properties of P can be deduced from properties of P_0.

As outlined in Chapter 1 on metastability, we assume that the molecular dynamics that we observe are described by a Markov chain with transfer operator T, which we want to analyze through another simple Markov chain with block-diagonal transition matrix and transfer operator T_0. We will later assume that the two Markov chains are "close" in the sense that the transfer operators T and T_0 are close in operator norm. This closeness and its implications on the spectral properties of T and T_0 are systematically studied in perturbation theory for linear operators. As our main approach relies on these spectral properties, we discuss the basics of perturbation theory in this section. This theory is actually a rather large mathematical topic on its own with a long history (see the introductory chapters in Kato (1995); Baumgärtel (1985)). We want to emphasize that we do not discuss perturbation theory in the sense used in other areas, e.g. in dynamical systems or in oscillation theory. In these cases, the unperturbed system usually corresponds to easily solvable equations while the actual analysis focuses on stability properties of the perturbed system. However, the methods employed and the respective applications are quite different from the ones for linear operators which we will use exclusively here. The material discussed here

is loosely based on the standard books on the topic by Kato and Baumgärtel. As before, we present the theory as we see fit for our purposes, largely simplifying the complexity of the subject. For proofs and a more detailed presentation, readers can consult the literature.

The main idea is as follows. We are given a family of linear operators $(T(\varepsilon))_{\varepsilon\in\mathbb{R}}$ on some normed space $\mathcal{X}$. As in the last section, for simplicity we will stay in the finite-dimensional setting, i.e. $\mathcal{X} = \mathbb{C}^N$, for some $N \in \mathbb{N}$, and linear operators can be considered as $N \times N$ dimensional matrices. We think of $T(\varepsilon)$ as the perturbation of an unperturbed operator $T_0 = T(0)$. In order to quantify this, in perturbation theory it is typically assumed that $T_\varepsilon = T(\varepsilon)$ can be expanded around T_0 as a convergent power series

$$T_\varepsilon \quad = \quad T_0 + \varepsilon T^{(1)} + \varepsilon^2 T^{(2)} + \cdots , \tag{2.3.1}$$

in some neighborhood $\mathcal{U} \subset \mathbb{R}$ of 0, where the $T^{(k)}$ are also linear operators. In applications it is often sufficient to neglect higher order terms and to consider only linear perturbations of T_0, i.e.

$$T_\varepsilon \quad = \quad T_0 + \varepsilon L, \tag{2.3.2}$$

where $\varepsilon \in \mathcal{U}$ is assumed to be small and $L = T^{(1)}$ is another linear operator. In fact, this is the original setting considered by Schrödinger (see Baumgärtel (1985)) and it is the setting which we assume from now on. However, note that all results in this section also hold in the general setting of (2.3.1).

Our goal is to analyze how the spectral properties of T_ε change with ε, depending on T_0 and L. We therefore want to study the eigenvalue problem

$$T_\varepsilon f(\varepsilon) \quad = \quad \lambda(\varepsilon) f(\varepsilon), \tag{2.3.3}$$

depending on $\varepsilon \in \mathcal{U}$. An important question is when the eigenvalues $\lambda(\varepsilon)$ and eigenvectors $f(\varepsilon)$ can be expanded as power series around some $\lambda(0)$ and $f(0)$, as well. This is necessary to ensure that spectral properties of T_ε change at the same order as T_ε itself. Perturbation theory is not restricted to holomorphic expansions. However, this case is the most classic setting and it is enough for our purposes. Moreover, even if this strong restriction is applied, the problem remains difficult enough. The most well-known results concern *self-adjoint perturbations*, i.e. T_ε is a self-adjoint linear operator for every ε. They form the foundation of the theory and the basis of our considerations later. In the rest of this section we always consider perturbations of T_0. This is not a restriction and we can similarly consider perturbations and holomorphic expansions around any T_ε for $\varepsilon \in \mathcal{U}$.

Theorem 2.10 (Kato (1995, p.120))**.** *Suppose the perturbation T_ε in (2.3.2) is self-adjoint for every $\varepsilon \in \mathcal{U}$. Then there exists a neighborhood of 0 such that we have for all ε in this neighborhood:*

(i) The perturbed eigenvalues $\lambda(\varepsilon)$ of T_ε are holomorphic perturbations of

eigenvalues of T_0, i.e. the eigenvalues can be written as power series in ε:

$$\lambda(\varepsilon) = \lambda(0) + \varepsilon\lambda^{(1)} + \varepsilon^2\lambda^{(2)} + \cdots$$

for some scalars $\lambda^{(i)}$.

(ii) The corresponding eigenvectors are orthonormal (with respect to the euclidean scalar product) and can be written as holomorphic functions of ε:

$$f(\varepsilon) = f(0) + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \cdots$$

for some vectors $f^{(i)}$.

For a proof with tools which we will introduce later in this section see Section 2.3.4. The main part of this thesis is concerned with non-selfadjoint perturbations T_ε. Unfortunately, the corresponding results are more difficult and not as easily accessible as in the self-adjoint case. In particular, a detailed study requires considerable knowledge of complex analysis for operator-valued functions. We emphasize the central ideas as they are used in the other chapters later on. We begin with a short reminder of some general facts on the eigenvalue problem for matrices. This is followed by the perturbation of the eigenvalue problem with a focus on the perturbation of the eigenvalues. After that we treat the perturbation of the corresponding eigenvectors. Finally, we discuss the special case where the unperturbed eigenvalue is semisimple. The last subsection is indeed the most important one for us and contains most of theorems we need later on.

2.3.1 The eigenvalue problem

Let $T = T_\varepsilon$ for a fixed $\varepsilon \in \mathbb{R}$. Let $\lambda_1, \ldots, \lambda_p$, $p \in \mathbb{N}$, be the distinct eigenvalues of T, i.e. they are the roots of the characteristic polynomial

$$\rho_T(\lambda) := \det(T - \lambda I) = 0,$$

where I is the $N \times N$ identity matrix. To each eigenvalue λ_k, $k = 1, \ldots, p$, we associate two important values: the algebraic multiplicity $m_k \in \mathbb{N}$ and the geometric multiplicity $g_k \in \mathbb{N}$. m_k is the multiplicity of λ_k as a root of ρ_T, while $g_k = \dim(\tilde{E}_k)$ is the dimension of the *eigenspace* $\tilde{E}_k = \ker(T - \lambda_k I)$. It always holds that $g_k \leq m_k$. If $m_k = 1$, then we call λ_k *simple*. If, on the other hand, $g_k = m_k$, then we call λ_k *semisimple*. If all λ_k are semisimple, then T is *diagonalizable*. In this case $\mathcal{X} = \tilde{E}_1 \oplus \cdots \oplus \tilde{E}_p$ and we can find a basis of eigenvectors $f_1, \ldots, f_N$, where every f_i lies in some eigenspace $\tilde{E}_k$, i.e. $Tf_i = \lambda_k f_i$. In many cases, however, we have $g_k < m_k$ for some k and thus we have to generalize the above concepts. The most important conclusions of T being diagonalizable is that T is *invariant* on the eigenspaces, i.e. $T\tilde{E}_k \subset \tilde{E}_k$, and that T takes a very simple form on these spaces (it is basically a multiplication operator with eigenvalues as factors). These properties can be generalized by

introducing the *generalized eigenspaces* $E_k = \ker((T-\lambda_k I)^{m_k})$. It can be shown that $TE_k \subset E_k$, $\tilde{E}_k \subset E_k$, and $\ker((T-\lambda_k I)^{m_k+1}) = \ker((T-\lambda_k I)^{m_k}) = E_k$. Hence, we can say that E_k is the maximal invariant subspace of T corresponding to the eigenvalue λ_k. A natural object with respect to E_k is the corresponding *eigenprojection* Q_k which projects any vector $x \in \mathcal{X}$ to E_k. The main properties of the generalized eigenspaces are summed up in the following proposition.

Proposition 2.11. *We have the following decompositions of $\mathcal{X}$ and T:*

(i) $\mathcal{X} = E_1 \oplus \cdots \oplus E_p$ *and* $\dim E_k = m_k$ *for all* $k = 1, \ldots, p$,

(ii) (Jordan decomposition) $T = Q+D$, *where* $Q = \sum_{k=1}^{p} \lambda_k Q_k$, $D = \sum_{k=1}^{p} D_k$ *and where* $D_k = (T - \lambda_k I)Q_k$ *is the* eigennilpotent *corresponding to* λ_k.

Clearly, the operators D_k are also invariant on the spaces E_k. The Jordan decomposition shows that T has a simple structure on the generalized eigenspaces with the restriction that vectors in E_k are not necessarily eigenvectors. Observe furthermore the following simple fact.

Corollary 2.12. *The eigenvalue λ_k is semisimple if and only if $D_k = 0$.*

Proof. This follows immediately from the fact that λ_k is semisimple if and only if there exists a basis of m_k eigenvectors $f_1, \ldots, f_{m_k}$ of E_k. This is, however, possible if only if for all such eigenvectors f we have

$$\lambda_k f = Tf = \lambda_k Q_k f + D_k f = \lambda_k f + D_k f$$

which is satisfied if only if $D_k f = 0$ for all f. □

Proof of Proposition 2.11. For interested readers, we want to describe shortly how Proposition 2.11 can be obtained in an elegant way using complex analysis for operator-valued functions. We use relevant concepts in an intuitive fashion similar to classical complex analysis. For details see Kato (1995, I.5.2-I.5.5). The key idea is to recognize the eigenvalues λ_k as singularities of the operator-valued *resolvent* function:

$$R(\xi) = R(\xi, T) = (T - \xi I)^{-1}, \quad \xi \in \mathbb{C} \backslash \sigma(T), \tag{2.3.4}$$

where $\sigma(T) = \{\lambda_1, \ldots, \lambda_p\}$ is the spectrum of T. R satisfies the *first resolvent equation*

$$R(\xi) - R(\nu) = (\xi - \nu) R(\xi) R(\nu), \quad \xi, \nu \in \mathbb{C} \backslash \sigma(T).$$

From this and well-known results on von-Neumann series we obtain for $|\nu - \xi| < \|R(\xi)\|^{-1}$ (use any norm) the *first Neumann series for the resolvent:*

$$R(\nu) = (I + (\xi - \nu) R(\xi))^{-1} R(\xi) = \sum_{k=0}^{\infty} (\nu - \xi)^k R(\xi)^{k+1}. \tag{2.3.5}$$

Consequently, R is holomorphic with the eigenvalues λ_k as its only singularities. The starting point of the spectral analysis is thus to study the Laurent series of R around an eigenvalue λ_k

$$R(\xi) = \sum_{n=-\infty}^{\infty} (\xi - \lambda_k)^n A_n$$

with operator coefficients

$$A_n = \frac{1}{2\pi i} \oint_\Gamma (\xi - \lambda_k)^{-n-1} R(\xi)\, d\xi \tag{2.3.6}$$

where Γ is a small circle around λ_k not containing any other $\lambda_j \neq \lambda_k$. Then *define* $Q_k = -A_{-1}$, $D_k = -A_{-2}$. Through analyzing the properties of the A_n, it is then more or less easy to prove the proposition. In particular, R is holomorphic at infinity and we obtain by residue calculus

$$\sum_{k=1}^{p} Q_k = -\frac{1}{2\pi i} \oint_\Gamma R(\xi)\, d\xi = I, \quad Q_k Q_j = \delta_{kj} Q_k, \tag{2.3.7}$$

where Γ is this time a circle around all eigenvalues of T and where $\delta_{jj} = 1$, $\delta_{ij} = 0$ for $i \neq j$. This yields the decomposition $\mathcal{X} = E_1 \oplus \ldots \oplus E_p$. Moreover, any Q_k commutes with T, since

$$\begin{aligned} Q_k T &= -\frac{1}{2\pi i} \oint_\Gamma R(\xi) T d\xi = -\frac{1}{2\pi i} \oint_\Gamma R(\xi)(T - \xi I)\, d\xi - \frac{1}{2\pi i} \oint_\Gamma R(\xi)\xi d\xi \\ &= -\frac{1}{2\pi i} \oint_\Gamma R(\xi)\xi d\xi = -\frac{1}{2\pi i} \oint_\Gamma (T - \xi I) R(\xi)\, d\xi - \frac{1}{2\pi i} \oint_\Gamma \xi R(\xi)\, d\xi \\ &= -\frac{1}{2\pi i} \oint_\Gamma T R(\xi)\, d\xi = T Q_k. \end{aligned} \tag{2.3.8}$$

On the other hand, from (2.3.4) we obtain by multiplication with its right-hand side $TR(\xi) = I + \xi R(\xi)$ and thus, multiplying (2.3.6) by T from the left

$$\begin{aligned} T A_n &= \frac{1}{2\pi i} \oint_\Gamma (\xi - \lambda_k)^{-n-1} T R(\xi)\, d\xi \\ &= \frac{1}{2\pi i} \oint_\Gamma (\xi - \lambda_k)^{-n-1} \xi R(\xi)\, d\xi \\ &= \frac{1}{2\pi i} \oint_\Gamma (\xi - \lambda_k)^{-n} R(\xi)\, d\xi + \frac{\lambda_k}{2\pi i} \oint_\Gamma (\xi - \lambda_k)^{-n-1} R(\xi)\, d\xi \\ &= A_{n-1} + \lambda_k A_n. \end{aligned}$$

In particular, for $n = -1$ we obtain $TQ_k = D_k + \lambda_k Q_k$, which is exactly the Jordan decomposition for λ_k. □

Finally, we want to remark on another well-known property of the generalized eigenspaces which will be used in Section 3.3.1. We give the proof since it is short. For $p \in \mathbb{N}$ and $\lambda \in \mathbb{R}$ we call $N_{\lambda,p} = \ker(T - \lambda I)^p$ the *generalized*

eigenspace of order p. Note that $E_k = N_{\lambda_k, m_k}$ for an eigenvalue λ_k with algebraic multiplicity m_k and $N_{\lambda,p} \subset N_{\lambda,p+1}$.

Proposition 2.13. *If $\lambda \neq \mu$ are eigenvalues of T, then for all $p, k \in \mathbb{N}$*

$$(T - \lambda I)^p \left(N_{\mu,k} \backslash N_{\mu,k-1}\right) = N_{\mu,k} \backslash N_{\mu,k-1}.$$

Proof. First let $p = k = 1$ and consider $h \in N_{\mu,1}$, i.e. $(T - \mu I)h = 0$. Then

$$(T - \lambda I)\, h = (T - \mu I)\, h + (\mu - \lambda)\, h = (\mu - \lambda)\, h \tag{2.3.9}$$

which implies " $\subset$ " in the statement for this case. For $p = 1$ and any $k \in \mathbb{N}$ we have for $h \in N_{\mu,k} \backslash N_{\mu,k-1}$ that $(T - \mu I)h \in N_{\mu,k-1}$ and $h \neq 0$. Therefore, as before

$$(T - \lambda I)\, h = (T - \mu I)\, h + (\mu - \lambda)\, h \in N_{\mu,k} \backslash N_{\mu,k-1}.$$

This proves " $\subset$ " for $p = 1$ and all $k \in \mathbb{N}$. For arbitrary $p, k \in \mathbb{N}$ the inclusion " $\subset$ " follows by induction. We show now the other inclusion. Let again first $p = k = 1$ and consider again $h \in N_{\mu,1}$. Then (2.3.9) implies that $\tilde{h} = \frac{1}{\mu - \lambda} h$ is mapped to h by $T - \lambda I$ and hence $N_{\mu,1} \subset (T - \lambda I) N_{\mu,1}$. We show the inclusion for $p = 1$ and general k by induction. Assume that the inclusion holds for k and let $h \in N_{\mu,k+1} \backslash N_{\mu,k}$. Then $(T - \mu I)h \in N_{\mu,k}$ and by the induction hypothesis there exists $h_1 \in N_{\mu,k} \backslash N_{\mu,k-1}$ with $(T - \lambda I)h_1 = (T - \mu I)h$. This implies

$$(T - \lambda I)\, h_1 - (T - \lambda I)\, h = (\lambda - \mu)\, h$$

and hence, $\tilde{h} = \frac{h_1 - h}{\lambda - \mu}$ is mapped to h by $T - \lambda I$ which proves the inclusion in this case. For general p, k the inclusion follows again by induction. □

2.3.2 Perturbation of the eigenvalue problem

We return to the general family of operators $(T_\varepsilon)_{\varepsilon \in \mathbb{R}}$. We want to understand how the eigenvalue problem depends on ε. For each $\varepsilon \in \mathcal{U}$, the eigenvalues of T_ε are again precisely the roots of the characteristic polynomial

$$\rho_{T_\varepsilon}\left(\lambda\left(\varepsilon\right)\right) = \det\left(T_\varepsilon - \lambda\left(\varepsilon\right) I\right) \quad = \quad 0. \tag{2.3.10}$$

Expanding the determinant from the components of T_ε, we see that $\rho_{T_\varepsilon}\left(\lambda\left(\varepsilon\right)\right)$ is a polynomial in $\lambda(\varepsilon)$ with coefficients $a_k(\varepsilon)$, $k = 0, \ldots, N = \dim \mathcal{X}$, i.e.

$$(-1)^N \lambda\left(\varepsilon\right)^N + a_{N-1}\left(\varepsilon\right) \lambda\left(\varepsilon\right)^{N-1} + \cdots + a_1\left(\varepsilon\right) \lambda\left(\varepsilon\right) + a_0\left(\varepsilon\right) \;=\; 0. \tag{2.3.11}$$

As T_ε is holomorphic in ε, a_k's are holomorphic in ε, as well. There are two major problems for the analysis of the roots of ρ_{T_ε}. First of all, it is not clear if or how the holomorphic expansion of T_ε implies any relation between the eigenvalues for different ε. In particular, without a careful analysis, the holomorphicity of the coefficients a_k does not imply immediately that the roots, i.e. the eigenvalues, are continuous in ε, let alone holomorphic. A second major problem is that

the number of eigenvalues may change for different ε and it is not clear if this happens "continuously". For example, eigenvalues may simply vanish or they may "split up". Consider the following simple examples from Kato (1995, p. 64) to demonstrate these issues.

Example 2.14. a) The matrix

$$T_\varepsilon = \begin{pmatrix} 0 & 1 \\ \varepsilon & 0 \end{pmatrix}$$

has eigenvalues $\lambda_1(\varepsilon) = \varepsilon^{1/2}$, $\lambda_2(\varepsilon) = -\varepsilon^{1/2}$ ($(\cdot)^{1/2}$ is the complex square root). Consequently, at $\varepsilon = 0$ the only eigenvalue is 0, while for any $\varepsilon > 0$ there are two distinct eigenvalues. Moreover, both eigenvalues are clearly not holomorphic at 0.

b) The matrix

$$T_\varepsilon = \begin{pmatrix} \varepsilon & 1 \\ 0 & 0 \end{pmatrix}$$

has eigenvalues $\lambda_1(\varepsilon) = 0$ and $\lambda_2(\varepsilon) = \varepsilon$. Hence, again, for $\varepsilon = 0$ there is only one eigenvalue while there are two distinct eigenvalues for any $\varepsilon > 0$. On the other hand, this time the functions λ_1, λ_2 are holomorphic for all ε.

From these examples we conclude that the eigenvalues are not holomorphic for all ε, in general. And even if they are, then it may happen that eigenvalues split such that the overall number of eigenvalues changes. These observations are typical for the general theory. In fact, it is possible to show that the roots $\lambda(\varepsilon)$ of ρ_{T_ε} are functions which are holomorphic on any compact set $\tilde{\mathcal{U}} \subset \mathcal{U}$ with only finitely many *exceptional points* (see Kato (1995, II.1.1)). The point $\varepsilon = 0$ is the only exceptional point in both examples above. Deep results from complex analysis yield that the behavior of $\lambda(\varepsilon)$ at such an exceptional point ε_0 is still somewhat regular in the sense that there always exists a *Puiseux expansion*, i.e. a series expansion with fractional powers:

$$\lambda(\varepsilon) \quad = \quad \lambda(\varepsilon_0) + (\varepsilon - \varepsilon_0)^{1/p} \lambda^{(1)} + (\varepsilon - \varepsilon_0)^{2/p} \lambda^{(2)} + \cdots, \quad (2.3.12)$$

where each $\lambda^{(k)} \in \mathbb{C}$, $p \in \mathbb{N}$. As the powers k/p are always positive, it follows that the $\lambda(\varepsilon)$ are always continuous in ε and if $p = 1$, then $\lambda(\varepsilon)$ is even holomorphic in ε. If $p \neq 1$, then the rate of change close to ε_0 is of order $\varepsilon^{1/p}$ and thus large compared to the change of T_ε itself. Moreover, the number of distinct eigenvalues $\lambda(\varepsilon)$ remains constant on all of $\mathcal{U}$ and decreases only at exceptional points (see also Kato (1995, II.1.1)). In particular, splitting of eigenvalues happens only at exceptional points. As in the introduction of this section, from now on we consider without loss of generality only the behavior around $\varepsilon_0 = 0$. We will not explain how to obtain the exceptional points or their properties from ρ_{T_ε}. For more details see Kato (1995, II.1.1).

Eigenvalue splitting is crucial for this thesis. The main idea of our algorithms

for metastability are based on finding *dominant eigenvalues*, i.e. eigenvalues which are close to 1 (see Chapter 4). If T_0 has $\lambda(0) = 1$ as an eigenvalue, then we would like to know which eigenvalues $\lambda(\varepsilon)$ of T_ε eventually converge to 1 as $\varepsilon \to 0$. More generally, for any eigenvalue $\lambda(0)$ of T_0 and $\varepsilon \in \mathcal{U}$ we call the set of eigenvalues $\lambda(\varepsilon)$ of T_ε such that $\lambda(\varepsilon) \to \lambda(0)$ as $\varepsilon \to 0$ the $\lambda(0)$-*group* of T_ε. From continuity and discreteness of the spectrum we obtain the following lemma.

Lemma 2.15 (Baumgärtel (1985, p.115))**.** *Let U be an open disk containing only $\lambda(0)$ but not any other eigenvalue of T_0. Then there exists $\varepsilon^* > 0$ such that for all $\varepsilon < \varepsilon*$, $\sigma(T_\varepsilon) \cap U$ is exactly the $\lambda(0)$-group of T_ε.*

At least in theory, for small ε, we are thus able to separate the dominant eigenvalues of T_ε from other eigenvalues. We want to emphasize again that we *always* have continuity for the eigenvalues $\lambda(\varepsilon)$ when $\varepsilon \to 0$, but in general $\lambda(\varepsilon)$ is *not* holomorphic in ε.

2.3.3 Perturbation of eigenprojections

In the last subsection we have seen that the eigenvalues $\lambda(\varepsilon)$ are always perturbed continuously, but the perturbation is in general not holomorphic. It is then natural to ask about the perturbation of the associated (generalized) eigenvectors. For this we study the associated eigenprojections Q_ε. Consider first the examples from above.

Example (continuation of Example 2.14)**.** a) From the proof of Proposition 2.11 we know that for any $\varepsilon \in \mathbb{R}$ the eigenprojections satisfy $Q_{k,\varepsilon} = -\frac{1}{2\pi i} \oint_{\Gamma_k(\varepsilon)} R(\xi, \varepsilon)\, d\xi$, $k = 1, 2$, where $R(\cdot, \varepsilon)$ is the resolvent function of T_ε and $\Gamma_k(\varepsilon)$ is a circle around $\lambda_k(\varepsilon)$ which does not contain any other eigenvalue. Evaluating the contour integral shows that for $\varepsilon > 0$

$$Q_{1,\varepsilon} = \frac{1}{2}\begin{pmatrix} 1 & \varepsilon^{-1/2} \\ \varepsilon^{1/2} & 1 \end{pmatrix}, \quad Q_{2,\varepsilon} = \frac{1}{2}\begin{pmatrix} 1 & -\varepsilon^{-1/2} \\ -\varepsilon^{1/2} & 1 \end{pmatrix}$$

and $Q_{1,0} = 0$ (there is only one eigenvalue at 0). However, while the eigenvalues are always continuous in $\varepsilon = 0$, the eigenprojections have pole singularities there.

b) By the similar argument as in the first example we can show that

$$Q_{1,\varepsilon} = \begin{pmatrix} 1 & \varepsilon^{-1} \\ 0 & 0 \end{pmatrix}, \quad Q_{2,\varepsilon} = \begin{pmatrix} 0 & -\varepsilon^{-1} \\ 0 & 1 \end{pmatrix}$$

for $\varepsilon > 0$ and $Q_{1,0} = 0$. In this example the eigenvalues are holomorphic in $\varepsilon = 0$, but the eigenprojections are not. Indeed, they have pole singularities there again.

These examples show that the eigenprojections are not everywhere holomorphic, but also not always continuous like the eigenvalues either. In particular, this means that we cannot expect the (generalized) eigenfunctions to be holomorphic or continuous. Note that the points of irregular behavior in the examples are exactly the exceptional points. Under some mild assumptions we can guarantee that the eigenfunctions are also holomorphic at some exceptional points (see below). There is, however, a different, maybe rather surprising, way to deal with the perturbation of the eigenprojections. While the eigenprojections themselves are not always holomorphic, the *sum* of eigenprojections corresponding to eigenvalues of the same $\lambda(0)$-group of T_ε are always holomorphic! This can be easily seen in the examples, as the sum of the eigenprojections is in both cases the identity matrix, for all $\varepsilon \geq 0$. We therefore call

$$\Pi_{\lambda(0),\varepsilon} \quad = \quad \sum_{k=1}^{n_{\lambda(0)}} Q_{k,\varepsilon}$$

the *total eigenprojection* of the $\lambda(0)$-group of T_ε, where $\lambda_1(\varepsilon), \ldots, \lambda_{n_{\lambda(0)}}(\varepsilon)$ are the distinct eigenvalues, i.e. $n_{\lambda(0)} \leq m_{\lambda(0)}$, in the $\lambda(0)$-group. We further call $\mathcal{E}_{\lambda(0)}(\varepsilon) = E_1(\varepsilon) \oplus \ldots \oplus E_{n_{\lambda(0)}}(\varepsilon)$ the *total eigenspace* of the $\lambda(0)$-group where the $E_k(\varepsilon)$ are the generalized eigenspaces corresponding to $\lambda_k(\varepsilon)$. Hence, $\Pi_{\lambda(0),\varepsilon}$ projects vectors in $\mathcal{X}$ onto $\mathcal{E}_{\lambda(0)}(\varepsilon)$. We sum up the discussion so far in the next theorem.

Theorem 2.16 (Baumgärtel (1985, p.116))**.** *For any eigenvalue $\lambda(0)$ of T_0 the total eigenprojection $\Pi_{\lambda(0),\varepsilon}$ is holomorphic for all $\varepsilon \in \mathcal{U}$.*

Proof. Continuing the exposition from above we sketch the main ideas behind the proof of this theorem (see Kato (1995, II.1.3)). From the proof of Proposition 2.11 we know that

$$\Pi_{\lambda(0),\varepsilon} = \sum_{k=1}^{n_{\lambda(0)}} Q_{k,\varepsilon} = -\frac{1}{2\pi i} \oint_\Gamma R(\xi,\varepsilon)\, d\xi, \tag{2.3.13}$$

where $R(\xi,\varepsilon) = (T_\varepsilon - \xi I)^{-1}$ is the resolvent function for $\varepsilon \in \mathcal{U}$, and Γ is any contour around the $\lambda(0)$-group of T_ε, not containing any other eigenvalues of T_ε. By Lemma 2.15 this contour Γ exists, as long as ε is small enough. In order to conclude that $\Pi_{\lambda(0),\varepsilon}$ is holomorphic at $\varepsilon = 0$, it is enough to show that R is holomorphic in ξ and ε. In the proof of Proposition 2.11 we showed only that $R(\cdot,\varepsilon)$ is holomorphic in ξ for fixed ε. Let $\xi \in \mathbb{C}$ be arbitrary but distinct from any eigenvalue of T_ε for small enough ε. This is, for instance, satisfied if ξ lies on the contour Γ above. Then $R(\xi,\varepsilon)$ and $R(\xi,0)$ are well-defined. Assuming that (2.3.2) is satisfied, we can write

$$T_\varepsilon - \xi I = T_0 - \xi I + \varepsilon L = (I + \varepsilon L R(\xi,0))(T_0 - \xi I).$$

From the theory of Neumann series we then see that for sufficiently small ε the

operator $I + \varepsilon LR(\xi, 0)$ is invertible and that

$$\begin{aligned} R(\xi,\varepsilon) &= R(\xi,0)\left(I+\varepsilon LR(\xi,0)\right)^{-1} = R(\xi,0)\sum_{k=0}^{\infty}\left(-\varepsilon LR(\xi,0)\right)^{k} \\ &= R(\xi,0)+\sum_{k=1}^{\infty}\varepsilon^{k}A_{k}(\xi), \end{aligned} \tag{2.3.14}$$

for some operators A_k which are holomorphic in ξ, where

$$A_k(\xi) = (-1)^k R(\xi,0)\left(LR(\xi,0)\right)^k. \tag{2.3.15}$$

Hence,

$$\begin{aligned} \Pi_{\lambda(0),\varepsilon} &= -\frac{1}{2\pi}\oint_{\Gamma} R(\xi,0)\,d\xi - \sum_{k=1}^{\infty}\varepsilon^{k}\frac{1}{2\pi}\oint_{\Gamma}A_k(\xi)\,d\xi \\ &= \Pi_{\lambda(0),0}+\sum_{k=1}^{\infty}\varepsilon^{k}\tilde{A}_k \end{aligned} \tag{2.3.16}$$

for $\tilde{A}_k = -\frac{1}{2\pi}\oint_{\Gamma} A_k(\xi)\,d\xi$. This proves that $\Pi_{\lambda(0)}$ is holomorphic in ε. □

An interesting question is how "big" $\mathcal{E}_{\lambda(0)}(\varepsilon)$ is compared to $\mathcal{E}_{\lambda(0)}(0) = E_{\lambda(0)}$. The theorem implies that $\Pi_{\lambda(0),\varepsilon}$ is just a continuous perturbation of $\Pi_{\lambda(0),0}$ and we can conclude from Lemma I.4.10 of Kato (1995) that the range $\Pi_{\lambda(0),\varepsilon}(\mathcal{X})$ is isomorphic to the range $\Pi_{\lambda(0),0}(\mathcal{X})$. At $\varepsilon = 0$, the total projection is just the eigenprojection $Q_{\lambda(0),0}$ of $\lambda(0)$ whose dimension is equal to the algebraic multiplicity $m_{\lambda(0)}$ of $\lambda(0)$ according to Proposition 2.11. Hence,

$$\dim \mathcal{E}_{\lambda(0)}(\varepsilon) = \dim \mathcal{E}_{\lambda(0)}(0) = m_{\lambda(0)}. \tag{2.3.17}$$

2.3.4 Perturbation of semisimple eigenvalues

In the previous subsections we discussed that the eigenvalue perturbations are always continuous, but they may fail to be holomorphic. Moreover, the total eigenprojections are always holomorphic, while the eigenprojections may not be. In this subsection, we briefly study the special case where the unperturbed eigenvalue $\lambda(0)$ is semisimple. This will be the case in the following chapters. The following principle is called *reduction process* (see Kato (1995, II.2.3)). Let $\lambda(0)$ be a semisimple eigenvalue of the unperturbed operator T_0 with algebraic multiplicity m. In order to obtain the $\lambda(0)$-group eigenvalues of T_ε, it is sufficient to study the projected operator $T_\varepsilon \Pi_{\lambda(0),\varepsilon}$, since λ is a $\lambda(0)$-group eigenvalue of T_ε if and only if it is one of $T_\varepsilon \Pi_{\lambda(0),\varepsilon}$ (this is true at least for non-zero perturbations of $\lambda(0)$, for the general case see Kato (1995, II.2.1)). Define the

operator $T_\varepsilon^{(1)} : \mathcal{E}_{\lambda(0)}(\varepsilon) \to \mathcal{E}_{\lambda(0)}(\varepsilon)$ by

$$T_\varepsilon^{(1)} = \frac{1}{\varepsilon} \left(T_\varepsilon - \lambda(0) I\right) \Pi_{\lambda(0),\varepsilon}. \tag{2.3.18}$$

$T_\varepsilon^{(1)}$ is well-defined, since T_ε is invariant on $\mathcal{E}_{\lambda(0)}(\varepsilon)$. Intuitively, this operator describes the behavior of T_ε after *subtracting out* first order terms. We have then the following:

Lemma 2.17. *If $\lambda(0)$ is semisimple, then $T_\varepsilon^{(1)}$ is holomorphic at $\varepsilon = 0$.*

Proof. We sum up the discussion of Kato (1995, p. 77 ff). Since

$$\left(T_\varepsilon - \lambda\left(0\right) I\right) R\left(\xi, \varepsilon\right) = I + \left(\xi - \lambda\left(0\right)\right) R\left(\xi, \varepsilon\right),$$

we can conclude from (2.3.13) that

$$\begin{aligned} \left(T_\varepsilon - \lambda(0) I\right) \Pi_{\lambda(0),\varepsilon} &= -\frac{1}{2\pi i} \oint_\Gamma \left(T_\varepsilon - \lambda(0) I\right) R\left(\xi, \varepsilon\right) \, d\xi \\ &= -\frac{1}{2\pi i} \oint_\Gamma \left(\xi - \lambda(0)\right) R\left(\xi, \varepsilon\right) \, d\xi, \end{aligned}$$

where we use that the contour integral over constant functions vanishes. Then (2.3.14), (2.3.16) and (2.3.6) imply that this is equal to

$$\begin{aligned} &- \frac{1}{2\pi i} \oint_\Gamma \left(\xi - \lambda\left(0\right)\right) R\left(\xi, 0\right) d\xi + \sum_{k=1}^{\infty} \varepsilon^k \left(\frac{(-1)}{2\pi i} \oint_\Gamma \left(\xi - \lambda\left(0\right)\right) A_k(\xi) d\xi \right) \\ &= D + \sum_{k=1}^{\infty} \varepsilon^k B_k \end{aligned}$$

for operators B_k and where D is the nilpotent matrix corresponding to $\lambda(0)$ from Proposition 2.11. From Corollary 2.12 we know that D vanishes. We can therefore divide by ε to obtain

$$T_\varepsilon^{(1)} = \sum_{k=0}^{\infty} B_{k+1} \varepsilon^k, \tag{2.3.19}$$

i.e. $T_\varepsilon^{(1)}$ is holomorphic at $\varepsilon = 0$. □

What is the relation between T_ε and $T_\varepsilon^{(1)}$? If $\lambda^{(1)}(\varepsilon) \neq 0$ is an eigenvalue of $T_\varepsilon^{(1)}$ for an eigenvector $f \in \mathcal{E}_{\lambda(0)}(\varepsilon)$, then $\Pi_{\lambda(0),\varepsilon} f = f$ and therefore

$$\varepsilon \lambda^{(1)}(\varepsilon) f = \varepsilon T_\varepsilon^{(1)} f = \left(T_\varepsilon - \lambda\left(0\right) I\right) \Pi_{\lambda(0),\varepsilon} f = T_\varepsilon f - \lambda\left(0\right) f,$$

such that

$$T_\varepsilon f = \left(\lambda\left(0\right) + \varepsilon \lambda^{(1)}\left(\varepsilon\right)\right) f.$$

Consequently, f is eigenvector of T_ε for the eigenvalue $\lambda(0) + \varepsilon\lambda^{(1)}(\varepsilon)$. The discussion of Section 2.3.2 applies also to $T_\varepsilon^{(1)}$ and $\lambda^{(1)}(\varepsilon)$ such that $\lambda^{(1)}(\varepsilon)$ is continuous at $\varepsilon = 0$ and, in particular, has a Puiseux expansion as in (2.3.12) such that

$$\lambda(0) + \varepsilon\lambda^{(1)}(\varepsilon) = \lambda(0) + \varepsilon\lambda^{(1)}(0) + o(\varepsilon).$$

Moreover, we can show that $\lambda^{(1)} = \lambda^{(1)}(0)$ is an eigenvalue of $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$, where L is the first order perturbation operator in (3.2.1). Indeed, from

$$\begin{aligned} 0 &= (T_0 - \lambda(0) I)\,\Pi_{\lambda(0),0} = \Pi_{\lambda(0),0}\,(T_0 - \lambda(0) I), \\ \Pi_{\lambda(0),\varepsilon} &= \Pi_{\lambda(0),0} + \varepsilon\tilde{A}_1 + o(\varepsilon) \end{aligned}$$

(see (2.3.16)), we can conclude that

$$\begin{aligned} T_\varepsilon^{(1)} &= \Pi_{\lambda(0),\varepsilon} T_\varepsilon^{(1)} \\ &= \frac{1}{\varepsilon}\Pi_{\lambda(0),\varepsilon}\,(T_0 - \lambda(0) I)\,\Pi_{\lambda(0),\varepsilon} + \Pi_{\lambda(0),\varepsilon} L \Pi_{\lambda(0),\varepsilon} \\ &= \Pi_{\lambda(0),\varepsilon} L \Pi_{\lambda(0),\varepsilon} + o(1), \end{aligned}$$

such that by continuity and letting $\varepsilon \to 0$

$$0 = \det\left(T_\varepsilon^{(1)} - \lambda^{(1)}(\varepsilon) I\right) \to \det\left(\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0} - \lambda^{(1)}(0) I\right).$$

Hence, $\lambda^{(1)}$ is an eigenvalue of $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$ by (2.3.10). We sum up this discussion in the following Theorem:

Theorem 2.18 (Reduction process, Kato (1995, Theorem 2.3, p.82))**.** *Let $T_\varepsilon = T_0 + \varepsilon L$ and let $\lambda(0)$ be a semisimple unperturbed eigenvalue. Denote by $\lambda^{(1)}$ a non-zero eigenvalue of $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$. Then the $\lambda(0)$-group eigenvalues of T_ε belongs to a $\lambda(0) + \varepsilon\lambda^{(1)}$-group and are of the form $\lambda(0) + \varepsilon\lambda^{(1)} + o(\varepsilon)$.*

The main implications of this are that the eigenvalues of perturbed semisimple eigenvalues are differentiable (not necessarily holomorphic) and that the first order eigenvalues are related to the perturbation operator L. That is, having a semisimple unperturbed eigenvalue gives even more structure that can be exploited. If $\lambda^{(1)}$ is semisimple, too, then we can repeat the reduction procedure and obtain a holomorphic operator $T_\varepsilon^{(2)}$ such that its zero order approximation yields an eigenvalue $\lambda^{(2)}$ and $\lambda(0) + \varepsilon\lambda^{(1)} + \varepsilon^2\lambda^{(2)} + o(1)$ is an eigenvalue of T_ε. If $\lambda^{(2)}$ is again semisimple, then we can apply this procedure again, and so on. If the resulting eigenvalues $\lambda^{(k)}$ are all semisimple, we can, in principle, continue this procedure infinitely often. We thus obtain explicitly the holomorphic expansions of all eigenvalues in the $\lambda(0)$-group of T_ε. A special case of this situation is when T_0 and L are self-adjoint (see Kato (1995, p. 120) for details). Then all eigenvalues of T_0 are semisimple and T_ε is self-adjoint for all ε. Since T_ε and $\Pi_{\lambda(0),\varepsilon}$ commute (all eigenprojections commute with T_ε, see (2.3.8)), (2.3.18) shows that $T_\varepsilon^{(1)}$ is self-adjoint for all ε, as well. Therefore all eigenvalues of $T_0^{(1)}$ are semisimple and the reduction procedure can be applied

again. The same reasoning can be used for all the $\lambda^{(k)}$ and, consequently, the eigenvalues of T_ε are holomorphic. Together with (*iii*) from Theorem 2.21 below this provides a proof of Theorem 2.10.

Remark 2.19. It is worth emphasizing that T_0 being self-adjoint does not imply more than that its eigenvalues are semisimple. If L is not self-adjoint, then we *cannot* conclude in general that the eigenvalues of T_ε are holomorphic. This is not even true, if $T_\varepsilon = T_0 + \varepsilon L$ is diagonalizable for all ε in some neighborhood of 0. Consider for this the following example from Kato (1995, p.86).

Example 2.20. Let

$$T_\varepsilon = T_0 + \varepsilon L = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Its eigenvalues are of the form

$$\pm\varepsilon^{3/2} + \cdots, \quad 1 + \varepsilon^3 + \cdots.$$

That is, even though T_0 is symmetric, the first two perturbed eigenvalues are not holomorphic at $\varepsilon = 0$.

For our purposes, the following results about eigenvectors, which extend the discussion in the beginning of this subsection, will be important.

Theorem 2.21 (Baumgärtel (1985, Corollary 4 and Theorem 3, p.269))**.** *Let $\lambda(0)$ be a semisimple unperturbed eigenvalue with algebraic multiplicity m. Then we have:*

(i) For small ε the generalized eigenvectors $f_i(\varepsilon)$, $i = 1, \ldots, m$, of the $\lambda(0) + \varepsilon\lambda_i^{(1)}$-group of T_ε can be chosen such that they are continuous at $\varepsilon = 0$ and span the total eigenspace $\mathcal{E}_{\lambda(0)}(\varepsilon)$.

(ii) The unperturbed generalized eigenvectors $f_i(0)$ are non-zero and they are eigenvectors of $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$ corresponding to the eigenvalues $\lambda_i^{(1)}$, i.e.

$$\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0} f_i(0) \quad = \quad \lambda_i^{(1)} f_i(0).$$

(iii) If $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$ has only simple eigenvalues, then the eigenvalues $\lambda_i(\varepsilon)$ and generalized eigenvectors $f_i(\varepsilon)$ of $T(\varepsilon)$ are holomorphic.

Finally, for later purposes we explicitly give the first order coefficient $\tilde{A}_1$ in the series expansion of the projection $\Pi_{\lambda(0),\varepsilon}$, which is holomorphic by Theorem 2.16.

Theorem 2.22 (Kato (1995, p.40))**.** *Let $\lambda(0)$ be a semisimple eigenvalue. Then the total eigenprojection $\Pi_{\lambda(0),\varepsilon}$ has the series expansion*

$$\Pi_{\lambda(0),\varepsilon} \quad = \quad \Pi_{\lambda(0),0} + \varepsilon \Pi_{\lambda(0)}^{(1)} + \mathcal{O}\left(\varepsilon^2\right),$$

where

$$\begin{aligned} \Pi^{(1)}_{\lambda(0)} &= -\Pi_{\lambda(0),0} L H - H L \Pi_{\lambda(0),0}, \\ H &= -\sum_{i=1}^{k} \left[(1-\beta_i)^{-1} Q_i + \sum_{j=1}^{n_i-1} (1-\beta_i)^{-j-1} D_i^j \right], \end{aligned} \tag{2.3.20}$$

for repeated eigenvalues $\beta_1, ..., \beta_k$ *of* T_0 *different from* 1 *with multiplicities* n_i*, eigenprojections* Q_i *and eigennilpotents* D_i*.*

Chapter 3

Generalized Reversibility

As outlined in Chapter 1 we study the stochastic dynamics of certain Markov processes through the spectral properties of the associated transfer operators. Indeed, we will see in the next chapter how metastability of such a process can be described based only on eigenvectors and eigenvalues of the transfer operator. The spectral analysis of an operator is typically easiest when the operator is self-adjoint since the spectral theorem shows that the complicated actions of the operator can be decomposed into simple actions on small invariant subspaces, which are the respective eigenspaces. If the Markov process has an invariant measure, then self-adjointness of the transfer operator corresponds to a detailed balance condition of the transition probabilities which was formulated in (2.2.2) for the case of Markov chains. The physical interpretation of the detailed balance condition is that the underlying dynamics are reversible. Reversibility is often a very restrictive assumption, which although simplifies the mathematical analysis, might not exist in some interesting physical dynamics, e.g. Langevin dynamics. Our main goal in this chapter is thus to generalize the concept of reversibility to cover more general physical systems while maintaining enough useful mathematical structure. The leading example for our work is the Langevin process whose transfer operator is in general not self-adjoint. Simulations and empirical evidence, however, show that this process has several features which are reminiscent of reversible processes. In particular, the *dominant* eigenvalues, i.e. the eigenvalues close to 1, are real-valued. Moreover, while the Langevin process is in general not reversible, the associated transfer operator always satisfies an *extended detailed balance* (see Chapter 1).

In this chapter, we will generalize the concept of reversibility in two ways. The first one is the extended detailed balance condition which directly generalizes the detailed balance condition of (2.2.2). The second one is the so-called *weak reversibility*, which essentially requires the transfer operator to be self-adjoint in the eigenspaces corresponding to the dominant eigenvalues. After introducing these two conditions, we analyze how they affect the spectral properties of the

transfer operators. In particular, we will explain why the dominant eigenvalues are real and in what sense the operators are "almost" self-adjoint. The main tool for the analysis is perturbation theory for linear operators as introduced in the previous chapter. This approach is justified since the dynamical systems that we consider depend fundamentally on the temperature of the system. The temperature can then be interpreted as a perturbation parameter, leading to a very simple system when approaching a specific temperature. As mentioned in the last chapter, we consider for simplicity only Markov processes in discrete time. They usually serve as close approximations to general Markov processes and are therefore the prime objects in simulations. Moreover, on the mathematical side, the analysis is simplified and the relevant properties we are after can be identified easily.

Previously, Hérau et al. (2008, 2011) analyzed the spectrum of some specific perturbed irreversible processes, as well. In the first section, we will therefore compare our approach to this prior work. In the second section we study how the perturbation theory of the last chapter can be applied to Markov chains and the associated transfer operators. In the third section, the aforementioned generalized concepts of reversibility are introduced. The fourth section, finally, discusses the application of these concepts to the spectral properties of the transfer operators.

In the following, we will use notation and concepts from Chapter 2 without further reference.

3.1 Comparison with previous approach from the literature

A similar study on dominant eigenvalues has actually been carried out before in Hérau et al. (2008, 2011). Hérau et al. consider an operator of Kramers-Fokker-Planck type, which is essentially a generator of some associated Markov semigroup. They show for small temperature that the eigenvalues of the operator, which are close to 0, are all real-valued. Moreover, the authors show that the corresponding eigenvectors are "almost" orthogonal with respect to some Hermitian form defined by using the concept of PT symmetry, which corresponds to the extended detailed balance condition in this thesis. Here we are interested in this particular problem of spectral analysis but in a different setting. We do not restrict ourselves to operators of a certain physical dynamics, but any transfer operators that satisfy an extended detailed balance condition.

3.2 Perturbation analysis of Markov Chains

We assume that the physical process we are modeling can be described by a Markov chain $X^{(\varepsilon)} = (X_n^{(\varepsilon)})_{n\in\mathbb{N}_0}$ where $\varepsilon \geq 0$ is a model parameter, e.g. temperature. Let $\mu_\varepsilon > 0$ be an invariant measure of $X^{(\varepsilon)}$ and let T_ε be the associated transfer operator defined in (2.2.1), i.e. T_ε is an operator on $\mathcal{X} = \mathbb{C}^N$, with $N < \infty$ being the cardinality of the state space S. We want to study properties of $X^{(\varepsilon)}$ by analyzing spectral properties of T_ε. Doing so by means of perturbation theory requires two key assumptions:

1. $X^{(0)}$ is a comparably simple Markov chain such that T_0 has "nice" properties;
2. $X^{(\varepsilon)}$ arises as a perturbation of $X^{(0)}$ in the sense that T_ε is a perturbation of T_0 as described in the previous chapter.

These assumptions will be made precise in the next two subsections. With respect to the perturbation, in the following, we always assume that T_ε is a *linear perturbation* of T_0, i.e. there exists another operator L, satisfying certain model-specific properties, such that

$$T_\varepsilon \quad = \quad T_0 + \varepsilon L, \quad \varepsilon \geq 0. \tag{3.2.1}$$

From perturbation theory (see Section 2.3) we know that the spectral properties of T_ε are related to those of T_0. In fact, it is not necessary to assume *a priori* that the perturbation is linear. The linear case is often easier to handle, as we have seen in the section on perturbation theory. For us, it becomes essential in the weak reversibility condition below and for simulations (see Section 4.4.4). In the next two subsections we will derive assumptions on T_0 and T_ε which are crucial for our analysis.

Remark 3.1. It may seem slightly unintuitive to assume that the transfer operators are perturbed, instead of the transition matrices P_ε of $X^{(\varepsilon)}$. However, equation 3.2.1 is essentially equivalent to assuming that the transition matrices P_ε are perturbed holomorphically, i.e. $P_\varepsilon = P^{(0)} + \varepsilon P^{(1)} + \cdots$ for some matrices $P^{(i)}$, as long as $X^{(\varepsilon)}$ is irreducible, which we will assume further below. Indeed, (3.2.1) and Proposition 2.8 show that we can recover the transition matrices P_ε and the invariant measures μ_ε from T_ε. From the proof of Proposition 2.8 it follows that then the defined μ_ε and P_ε will depend holomorphically on ε, as well. On the other hand, a holomorphic perturbation of P_ε is reflected in a holomorphic perturbation of their unique normalized left eigenvectors μ_ε. This, in turn, immediately implies that T_ε depends holomophically on ε, as well, by its definition on (2.2.1). In the following we can therefore without any restriction assume that (3.2.1) is satisfied.

3.2.1 Uncoupled Markov chain

As outlined earlier our final goal is to find metastable partitions of the state space. Since we look for decompositions of the whole state space, we define

Definition 3.2. Let $S_1, \ldots, S_m$ be disjoint subsets of S. If $\bigcup_{k=1}^m S_k = S$, then we call $\mathfrak{S} = \{S_1, \ldots, S_m\}$ a *full partition* of S. We call a Markov chain X *uncoupled,* if there exists a full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ such that for all $i, j = 1, \ldots, m$,

$$\mathbb{P}\left(X_1 \in S_j \,|X_0 \in S_i\right) \quad = \quad \delta_{ij}. \tag{3.2.2}$$

From a modeling point of view it makes sense to assume that the metastable partition of the system for small ε is a small perturbation of a *perfectly stable* or *invariant* partition at $\varepsilon = 0$. To be precise, we assume the following:

Assumption 3.3. *The Markov chain $X^{(0)}$ is uncoupled.*

Intuitively speaking, this means when the uncoupled Markov chain $X^{(0)}$ starts in some invariant subset S_i, then it will remain in S_i for an infinitely long time. For the transition matrix P_0 of $X^{(0)}$ this assumption implies that $P_0(x, y)$ is zero if x and y lie in two different invariant subsets $S_i, S_j, i \neq j$. Hence, up to a permutation of the states in S, P_0 is block-diagonal with stochastic matrices Q_i, $i = 1, \ldots, m$, such that $Q_i(x, y) = P_0(x, y)$ for all $x, y \in S_i$, i.e.

$$\Sigma^\top P_0 \Sigma \quad = \quad \begin{pmatrix} Q_1 & 0 & \cdots & 0 \\ 0 & Q_2 & \cdots & 0 \\ \cdot & \cdot & \cdots & \cdot \\ 0 & \cdots & 0 & Q_3 \end{pmatrix}$$

where Σ is a permutation matrix. We assume additionally that the Markov chains corresponding to the block transition matrices Q_i have unique invariant measures η_i. Since those chains correspond to $X^{(0)}$ starting in S_i, this can be formulated easily by assuming that

Assumption 3.4. *Conditional on $X_0^{(0)} \in S_i$, $X^{(0)}$ has unique invariant measure η_i.*

In particular, from Definition 2.6 and Theorem 2.7 it is sufficient to assume that the Markov chains corresponding to the Q_i's are ergodic. Extending the measures η_i to all of S, we can assume that they are supported on S_i, i.e. $\eta_i(S_i) = 1$ and $\eta_i(S \setminus S_i) = 0$. From the two Assumptions 3.3 and 3.4 above it then follows that every probability measure of the form $\mu_0 = \sum_{i=1}^m \beta_i \eta_i$ with non-negative coefficients β_i is an invariant measure of $X^{(0)}$. In particular, if $m > 1$, then $X^{(0)}$ does not have a unique invariant measure.

Assumptions 3.3 and 3.4 are the two "nice" assumptions which we mentioned in the beginning of the section. The next two lemmas describe their implications

on the spectral properties of the transfer operator T_0, first for the case that $m = 1$ and then for the general case $m \geq 1$.

Lemma 3.5. *Let $X = (X_n)_{n\in\mathbb{N}_0}$ be a Markov chain with unique invariant measure μ and transfer operator T. Then it holds:*

(i) The eigenvalue 1 of T has algebraic and geometric multiplicity 1. In particular, the function $\mathbf{1}(x) = 1$ for all $x \in S$, is the only eigenvector (up to scalar multiples) of T corresponding to the eigenvalue 1.

(ii) The function $\mathbf{1}$ is $\langle\cdot,\cdot\rangle_\mu$-orthogonal to all generalized eigenvectors y of T corresponding to eigenvalues with absolute value less than 1.

Proof. (i) Since μ is unique, it follows that $\mu > 0$. Then the statement is implied by Proposition 2.8 and Theorem 2.4.

(ii) Let y be a generalized eigenvector for an eigenvalue λ with $|\lambda| < 1$, i.e. $(T - \lambda I)^k y = 0$ for some $k \in \mathbb{N}$. The binomial theorem implies

$$0 = \sum_{l=0}^{k} \binom{k}{l} T^{k-l} (-\lambda)^l y = \sum_{l=0}^{k-1} \binom{k}{l} T^{k-l} (-\lambda)^l y + (-\lambda)^k y,$$

and consequently

$$(-\lambda)^k y = -\sum_{l=0}^{k-1} \binom{k}{l} T^{k-l} (-\lambda)^l y. \tag{3.2.3}$$

Observe that the properties of μ and $\mathbf{1}$ imply for any $z \in \mathcal{X}$

$$\langle z, \mathbf{1}\rangle_\mu = \sum_{x\in S} \mu(x)\, z(x) = \langle z, \mu\rangle = z^\top \mu = z^\top T^\top \mu = \langle Tz, \mu\rangle = \langle Tz, \mathbf{1}\rangle_\mu \tag{3.2.4}$$

and thus by induction

$$\langle z, \mathbf{1}\rangle_\mu \quad = \quad \left\langle T^l z, \mathbf{1}\right\rangle_\mu, \quad l \in \mathbb{N}.$$

Together with (3.2.3) we therefore obtain for $z = y$

$$\begin{aligned}
(-\lambda)^k \langle y, \mathbf{1}\rangle_\mu &= \left\langle (-\lambda)^k y, \mathbf{1}\right\rangle_\mu \\
&= \left\langle -\sum_{l=0}^{k-1} \binom{k}{l} T^{k-l} (-\lambda)^l y, \mathbf{1}\right\rangle_\mu \\
&= -\sum_{l=0}^{k-1} \binom{k}{l} \left\langle T^{k-l} (-\lambda)^l y, \mathbf{1}\right\rangle_\mu \\
&= \left(-\sum_{l=0}^{k-1} \binom{k}{l} (-\lambda)^l\right) \langle y, \mathbf{1}\rangle_\mu .
\end{aligned}$$

Hence, either $\langle y, \mathbf{1} \rangle_\mu = 0$ or $(1-\lambda)^k = \sum_{l=0}^{k} \binom{k}{l} (-\lambda)^l = 0$. As we assumed $|\lambda| < 1$, we conclude $\langle y, \mathbf{1} \rangle_\mu = 0$. □

Lemma 3.6. *Let $X = (X_n)_{n \in \mathbb{N}_0}$ be an uncoupled Markov chain with full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ such that conditional on $X_0 \in S_i$ the process X has unique invariant measure η_i for $i = 1, \ldots, m$. Let χ_i be the indicator function for the set S_i and let T be the transfer operator of X with respect to some invariant measure $\mu = \sum_{i=1}^{m} \beta_i \eta_i$, $\beta_i > 0$. Then it holds:*

(i) Every eigenvector f of T corresponding to the eigenvalue 1 is a linear combination of χ_i's.

(ii) The eigenvalue 1 of T is semisimple and the dimension of the corresponding eigenspace E_1 is m.

(iii) There exists a basis of E_1 which is $\langle \cdot, \cdot \rangle_\mu$-orthonormal and consists of eigenvectors f_i, $i = 1, \ldots, m$, of T corresponding to the eigenvalue 1.

(iv) Each f_i is $\langle \cdot, \cdot \rangle_\mu$-orthogonal to all generalized eigenvectors g of T corresponding to eigenvalues with absolute value less than 1.

Proof. (i) Let $f \neq 0$ be an eigenvector of T corresponding to the eigenvalue 1. From (3.2.2) it follows that the entries $P(x, y)$ of the transition matrix of X are zero if x and y are not elements of the same set S_i. Since the sets S_i's are disjoint, we have for $y \in S_i$ that $\mu(y) = \beta_i \eta_i(y)$ and thus

$$\begin{aligned} (Tf)(y) &= \frac{1}{\left(\sum_{i=1}^{m} \beta_i \eta_i\right)(y)} \sum_{x \in S} P(x, y) f(x) \left(\sum_{i=1}^{m} \beta_i \eta_i \right)(x) \\ &= \frac{1}{\eta_i(y)} \sum_{x \in S_i} P(x, y) f(x) \eta_i(x) \\ &= (T_i f)(y), \end{aligned} \tag{3.2.5}$$

where T_i is the transfer operator of the Markov chain X, starting in S_i. Since $f \neq 0$ is an eigenvector of T, this implies that

$$(T_i f)(y) = (Tf)(y) = f(y)$$

for all $y \in S_i$, i.e. $f \neq 0$ is also an eigenvector of T_i for the eigenvalue 1. Since the Markov chain corresponding to T_i has unique invariant measure η_i, it follows from Lemma 3.5 that $f(y) = \alpha_i$ for all $y \in S_i$ and some $\alpha_i \in \mathbb{C} \backslash \{0\}$. This is true for all $i = 1, \ldots, m$ such that $f = \sum_{i=1}^{m} \alpha_i \chi_i$.

(ii) By part (i), the eigenspace corresponding to the eigenvalue 1 has dimension m, i.e. the geometric multiplicity is m. We want to prove that all generalized eigenvectors corresponding to eigenvalue 1 are already eigenvectors. We therefore consider a generalized eigenvector $f \neq 0$ corresponding to the eigenvalue 1, i.e. $(T - I)^l (f) = 0$ for some $l \geq 1$. Similar calculations as in (3.2.5) show that

$(T_i - I)^l(f)(y) = 0$ for all $y \in S_i$, i.e. $f\chi_i$ is also a generalized eigenvector for each T_i, $i = 1, \ldots, m$. By Lemma 3.5, $f\chi_i$ is already an eigenvector of block T_i, i.e. $l = 1$. We therefore conclude that geometric and algebraic multiplicity coincide, i.e. 1 is a semisimple eigenvalue.

(iii) Clear.

(iv) By part (i), $f_i = \sum_{k=1}^m \alpha_k \chi_k$ for some $\alpha_k \in \mathbb{R}$. It is thus sufficient to show the statement for χ_k instead of f_i. Let g be a generalized eigenvector of T for any eigenvalue λ with $|\lambda| < 1$, i.e. $(T - \lambda I)^l(g) = 0$ for some $l \geq 1$. As in part (ii) this implies $(T_i - \lambda I)^l(g\chi_i) = 0$ for all $i = 1, \ldots, m$, i.e. $g\chi_i$ is a generalized eigenvector of T_i for the eigenvalue λ. In particular, $g\chi_k$ is an eigenvector of T_k. We then obtain immediately from Lemma 3.5 that

$$\begin{aligned}
\langle g, \chi_k \rangle_\mu &= \sum_{x \in S} g(x)\, \chi_k(x) \left(\sum_{j=1}^m \beta_j \eta_j \right)(x) \\
&= \beta_k \sum_{x \in S_k} g(x)\, \chi_k(x)\, \eta_k(x) \\
&= \beta_k \langle g\chi_k, \chi_k \rangle_{\eta_k} \\
&= 0
\end{aligned}$$

which proves the claim. □

Lemma 3.6 shows, in particular, that eigenvectors with respect to $\lambda = 1$ can be expressed either as linear combinations of the f_i or the indicator functions χ_i.

3.2.2 Nearly uncoupled Markov chain

Our approach relies on the hope that $X^{(\varepsilon)}$ is a *nearly uncoupled* Markov chain in the sense that for a small perturbation $\varepsilon > 0$ we can ensure metastability of the partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ which is the partition from Assumption 3.3. From here on we assume the following:

Assumption 3.7. *$X^{(\varepsilon)}$ has a unique invariant measure μ_ε for $\varepsilon > 0$.*

The main assumption made in the beginning of the section is that the transfer operator T_ε arises as a linear perturbation from T_0 by εL for some perturbation operator L. While the spectrum of T_0 is rather easy to analyze, as we saw in the previous subsection, the spectrum of T_ε can only be accessed by means of perturbation theory, as outlined in Section 2.3. As will be seen in the following chapter, the metastability of the system can be described conveniently via the $\lambda(0)$-group eigenvalues of T_ε, where $\lambda(0)$ denotes (throughout this thesis) the eigenvalue 1 of T_0, and the associated eigenvectors. Since the $\lambda(0)$-group eigenvalues converge to 1, they are called *dominant* eigenvalues (when they are

close enough to 1). From Assumption 3.3 the Markov chain $X^{(0)}$ is uncoupled with stable partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$. Lemma 3.6 implies then that $\lambda(0)$ is semisimple and has algebraic multiplicity m. For small $\varepsilon > 0$ the total eigenspace of the $\lambda(0)$-group always has the same dimension, i.e.

$$\dim \mathcal{E}_{\lambda(0)}(\varepsilon) = \dim \mathcal{E}_{\lambda(0)}(0) = m$$

(see (2.3.17) and the discussion there). In particular, the $\lambda(0)$-group has at most m different eigenvalues. We denote by

$$\lambda_1(\varepsilon), \ldots, \lambda_m(\varepsilon)$$

the *repeated* $\lambda(0)$-group perturbed eigenvalues of T_ε. The $\lambda_i(\varepsilon)$ are thus not necessarily unique, except for $\lambda_i(\varepsilon) = 1$. Similarly, let

$$f_1(\varepsilon), \ldots, f_m(\varepsilon)$$

denote the corresponding $\lambda(0)$-group generalized eigenvectors of T_ε. From Theorem 2.21 we obtain that $f_i(\varepsilon)$'s span $\mathcal{E}_{\lambda(0)}(\varepsilon)$. Moreover, the eigenvalues $\lambda_i(\varepsilon)$ and the eigenvectors $f_i(\varepsilon)$ are continuous in ε, i.e. $\lambda_i(\varepsilon) \to \lambda(0)$ and $f_i(\varepsilon) \to f_i(0)$ as $\varepsilon \to 0$. Similarly, we can also show that the invariant measures μ_ε are continuous in ε.

Lemma 3.8. *Under Assumptions 3.3, 3.4, and 3.7 the invariant measures μ_ε are continuous at $\varepsilon = 0$.*

Proof. By Remark 3.1 the transition matrices P_ε of $X^{(\varepsilon)}$ and thus the respective transpose matrices $P_\varepsilon^\top$ are holomorphic at $\varepsilon = 0$. Since $\lambda(0) = 1$ is a semisimple eigenvalue of $P_0^\top$, Theorem 2.21 applies also to $P_\varepsilon^\top$ such that the generalized eigenvectors of $P_\varepsilon^\top$ belonging to the $\lambda(0)$-group can be chosen to be continuous. As μ_ε is the unique normalized left eigenvectors of P_ε for the eigenvalue 1, μ_ε itself is already continuous at $\varepsilon = 0$. □

Remark 3.9. We emphasize that T_ε is in general not a self-adjoint operator and, hence, T_ε can be non-diagonalizable. Therefore, not every $f_i(\varepsilon)$ is necessarily an eigenvector.

3.3 Two concepts of generalized reversibility

Using the notation of the previous subsection, we are now ready to generalize the concept of reversibility.

3.3.1 The extended detailed balance condition

This section aims to present the first form of generalized reversibility condition, namely the *extended detailed balance*. Such a condition is found, for example, in Langevin dynamics in terms of momentum reversal (see Chapter 1). The extended detailed balance is our main interest in this thesis. We will prove that it implies important results about the spectrum of the transfer operator. Let us begin by giving the definition of the condition.

Definition 3.10. Let $a : S \to S$ be an involution, i.e. a is one-to-one with $a^2 = a$. Let X be a Markov chain with transition matrix P, transfer operator T and invariant measure μ. Define furthermore the operator $A : \mathcal{X} \to \mathcal{X}$, where

$$Af\left(x\right) \quad := \quad f\left(a\left(x\right)\right), \quad x \in S. \tag{3.3.1}$$

We say that X (or P or T) satisfies *extended detailed balance* with respect to A and μ, if for all $x, y \in S$ it holds that

$$\mu(x)P(x,y) \quad = \quad \mu(a(y))P(a(y),a(x)). \tag{3.3.2}$$

Obviously, if $a(x) = x$ for all $x \in S$, the extended detailed balance reduces to the classical detailed balance condition in (2.2.2). A is an involution, as well, but this time on $\mathcal{X}$ instead of S. We derive now a few properties of A with respect to T and μ.

Lemma 3.11. *Let T be a transfer operator that satisfies extended detailed balance with respect to an involution A and a measure μ. Then it holds:*

(i) $A\mu = \mu$, *i.e. μ is invariant under a.*

(ii) *A is self-adjoint with respect to $\langle \cdot, \cdot \rangle_\mu$.*

(iii) *The adjoint of T with respect to $\langle \cdot, \cdot \rangle_\mu$ is given by $T^* = ATA$.*

Proof. (i) By definition of the invariant measure and the extended detailed balance condition, we have for $y \in S$

$$\mu(y) = \sum_{x \in S} P(x,y)\mu(x) = \sum_{x \in S} \mu(a\left(y\right))P(a\left(y\right), a\left(x\right)).$$

Set $z = a\left(x\right)$, then $\mu(y) = \mu(a\left(y\right)) \sum_{z \in S} P(a\left(y\right), z) = \mu(a\left(y\right))$, i.e. $A\mu = \mu$.

(ii) $\langle f, Ag \rangle_\mu = \sum_x f(x)\overline{g(a\left(x\right))}\mu(x) = \sum_y f(a\left(y\right))\overline{g(y)}\mu(y) = \langle Af, g \rangle_\mu$, where we set $y = a\left(x\right)$ and use the fact from part *i)* that μ is invariant under a in the second equation.

(*iii*) For any $f, g \in \mathcal{X}$

$$\begin{aligned}
\langle f, Tg\rangle_\mu &= \sum_{x,y} f(y)\overline{g(x)}P(x,y)\mu(x) \\
&= \sum_{x,y} f(y)\overline{g(x)}P(a(y), a(x))\mu(a(y)) \\
&= \sum_{j,k} f(a(k))\overline{g(a(j))}P(k,j)\mu(k) \\
&= \langle TAf, Ag\rangle_\mu \\
&= \langle ATAf, g\rangle_\mu ,
\end{aligned}$$

where we use the extended detailed balance condition in the second equation and the fact that A is self-adjoint in the last equation. □

The lemma shows that T is not self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$, unless $A = I$. However, since A is only an involution, T^* is not "far away" from T. In fact, we can define a Hermitian form (which was also discussed in Hérau et al. (2011) in the context of PT symmetry) $\langle\cdot,\cdot\rangle_{A,\mu} : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ by

$$\langle f, g\rangle_{A,\mu} := \langle Af, g\rangle_\mu .$$

This is indeed a Hermitian form follows from the properties of $\langle\cdot,\cdot\rangle_\mu$ and the self-adjointness of A with respect to $\langle\cdot,\cdot\rangle_\mu$. In turns out that T behaves with respect to $\langle\cdot,\cdot\rangle_{A,\mu}$ almost like a self-adjoint operator. From Proposition 2.11 we know that T may not be diagonalizable by a basis of eigenvectors. Instead there is always a basis of generalized eigenvectors, decomposing $\mathcal{X}$ into a direct sum of generalized eigenspaces $E_k = \ker((T - \lambda_k I)^{m_k})$ for eigenvalues λ_k with algebraic multiplicity m_k. Recall also the generalized eigenspaces, of order p, $N_{\lambda,p} = \ker(T - \lambda I)^p$. We then obtain the following properties of T with respect to $\langle\cdot,\cdot\rangle_{A,\mu}$.

Lemma 3.12. *Let T be a transfer operator that satisfies extended detailed balance with respect to an involution A and a measure μ. Then it holds:*

(i) For any $f, g \in \mathcal{X}$

$$\langle Tf, g\rangle_{A,\mu} = \langle f, Tg\rangle_{A,\mu} .$$

(ii) Let λ_1, λ_2 be eigenvalues of T and let $f \in N_{\lambda_1,p_1}\backslash N_{\lambda_1,p_1-1}$ and $g \in N_{\lambda_2,p_2}\backslash N_{\lambda_2,p_2-1}$ be generalized eigenvectors for $p_1, p_2 \in \mathbb{N}$. If $\lambda_1 \neq \overline{\lambda_2}$, then $\langle f, g\rangle_{A,\mu} = 0$. This holds, in particular, for any two eigenpairs (λ_1, f) and (λ_2, g) of T (an eigenpair (λ, f) satisfies $Tf = \lambda f$).

Proof. (*i*) By definition of the Hermitian form $\langle\cdot,\cdot\rangle_{A,\mu}$

$$\langle Tf, g\rangle_{A,\mu} = \langle ATf, g\rangle_\mu = \langle f, T^*A^*g\rangle_\mu = \langle f, ATAA^*g\rangle_\mu$$

where the last equation is due to Lemma 3.11. Now, because A is $\langle\cdot,\cdot\rangle_\mu$-self-adjoint and also an involution, we have $ATAA^* = ATA^2 = AT$. Thus,

$$\langle Tf, g\rangle_{A,\mu} = \langle f, ATAA^* g\rangle_\mu = \langle f, ATg\rangle_\mu = \langle f, Tg\rangle_{A,\mu}.$$

(ii) Assume that $\lambda_1 \neq \overline{\lambda_2}$ and let $f \in N_{\lambda_1,p_1}\backslash N_{\lambda_1,p_1-1}$, $g \in N_{\lambda_2,p_2}\backslash N_{\lambda_2,p_2-1}$. From Proposition 2.13 we know that for any $k \in \mathbb{N}$

$$\left(T - \bar{\lambda}_2 I\right)^k \left(N_{\lambda_1,p_1}\backslash N_{\lambda_1,p_1-1}\right) \quad = \quad N_{\lambda_1,p_1}\backslash N_{\lambda_1,p_1-1}. \tag{3.3.3}$$

Therefore, we find $\tilde{f} \in N_{\lambda_1,p_1}\backslash N_{\lambda_1,p_1-1}$ such that $f = \left(T - \overline{\lambda}_2 I\right)^{p_2}\left(\tilde{f}\right)$. From part *(i)* we thus conclude that

$$\langle f, g\rangle_{A,\mu} = \left\langle \tilde{f}, (T - \lambda_2 I)^{p_2} g\right\rangle_{A,\mu} = 0.$$

□

Unfortunately, $\langle\cdot,\cdot\rangle_{A,\mu}$ is in general *not* a scalar product on $\mathcal{X}$. For example, if $S = \{0,1\}$ and $a(0) = 1$, $a(1) = 0$, and μ is any positive measure, then we have for the functions $f(0) = 1$, $f(1) = -1$ that

$$\langle f, f\rangle_{A,\mu} = Af(0) f(0) \mu(0) + Af(1) f(1) \mu(1) = -\mu(0) - \mu(1) < 0.$$

Hence, $\langle\cdot,\cdot\rangle_{A,\mu}$ is not positive definite and can therefore not induce a norm on $\mathcal{X}$. In fact, the choice of A with respect to any probability measure μ is rather arbitrary, i.e. there are many possible realizations of A for a given μ. On the other hand, we can find subspaces on which $\langle\cdot,\cdot\rangle_{A,\mu}$ is indeed positive definite. Define the subspaces

$$\mathcal{X}_\pm = \{f \in \mathcal{X} : f = \pm Af\} \tag{3.3.4}$$

and observe the following lemma which essentially shows that $\langle\cdot,\cdot\rangle_{A,\mu}$ cannot be positive definite in general, but that its restriction to $\mathcal{X}_+$ is.

Lemma 3.13. *Let μ be a probability measure on S and let A be an involution on $\mathcal{X}$ which is self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$. Then the spaces $\mathcal{X}_\pm$ satisfy:*

(i) *$\mathcal{X}_+$ and $\mathcal{X}_-$ are closed subspaces of $\mathcal{X}$ with respect to $\langle\cdot,\cdot\rangle_\mu$, we have the direct sum $\mathcal{X} = \mathcal{X}_+ \oplus \mathcal{X}_-$ and $\mathcal{X}_+ \perp_\mu \mathcal{X}_-$.*

(ii) *Let $f^\pm := P^\pm f$ be the orthogonal projection with respect to $\langle\cdot,\cdot\rangle_\mu$ on $\mathcal{X}_\pm$. Then $\langle f, f\rangle_{A,\mu} = ||f^+||_\mu^2 - ||f^-||_\mu^2$ for any $f \in \mathcal{X}$.*

(iii) *If $f \in \mathcal{X}_+$, and $f \neq 0$, then $\langle f, f\rangle_{A,\mu} > 0$.*

Proof. *(i)* A is continuous since it is self-adjoint. Hence,

$$\mathcal{X}_\pm = (I \mp A)^{-1}(0)$$

are closed. For any $f \in \mathcal{X}$, we can write

$$f(x) = \frac{1}{2}\left(f(x) + f(a(x))\right) + \frac{1}{2}\left(f(x) - f(a(x))\right).$$

In particular, we write $f = f^+ + f^-$ where $f^{\pm}(x) = \frac{1}{2}\left(f(x) \pm f(a(x))\right) \in \mathcal{X}_{\pm}$. Additionally $\mathcal{X}_+ \cap \mathcal{X}_- = \{0\}$ since the only vector that exists in both subspaces is the zero vector. That is we have $\mathcal{X} = \mathcal{X}_+ \oplus \mathcal{X}_-$. Next, let $f \in \mathcal{X}_+, g \in \mathcal{X}_-$. We need to show $< f, g >_\mu = \sum_x f(x)\overline{g(x)}\mu(x) = 0$. Since this series is absolutely convergent, the terms can be rearranged. Now let $x, y \in S$ such that $a(x) = y$.

(a) Assume $x = y$. Then necessarily $g(x) = -g(y) = -g(x) = 0$ and $f(x) = f(y)$ and $\mu(x) = \mu(y)$. Therefore $f(x)\overline{g(x)}\mu(x) = 0$.

(b) Let now $x \neq y$. Then $g(x) = -g(y)$, $f(x) = f(y)$ and $\mu(x) = \mu(y)$. Thus $f(x)\overline{g(x)}\mu(x) + f(y)\overline{g(y)}\mu(y) = 0$.

Therefore, $< f, g >_\mu = 0$.

(ii) From part (i) we can write f as $f = f^+ + f^-$ where $f^{\pm} \in \mathcal{X}_{\pm}$. Then

$$\begin{aligned}
\langle f, f\rangle_{A,\mu} &= \left\langle f^+ + f^-, f^+ + f^-\right\rangle_{A,\mu} \\
&= \left\langle A\left(f^+ + f^-\right), f^+ + f^-\right\rangle_{\mu} \\
&= \left\langle f^+ - f^-, f^+ + f^-\right\rangle_{\mu} \\
&= \left\langle f^+, f^+\right\rangle - \left\langle f^-, f^-\right\rangle_{\mu} \\
&= ||f^+||_\mu^2 - ||f^-||_\mu^2.
\end{aligned}$$

where we use the orthogonality of $\mathcal{X}_+$ and $\mathcal{X}_-$ in the fourth equation.

(iii) It follows from part (ii) that $\langle f, f\rangle_{A,\mu} = ||f^+||_\mu^2 - ||f^-||_\mu^2 = ||f||_\mu^2 - 0 > 0$. □

We will see later that this lemma is of high importance for our main results which focus on the eigenspaces of T for eigenvalues close to 1. In fact, we will consider in Subsection 3.4.1 operators where these eigenvectors *almost* lie in $\mathcal{X}_+$.

3.3.2 Weak reversibility in the $\mathcal{E}_{\lambda(0)}(0)$-eigenspace

Generalizing the concept of reversibility of the Markov processes $X^{(\varepsilon)}$ is related to dropping the assumption that the transfer operators T_ε's are self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$. The extended detailed balance from the previous section is based on an involution A and the associated Hermitian form such that T_ε are "almost" self-adjoint with respect to this Hermitian form. In fact, as we will see in Section 3.4.1, under weak conditions on A the operator T_0 is actually self-adjoint in $(\mathcal{E}_{\lambda(0)}(0), \langle\cdot,\cdot\rangle_{\mu_0})$ which is the crucial property we need, for instance,

to show that the dominant eigenvalues are real. Here, $\mathcal{E}_{\lambda(0)}(0) = E_{\lambda(0)}(0)$ is the total eigenspace of the $\lambda(0)$-group at $\varepsilon = 0$. It is therefore reasonable, instead of using the involution A, to consider smaller spaces where T_ε behaves like a self-adjoint operator. For our purposes, it turns out to be sufficient to consider $(\mathcal{E}_{\lambda(0)}(0), \langle\cdot,\cdot\rangle_{\mu_\varepsilon})$. This leads to

Definition 3.14. Let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be the full partition of the uncoupled Markov chain $X^{(0)}$ and let $\chi_1, \ldots, \chi_m$ be the corresponding indicator functions of the sets $S_1, \ldots, S_m$. Then T_ε satisfies the *weak reversibility condition in* $\mathcal{E}_{\lambda(0)}(0)$, if for all $k, l = 1, \ldots, m$,

$$\langle \chi_k, T_\varepsilon \chi_l \rangle_{\mu_\varepsilon} \quad = \quad \langle T_\varepsilon \chi_k, \chi_l \rangle_{\mu_\varepsilon} . \tag{3.3.5}$$

From Lemma 3.6 we know that the functions $\chi_1, \ldots, \chi_m$ span $\mathcal{E}_{\lambda(0)}(0)$. The condition (3.3.5) does not imply self-adjointness of T_ε in $(\mathcal{E}_{\lambda(0)}(0), \langle\cdot,\cdot\rangle_{\mu_\varepsilon})$ due to the possible lack of invariance of the subspace $\mathcal{E}_{\lambda(0)}(0)$ under T_ε.

Remark 3.15. We could more generally define weak reversibility such that T_ε satisfies for all $k, l = 1, \ldots, m$

$$\langle \chi_k, T_\varepsilon \chi_l \rangle_{\mu_\varepsilon} = \langle T_\varepsilon \chi_k, \chi_l \rangle_{\mu_\varepsilon} + o(\varepsilon) . \tag{3.3.6}$$

This condition clearly implies (3.3.5), but is much more general. In fact, it is *always* satisfied, if the eigenvalues in the $\lambda(0)$-group of T_ε and the corresponding eigenvectors satisfy $\lambda_k(\varepsilon) = 1 + o(\varepsilon)$, $f_k(\varepsilon) = \chi_k + o(\varepsilon)$ for all $k = 1, \ldots, m$ and for ε small enough. This is, for instance, the case if the $\lambda_k(\varepsilon)$ and $f_k(\varepsilon)$ are holomorphic in $\varepsilon = 0$ such that the first order terms vanish. Indeed, in that case

$$\begin{aligned}
\langle f_k(\varepsilon), f_l(\varepsilon) \rangle_{\mu(\varepsilon)} &= \lambda_l(\varepsilon) \langle f_k(\varepsilon), f_l(\varepsilon) \rangle_{\mu(\varepsilon)} + o(\varepsilon) \\
&= \langle f_k(\varepsilon), T_\varepsilon f_l(\varepsilon) \rangle_{\mu(\varepsilon)} + o(\varepsilon) = \langle \chi_k, T_\varepsilon \chi_l \rangle_{\mu(\varepsilon)} + o(\varepsilon) \\
\langle f_k(\varepsilon), f_l(\varepsilon) \rangle_{\mu(\varepsilon)} &= \lambda_k(\varepsilon) \langle f_k(\varepsilon), f_l(\varepsilon) \rangle_{\mu(\varepsilon)} + o(\varepsilon) \\
&= \langle T_\varepsilon f_k(\varepsilon), f_l(\varepsilon) \rangle_{\mu(\varepsilon)} + o(\varepsilon) = \langle T_\varepsilon \chi_k, \chi_l \rangle_{\mu(\varepsilon)} + o(\varepsilon) .
\end{aligned}$$

This implies (3.3.6). Since both (3.3.5) and (3.3.6) are in practice difficult to check, we use in the following the former condition for simplicity. Observe that (3.3.6) is indeed always satisfied, if we replace $o(\varepsilon)$ by $O(\varepsilon)$, as long as the eigenvalues and eigenvectors are holomorphic, which is therefore not very useful for us.

An important question at this point is, of course, which T_ε satisfies the weak reversibility condition. Before we study this question and also the consequences of weak reversibility for the spectrum of T_ε, we give here a very simple situation for which (3.3.5) is always satisfied.

Proposition 3.16. *If $m = 2$, then the weak reversibility condition in $\mathcal{E}_{\lambda(0)}(0)$ is satisfied for all $\varepsilon \geq 0$.*

Proof. In this case $\mathcal{E}_{\lambda(0)}(0)$ is spanned by exactly two indicator functions χ_1

and χ_2. Observe that the function $\mathbf{1}$, i.e. $\mathbf{1}(x) = 1$ for all $x \in S$, is always an eigenfunction of T_ε for the eigenvalue 1, since the corresponding transition matrix P_ε is a stochastic matrix. The same is true for the adjoint T_ε^*, as we see from Proposition 2.8. Hence,

$$\begin{aligned}\langle T_\varepsilon \chi_1, \chi_2\rangle_{\mu_\varepsilon} &= \langle T_\varepsilon\left(\mathbf{1}-\chi_2\right), \left(\mathbf{1}-\chi_1\right)\rangle_{\mu_\varepsilon} \\ &= \langle T_\varepsilon \mathbf{1}, \mathbf{1}\rangle_{\mu_\varepsilon} - \langle T_\varepsilon \mathbf{1}, \chi_1\rangle_{\mu_\varepsilon} - \langle T_\varepsilon \chi_2, \mathbf{1}\rangle_{\mu_\varepsilon} + \langle T_\varepsilon \chi_2, \chi_1\rangle_{\mu_\varepsilon} \\ &= 1 - \langle \mathbf{1}, \chi_1\rangle_{\mu_\varepsilon} - \langle \chi_2, \mathbf{1}\rangle_{\mu_\varepsilon} + \langle T_\varepsilon \chi_2, \chi_1\rangle_{\mu_\varepsilon} = \langle T_\varepsilon \chi_2, \chi_1\rangle_{\mu_\varepsilon}\,.\end{aligned}$$

□

As indicated in the beginning of this subsection, weak reversibility in the $\mathcal{E}_{\lambda(0)}(0)$-eigenspace is more general than the extended detailed balance condition which we show next. For this we have to focus on partitions which are "compatible" with the involution A in the following sense:

Definition 3.17. Let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be a full partition of S with associated indicator functions $\chi_1, \ldots, \chi_m$. Then the partition is called *A-invariant*, if $A\chi_i = \chi_i$ for all $i = 1, \ldots, m$.

Since an involution has only eigenvalues 1 and -1, this property is equivalent to asking for the indicator functions to be eigenvectors belonging to the eigenvalue 1 of A. In terms of the involution $a : S \to S$, A-invariance of a partition means that a state $x \in S_i$ is mapped by a to the same set. This allows us to show the following proposition.

Proposition 3.18. *Let $X^{(0)}$ be an uncoupled Markov chain with the associated full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ such that the indicators χ_i's of the sets S_i's span $\mathcal{E}_{\lambda(0)}(0)$. Assume that T_ε satisfies extended detailed balance with respect to an involution A and invariant measure μ_ε, and that $\mathfrak{S}$ is A-invariant. Then T_ε also satisfies the weak reversibility condition in $\mathcal{E}_{\lambda(0)}(0)$.*

Proof. From $A\chi_i = \chi_i$ for all $i = 1, \ldots, m$ and Lemma 3.12 it follows

$$\begin{aligned}\langle \chi_k, T_\varepsilon \chi_l\rangle_{\mu_\varepsilon} &= \langle \chi_k, T_\varepsilon \chi_l\rangle_{A,\mu_\varepsilon} = \langle T_\varepsilon^* \chi_k, \chi_l\rangle_{A,\mu_\varepsilon} \\ &= \langle A T_\varepsilon A \chi_k, \chi_l\rangle_{A,\mu_\varepsilon} = \langle T_\varepsilon \chi_k, \chi_l\rangle_{\mu_\varepsilon}\,.\end{aligned}$$

□

3.4 Generalized reversibility and spectral properties of the transfer operator

In this section we will apply the two concepts of generalized reversibility from above to derive interesting spectral properties of the transfer operators T_ε. We

are in the setting of Section 3.2.2, i.e. we consider a Markov chain $X^{(\varepsilon)} = (X_n^{(\varepsilon)})_{n\in\mathbb{N}_0}$ satisfying Assumptions 3.3, 3.4, and 3.7.

3.4.1 Consequences of extended detailed balance

In Section 3.3.1 we introduced the Hermitian form $\langle\cdot,\cdot\rangle_{A,\mu}$ and showed that a transfer operator T, which satisfies the extended detailed balance condition, behaves very similar to a self-adjoint operator. We have also shown that the Hermitian form is not a scalar product in general such that the operator T cannot be truly self-adjoint. In this subsection we assume that all transfer operators T_ε (or at least for small ε) satisfy the extended detailed balance condition. Since T_0 corresponds to an uncoupled Markov chain, we will show that the Hermitian form $\langle\cdot,\cdot\rangle_{A,\mu_\varepsilon}$ becomes a scalar product, at least on the total eigenspace $\mathcal{E}_{\lambda(0)}(\varepsilon)$ corresponding to the $\lambda(0)$-group. Consequently, many interesting properties of T_ε can be explained through this perturbation approach. We first show the main result in this subsection. The key to this result is to assume that a full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ of S exists and is A-invariant (see Definition 3.17).

Theorem 3.19. *Let $X^{(\varepsilon)}$ be a Markov chain satisfying Assumptions 3.3, 3.4, and 3.7. Let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be the full partition of the uncoupled Markov chain $X^{(0)}$ and assume that the transfer operators T_ε satisfy extended detailed balance with respect to an involution A and invariant measures μ_ε. If $\mathfrak{S}$ is A-invariant, then $\langle\cdot,\cdot\rangle_{A,\mu_\varepsilon}$ is a scalar product on $\mathcal{E}_{\lambda(0)}(\varepsilon)$ for sufficiently small $\varepsilon \geq 0$.*

Proof. Let $f_i(\varepsilon)$, $i = 1, \ldots, m$ be the generalized eigenvectors from Section 3.2.2 which span $\mathcal{E}_{\lambda(0)}(\varepsilon)$. The key idea is to apply the Gram-Schmidt procedure to find vectors $\tilde{f}_i(\varepsilon)$ which are pairwise "orthogonal" with respect to the Hermitian form $\langle\cdot,\cdot\rangle_{A,\mu_\varepsilon}$. This will turn out to be enough for our purposes. We proof the theorem in a number of different steps.

1. We first show that for ε small enough we have $\langle f_i(\varepsilon), f_i(\varepsilon)\rangle_{A,\mu_\varepsilon} > 0$ for all $i = 1, \ldots, m$. By Lemma 3.6 there exist $\alpha_{k,i} \in \mathbb{C}\backslash\{0\}$, $k = 1, \ldots, m$ such that

$$f_i(0) = \sum_{k=1}^{m} \alpha_{k,i}\chi_k.$$

As $\mathfrak{S}$ is A-invariant, we have $A\chi_k = \chi_k$ for all $k = 1, \ldots, m$ and, thus, by Lemma 3.13, $\chi_k \in \mathcal{X}_+$. Consequently, $f_i(0) \in \mathcal{X}_+$ for all i and hence $\langle f_i(0), f_i(0)\rangle_{A,\mu(0)} > 0$, by Lemma 3.13. Using Lemma 3.13 shows

$$\langle f_i(\varepsilon), f_i(\varepsilon)\rangle_{A,\mu_\varepsilon} = ||f_i^+(\varepsilon)||^2_{\mu_\varepsilon} - ||f_i^-(\varepsilon)||^2_{\mu_\varepsilon}. \tag{3.4.1}$$

By Theorem 2.21, the $f_i(\varepsilon)$ are continuous in ε and by Lemma 3.8 the invariant measure μ_ε is as well. We can therefore conclude by continuity that the right

hand side in (3.4.1) converges to

$$\|f_i^+(0)\|_{\mu_0} - \|f_i^-(0)\|_{\mu_0} = \|f_i(0)\|_{\mu_0} > 0,$$

where we use $f_i(0) \in \mathcal{X}_+$. Hence, we can find ε small enough such that (3.4.1) is positive for all $i = 1, \ldots, m$.

2. We next "orthogonalize" the $f_i(\varepsilon)$'s. Define inductively

$$\tilde{f}_i(\varepsilon) = f_i(\varepsilon) - \sum_{j=2}^{i} \frac{\left\langle f_i(\varepsilon), \tilde{f}_{j-1}(\varepsilon) \right\rangle_{A,\mu_\varepsilon}}{\left\langle \tilde{f}_{j-1}(\varepsilon), \tilde{f}_{j-1}(\varepsilon) \right\rangle_{A,\mu_\varepsilon}} \tilde{f}_{j-1}(\varepsilon).$$

This is clearly well-defined for $i = 1$ and $i = 2$ by the first step. Moreover,

$$\begin{aligned}
\left\langle \tilde{f}_1(\varepsilon), \tilde{f}_2(\varepsilon) \right\rangle_{A,\mu_\varepsilon} &= \left\langle f_1(\varepsilon), \tilde{f}_2(\varepsilon) \right\rangle_{A,\mu_\varepsilon} \\
&= \langle f_1(\varepsilon), f_1(\varepsilon) \rangle_{A,\mu_\varepsilon} \\
&\quad - \frac{\overline{\langle f_1(\varepsilon), f_1(\varepsilon) \rangle_{A,\mu_\varepsilon}}}{\langle f_1(\varepsilon), f_1(\varepsilon) \rangle_{A,\mu_\varepsilon}} \langle f_1(\varepsilon), f_1(\varepsilon) \rangle_{A,\mu_\varepsilon} \\
&= 0.
\end{aligned}$$

Let now $i \in \{3, \ldots, m\}$ be arbitrary and assume that for ε small enough, $\tilde{f}_j(\varepsilon)$'s have been chosen such that $\left\langle \tilde{f}_j(\varepsilon), \tilde{f}_j(\varepsilon) \right\rangle_{A,\mu_\varepsilon} > 0$ for all $1 \leq j < i$ and $\left\langle \tilde{f}_j(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} = 0$ for all $1 \leq j < k < i$. This, in particular, means that $\tilde{f}_i(\varepsilon)$ is well-defined as well. Moreover, for any $1 \leq k < i$

$$\begin{aligned}
\left\langle \tilde{f}_i(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} &= \left\langle f_i(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} \\
&\quad - \sum_{j=2}^{i} \frac{\left\langle f_i(\varepsilon), \tilde{f}_{j-1}(\varepsilon) \right\rangle_{A,\mu_\varepsilon}}{\left\langle \tilde{f}_{j-1}(\varepsilon), \tilde{f}_{j-1}(\varepsilon) \right\rangle_{A,\mu_\varepsilon}} \left\langle \tilde{f}_{j-1}(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} \\
&= \left\langle f_i(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} \\
&\quad - \frac{\left\langle f_i(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon}}{\left\langle \tilde{f}_k(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon}} \left\langle \tilde{f}_k(\varepsilon), \tilde{f}_k(\varepsilon) \right\rangle_{A,\mu_\varepsilon} \\
&= 0,
\end{aligned}$$

i.e. $\tilde{f}_i(\varepsilon)$ is "orthogonal" to all previously defined $\tilde{f}_k(\varepsilon)$'s. Observe that $\tilde{f}_k(\varepsilon)$'s are still continuous in ε. For $\varepsilon = 0$, we can argue as in step 1 that $\tilde{f}_i(0) \in \mathcal{X}_+$ such that $\left\langle \tilde{f}_i(0), \tilde{f}_i(0) \right\rangle_{A,\mu_0} > 0$. By continuity we thus have $\left\langle \tilde{f}_i(\varepsilon), \tilde{f}_i(\varepsilon) \right\rangle_{A,\mu_\varepsilon} > 0$ for ε small enough. This proves that we can find $\tilde{f}_i(\varepsilon) \in \mathcal{X}$ for ε small enough such that $\left\langle \tilde{f}_i(\varepsilon), \tilde{f}_i(\varepsilon) \right\rangle_{A,\mu_\varepsilon} > 0$ for all $i = 1, \ldots, m$ and $\left\langle \tilde{f}_i(\varepsilon), \tilde{f}_j(\varepsilon) \right\rangle_{A,\mu_\varepsilon} = 0$

for all $1 \leq j < i \leq m$.

3. We finally prove the claim. Since $\tilde{f}_j(\varepsilon)$'s from step 2 span $\mathcal{E}_{\lambda(0)}(\varepsilon)$, any vector $0 \neq u(\varepsilon) \in \mathcal{E}_{\lambda(0)}(\varepsilon)$ can thus be written as a linear combination of $\tilde{f}_i(\varepsilon)$'s, i.e.

$$u(\varepsilon) = \sum_{i=1}^{m} \beta_i(\varepsilon)\, \tilde{f}_i(\varepsilon)$$

for some $\beta_i(\varepsilon) \in \mathbb{C}$. Since $\langle \cdot, \cdot \rangle_{A,\mu_\varepsilon}$ is a Hermitian form, we have

$$\langle u(\varepsilon), u(\varepsilon) \rangle_{A,\mu_\varepsilon} = \sum_{i,j} \beta_i(\varepsilon)\, \overline{\beta_j}(\varepsilon) \left\langle \tilde{f}_i(\varepsilon), \tilde{f}_j(\varepsilon) \right\rangle_{A,\mu_\varepsilon}.$$

For ε small enough as in the previous step we conclude that

$$\langle u(\varepsilon), u(\varepsilon) \rangle_{A,\mu_\varepsilon} = \sum_{i=1}^{m} |\beta_i(\varepsilon)|^2 \left\langle \tilde{f}_i(\varepsilon), \tilde{f}_i(\varepsilon) \right\rangle_{A,\mu_\varepsilon} > 0.$$

As u is arbitrary, this proves the claim. □

The assumption that the full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$ is A-invariant is necessary for the statement. In fact, if this is not satisfied, then it can happen that $\langle f_i(0), f_i(0) \rangle_{A,\mu_0} \leq 0$, which of course implies that $\langle \cdot, \cdot \rangle_{A,\mu_\varepsilon}$ cannot be a scalar product on $\mathcal{E}_{\lambda(0)}(\varepsilon)$. This is illustrated in the following simple example.

Example 3.20. Consider the transition matrix

$$P_0 = \begin{pmatrix} 0.3 & 0.5 & 0.2 & 0 & 0 & 0 \\ 0.4 & 0.2 & 0.4 & 0 & 0 & 0 \\ 0.3 & 0.3 & 0.4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.3 & 0.4 & 0.3 \\ 0 & 0 & 0 & 0.5 & 0.2 & 0.3 \\ 0 & 0 & 0 & 0.2 & 0.4 & 0.4 \end{pmatrix}$$

with invariant measure $\mu_0 = \begin{pmatrix} \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \end{pmatrix}^\top$. The associated transfer operator T_0 satisfies extended balance with the involution

$$A = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

Then $f(0) = \begin{pmatrix} -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix}^\top$ is an eigenvector T_0 corresponding to the eigenvalue 1, but $\langle f(0), f(0) \rangle_{A,\mu_0} = -1$.

In physical applications, the A-invariance condition is, for example, satisfied in

the Langevin dynamics (see Chapter 1).

Theorem 3.19 has interesting consequences for the spectrum of T_ε for small $\varepsilon \geq 0$.

Corollary 3.21. *In the situation of the previous theorem we have for small $\varepsilon > 0$:*

(i) The $\lambda(0)$-group eigenvalues $\lambda_i(\varepsilon), i = 1, \ldots, m$, of T_ε are real-valued.

(ii) There exists an orthonormal basis of $(\mathcal{E}_{\lambda(0)}(\varepsilon), \langle \cdot, \cdot \rangle_{A,\mu_\varepsilon})$ consisting of eigenvectors of T_ε.

Proof. The previous Theorem 3.19 and Lemma 3.12 imply that T_ε is self-adjoint in $(\mathcal{E}_{\lambda(0)}(\varepsilon), \langle \cdot, \cdot \rangle_{A,\mu_\varepsilon})$. This shows both claims. In fact, in the proof of Theorem 3.19 we constructed an orthogonal basis of $(\mathcal{E}_{\lambda(0)}(\varepsilon), \langle \cdot, \cdot \rangle_{A,\mu_\varepsilon})$ explicitly, which can then be normalized. □

Remark 3.22. In the proof of Theorem 3.19 we started with a basis of generalized eigenvectors of $\mathcal{E}_{\lambda(0)}(\varepsilon)$. In Corollary 3.21 it turns out that all the vectors, for small ε, are actually already eigenvectors.

3.4.1.1 Dominant eigenvalues versus $\lambda(0)$-group eigenvalues

The statement of Theorem 3.19 is rather qualitative, since it only proves the existence of a small $\varepsilon > 0$ for which T_ε is actually self-adjoint with respect to the Hermitian form $\langle \cdot, \cdot \rangle_{A,\mu_\varepsilon}$. An interesting question is of course how small ε has to be in practice. A major problem when applying this theorem is to decide which eigenvalues belong to the $\lambda(0)$-group of T_ε. For small enough ε the eigenvalues of T_ε will concentrate around the eigenvalues of T_0. However, for a given transfer operator it is not clear if the *dominant* eigenvalues, i.e. the eigenvalues that cluster around 1, belong to the $\lambda(0)$-group or not. Moreover, even if we consider only a very small perturbation, the complex eigenvalues can appear as the dominant eigenvalues. This is clearly illustrated in the following example.

Example 3.23. Consider

$$T_\varepsilon = \begin{pmatrix} 0.98 & 0.01 & 0 & 0.01 & 0 \\ 0 & 0.99 & 0.01 & 0 & 0 \\ 0.02 & 0 & 0.98 & 0 & 0 \\ 0 & 0 & 0 & 0.50 & 0.50 \\ 0 & 0 & 0.01 & 0.49 & 0.50 \end{pmatrix}$$

which satisfies extended balance condition with respect to the involution

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

and the unique invariant measure $\mu_\varepsilon = \begin{pmatrix} \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{pmatrix}^T$. The eigenvalues of T_ε are

$\lambda_1(\varepsilon)$	$\lambda_2(\varepsilon)$	$\lambda_3(\varepsilon)$	$\lambda_4(\varepsilon)$	$\lambda_5(\varepsilon)$
1.0000	0.9930	$0.9760 + 0.0118\mathrm{i}$	$0.9760 - 0.0118\mathrm{i}$	0.0050

where there are four dominant eigenvalues, including the complex eigenvalues λ_3 and λ_4. To analyze this result, let us first assume T_ε is a perturbation of

$$T_0 = \begin{pmatrix} 0.99 & 0.01 & 0 & 0 & 0 \\ 0 & 0.99 & 0.01 & 0 & 0 \\ 0.01 & 0 & 0.99 & 0 & 0 \\ 0 & 0 & 0 & 0.50 & 0.50 \\ 0 & 0 & 0 & 0.50 & 0.50 \end{pmatrix}$$

with $m = 2$ blocks. Note that it holds $A\chi_i = \chi_i$, $i = 1, 2$. The eigenvalues of T_0 are $\{1, 1, 0.9850 + 0.0087\mathrm{i}, 0.9850 + 0.0087\mathrm{i}, 0.0000\}$. Hence, the $\lambda(0)$-group has two members and with sufficiently small ε, these two $\lambda(0)$-group eigenvalues are real.

Now let us assume that T_ε is instead a perturbation of

$$\widetilde{T}_0 = \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 & 0 \\ 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0 & 0.50 & 0.50 \\ 0 & 0 & 0 & 0.50 & 0.50 \end{pmatrix}$$

with $m = 4$ blocks. The eigenvalues of $\widetilde{T}_0$ are $\{1, 1, 1, 1, 0\}$ where there are four eigenvalues in the $\widetilde{\lambda}(0)$-group. One can see that even with a small ε, two of the $\widetilde{\lambda}(0)$-group eigenvalues are complex. This is due to the fact that the $\widetilde{T}_0$-invariant partition is not A-invariant.

3.4.1.2 Illustrative example

To better understand the results presented in Theorem 3.19 and Corollary 3.21, it is helpful to construct an example for illustration.

Example 3.24. Consider the matrix

$$T_0 = \begin{pmatrix} 0.7124 & 0.2876 & 0 & 0 & 0 \\ 0.2876 & 0.7124 & 0 & 0 & 0 \\ 0 & 0 & 0.0894 & 0.2539 & 0.6567 \\ 0 & 0 & 0.1379 & 0.6082 & 0.2539 \\ 0 & 0 & 0.7727 & 0.1379 & 0.0894 \end{pmatrix}$$

with $m = 2$ and the matrix

$$L = \begin{pmatrix} -0.3916 & -0.2816 & 0.1029 & 0.5221 & 0.0482 \\ -0.1416 & -0.3916 & 0.0010 & 0.2159 & 0.3163 \\ 0.3163 & 0.0482 & -0.0424 & -0.2147 & -0.1074 \\ 0.2159 & 0.5221 & -0.0609 & -0.4624 & -0.2147 \\ 0.0010 & 0.1029 & -0.0006 & -0.0609 & -0.0424 \end{pmatrix}.$$

Then $T_\varepsilon = T_0 + \varepsilon L$ is non-negative for all $0 \leq \varepsilon \leq \hat{\varepsilon} = \frac{0.2876}{0.2816}$ and thus a stochastic matrix. Note that the columns of T_ε sum to 1, that is $\mathbf{1}^T T_\varepsilon = \mathbf{1}^T$. So $\frac{1}{5}(\mathbf{1})$ is the unique invariant measure of T_ε for all $0 < \varepsilon \leq \hat{\varepsilon}$. Also, the matrices T_0 and L satisfy extended detailed balance with respect to μ_0 with

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

that preserves invariance of block decomposition of T_0. Then it follows that T_ε satisfies extended detailed balance with respect to μ_ε for all $\varepsilon > 0$.

Figure 3.4.1 shows the $\lambda(0)$-group eigenvalues $\lambda_1(\varepsilon)$ and $\lambda_2(\varepsilon)$ of T_ε for $0 \leq \varepsilon \leq \hat{\varepsilon}$. $\lambda_1(\varepsilon) = 1$ for all ε, while $\lambda_2(\varepsilon) = 1$ for $\varepsilon = 0$ and then decreases with the increasing ε until a certain point, which we will call ε_*, that it becomes a complex eigenvalue.

Let $f_2(\varepsilon)$ be an eigenvector corresponding to the eigenvalue $\lambda_2(\varepsilon)$. Then it is illustrated in Figure 3.4.2 that $\langle f_2(\varepsilon), f_2(\varepsilon)\rangle_{A,\mu_\varepsilon} > 0$ for all $\varepsilon < \varepsilon_*$. Note that the eigenvector $f_2(\varepsilon)$ can also be scaled such that $\langle f_2(\varepsilon), f_2(\varepsilon)\rangle_{A,\mu_\varepsilon} = 1$ for all $\varepsilon < \varepsilon_*$.

Furthermore, it is observed that at $\varepsilon = \varepsilon_*$, the eigenvalue $\lambda_2(\varepsilon)$ is not simple but clashes with another eigenvalue, denoted by $\beta(\varepsilon)$, of T_ε (see Figure 3.4.3). Let $g(\varepsilon)$ be a corresponding eigenvector of $\beta(\varepsilon)$, Figure 3.4.3 also illustrates the statement in Corollary 3.12 that is $\langle f_2(\varepsilon), g(\varepsilon)\rangle_{A,\mu_\varepsilon} = 0$ for $\varepsilon < \varepsilon_*$ and $\lambda_2(\varepsilon) = \overline{\beta(\varepsilon)}$ for $\varepsilon_* < \varepsilon < \hat{\varepsilon}$.

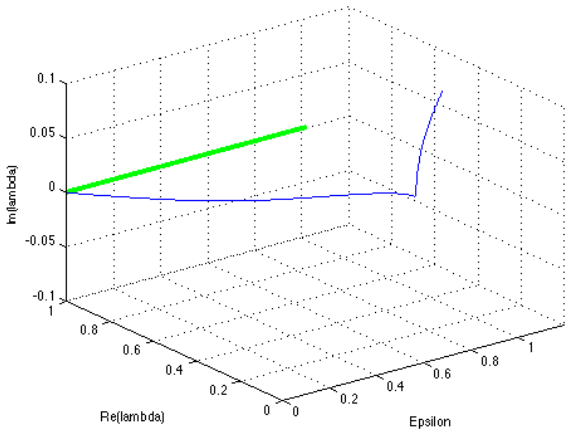

Figure 3.4.1: $\lambda(0)$-group eigenvalues. Green thick line: λ_1. Blue thin line: λ_2.

3.4.2 Consequences of weak reversibility

The next theorem extends Theorem 4.19 in Schütte and Sarich (2013). The main difference here is that we drop the assumption on T_0 being self-adjoint.

Theorem 3.25. *Let $X^{(\varepsilon)}$ be a Markov chain satisfying Assumptions 3.3, 3.4, and 3.7 with invariant measure μ_ε. If the transfer operator T_ε satisfy the weak reversibility condition in $\mathcal{E}_{\lambda(0)}(0)$, then the $\lambda(0)$-group eigenvalues of T_ε (with $\lambda(0) = 1$) are real-valued up to the first perturbation order.*

Proof. Since $\lambda(0) = 1$ is semisimple, by Theorem 2.18 the $\lambda(0)$-group eigenvalues of T_ε are of the form

$$\lambda_i(\varepsilon) \quad = \quad \lambda(0) + \lambda_i^{(1)}\varepsilon + o(\varepsilon).$$

Moreover, by Theorem 2.21

$$\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0} f_i(0) \quad = \quad \lambda_i^{(1)} f_i(0).$$

By Lemma 3.6 there exist $\alpha_{k,i} \in \mathbb{C}\backslash\{0\}$, $k = 1, \ldots, m$ such that

$$f_i(0) = \sum_{k=1}^{m} \alpha_{k,i} \chi_k$$

such that the weak reversibility assumption (3.3.5) implies, in particular, that

$$\langle f_i(0), T_\varepsilon f_j(0) \rangle_{\mu_\varepsilon} \quad = \quad \langle T_\varepsilon f_i(0), f_j(0) \rangle_{\mu_\varepsilon}.$$

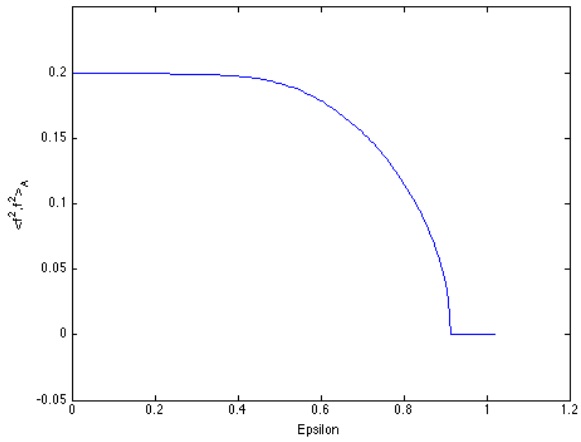

Figure 3.4.2: $\langle f_2(\varepsilon), f_2(\varepsilon)\rangle_{A,\mu_\varepsilon}$.

This can be written as

$$\begin{aligned} & \langle f_i(0), (T_0+\varepsilon L) f_j(0)\rangle_{\mu_\varepsilon} = \langle (T_0+\varepsilon L) f_i(0), f_j(0)\rangle_{\mu_\varepsilon} \\ \Leftrightarrow \quad & \varepsilon \langle f_i(0), L f_j(0)\rangle_{\mu_\varepsilon} = \varepsilon \langle L f_i(0), f_j(0)\rangle_{\mu_\varepsilon}. \end{aligned}$$

By the continuity of μ_ε (Lemma 3.8) for $\varepsilon \to 0$

$$\langle f_i(0), L f_j(0)\rangle_{\mu_0} = \langle L f_i(0), f_j(0)\rangle_{\mu_0}$$

from which we conclude that

$$\left\langle f_i(0), \Pi_{\lambda(0),0} L \Pi_{\lambda(0),0} f_j(0)\right\rangle_{\mu_0} = \left\langle \Pi_{\lambda(0),0} L \Pi_{\lambda(0),0} f_i(0), f_j(0)\right\rangle_{\mu_0}.$$

Therefore $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$ is self-adjoint in $(\mathcal{E}_{\lambda(0)}(0), \langle\cdot,\cdot\rangle_{\mu_0})$ and thus the eigenvalues $\lambda_1^{(1)}, \ldots, \lambda_m^{(1)}$ of $\Pi_{\lambda(0),0} L \Pi_{\lambda(0),0}$ are real-valued. This proves the theorem. □

All in all, we have seen in Section 3.3.2 that the weak reversibility in $\mathcal{E}_{\lambda(0)}(0)$ condition results in the λ_0-group eigenvalues being real-valued up to the first perturbation order. The extended detailed balance, on the other hand, yields a better yet result of real holomorphic $\lambda(0)$-group eigenvalues and eigenvectors of T_ε, as well as the orthogonality of the eigenvectors.

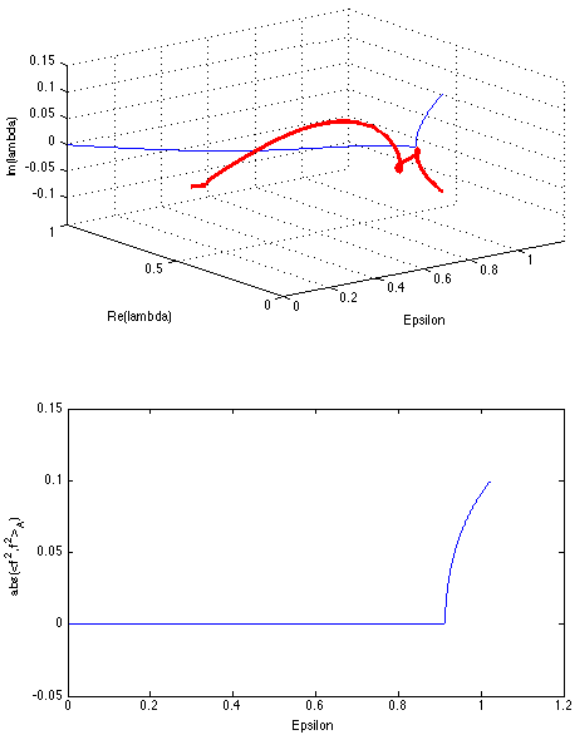

Figure 3.4.3: Top: Clash of eigenvalues. Red thick line: β. Blue thin line: λ_2. Bottom: $\left|\langle f_2(\varepsilon), g(\varepsilon)\rangle_{A,\mu_\varepsilon}\right|$.

Chapter 4

Metastability of EDB systems

In this chapter we study a Markov chain whose dynamics exhibits metastability. The main goal is to develop an algorithm to characterize *metastable* or *almost invariant* sets of the underlying Markov chain. A fair amount of research has been done to find metastable sets using various methods, ranging from the spectral approach of Dellnitz and Junge (2004); Deuflhard et al. (2000); Deuflhard and Weber (2005); Huisinga and Schmidt (2006) to the exit time approach of Bovier et al. (2000, 2002). However, all these works were done based on the assumption that the Markov process being considered is reversible. This motivates us to approach the same problem in a more general setting, namely with the extended detailed balance condition. Here, we hope to extend the idea of Deuflhard et al. (2000), where metastable sets are computed from the dominant eigenvalues and eigenvectors which are known to be real-valued due to the reversibility assumption. As shown in the previous chapter that a Markov chain with the extended detailed balance condition can actually have real dominant eigenvalues, the question then arises whether the same method can be applied to find metastable sets in this case. The extension is by no means trivial and requires special attention to mathematical technicalities, as we are now dealing with a transfer operator which is not necessarily self-adjoint.

We continue the study of the spectrum of T_ε from the previous chapter. We begin with the definition of metastability in Section 4.1, then present an algorithm to identify metastable sets including the mathematical justification in Section 4.2. In Section 4.3 we present some related work for non-reversible processes. At last, Section 4.4 contains numerical examples to illustrate the proposed algorithm.

4.1 Characterization of metastability

The concept of metastability is very intuitive in physics. Loosely speaking, we say that a system of particles is metastable if the system spends a long time is some configuration and jumps only rarely between different configurations. In the literature, there are many possible definitions of metastability which depend strongly on the underlying application (see, for example, Beltrán and Landim (2011); Bovier et al. (2001); Davies (1982); Huisinga et al. (2004); Schütte et al. (2001); Singleton (1984)). Our goal in this thesis is to study metastability with respect to a discrete time Markov chain $X = (X_n)_{n\in\mathbb{N}_0}$ on a finite state space S. In this case, we could analyze metastability pathwise in the sense that a set $B \subset S$ is metastable, if the time a given path spends in B is large compared to other sets. However, instead of this we give an analysis of the average case by characterizing metastability through the probability law $\mathbb{P} \circ X^{-1}$ of the process. For this, denote by P the related transition probability function and μ an invariant measure of X and define for two sets $B, C \subset S$ with $\mu(B), \mu(C) > 0$

$$P_\mu(B,C) \quad = \quad \frac{\sum_{x\in B, y\in C} P(x,y)\mu(x)}{\sum_{x\in B}\mu(x)}. \tag{4.1.1}$$

If μ is the initial distribution of X, i.e. $\mu(x) = \mathbb{P}_\mu(X_0 = x)$, $x \in S$, then this implies

$$P_\mu(B,C) = \frac{\mathbb{P}_\mu(X_0 \in B, X_1 \in C)}{\mathbb{P}_\mu(X_0 \in B)} = \mathbb{P}_\mu(X_1 \in C | X_0 \in B),$$

i.e. $P_\mu(B,C)$ is the probability to move from set B to set C in one step with initial distribution μ. In particular, $\mathbb{P}_\mu(B,B)$ is the probability to stay in B after starting in B. If this probability is large, then we think of B as metastable. This leads to following definition.

Definition 4.1. Consider $B \subset S$. We call B an *invariant* set with respect to P_μ, if

$$P_\mu(B,B) \quad = \quad 1. \tag{4.1.2}$$

and we say that B is *almost invariant* or *metastable,* if

$$P_\mu(B,B) \quad \approx \quad 1. \tag{4.1.3}$$

Moreover, let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be a full partition of S. If all S_i, $i = 1, \ldots, m$ are invariant, then we call the full partition $\mathfrak{S}$ *invariant*, and if all S_i are metastable, then we call $\mathfrak{S}$ *metastable*.

Our goal is to find metastable full partitions, as opposed to the core set approach as seen for example in Sarich (2011). Obviously, any such partition is not unique, since, for instance, the unions of invariant or metastable sets are still invariant or metastable. Furthermore, (4.1.3) does not provide a precise criterion for us

to determine whether some partition is more metastable than some others. In order to quantify the metastability of a full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$, we can use, for instance, the *metastability index*

$$M_\mu(\mathfrak{S}) \quad = \quad P_\mu(S_1, S_1) + \cdots + P_\mu(S_m, S_m).$$

As $0 \leq P_\mu(S_i, S_i) \leq 1$, the metastability index is a number between 0 and m. The closer it is to m, the more metastable the partition $\mathfrak{S}$ is. The metastability index is, of course, still a rather simple measure of metastability. It is nevertheless a powerful measure and has been widely used in algorithms in the literature (see Deuflhard et al. (2000); Deuflhard and Weber (2005)).

Another nice property of the metastability index is that we can express it with respect to the transfer operator T of X. To do so, denote by χ_i, $i = 1, \ldots, m$ the indicator functions with respect to a full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$. Then we obtain from the definition of the transfer operator T in (2.2.1) that

$$\begin{aligned} \sum_{x \in S_i, y \in S_j} P(x,y)\mu(x) &= \sum_{x,y \in S} P(x,y)\,\chi_i(x)\,\chi_j(y)\,\mu(x) \\ &= \sum_{y \in S} T\chi_i(y)\,\chi_j(y)\,\mu(y) \\ &= \langle T\chi_i, \chi_j \rangle_\mu . \end{aligned}$$

Similarly, the normalization is

$$\sum_{x \in S_i} \mu(x) = \sum_{x \in S} \chi_i(x)\,\chi_i(x)\,\mu(x) = \langle \chi_i, \chi_i \rangle_\mu = \|\chi_i\|_\mu^2.$$

Therefore, (4.1.1) can be written as

$$P_\mu(S_i, S_j) = \frac{\langle T\chi_i, \chi_j \rangle_\mu}{\|\chi_i\|_\mu^2} \tag{4.1.4}$$

and the metastability index is

$$M_\mu(\mathfrak{S}) \quad = \quad \frac{\langle T\chi_1, \chi_1 \rangle_\mu}{\|\chi_1\|_\mu^2} + \cdots + \frac{\langle T\chi_m, \chi_m \rangle_\mu}{\|\chi_m\|_\mu^2}.$$

We therefore expressed the metastability index in terms of the actions of the transfer operator.

4.2 Identification of metastable sets

The main goal in this section is to develop an algorithm to find metastable sets. The method involves computing the metastable decomposition from the sign structure of the dominant eigenvectors of T. This identification procedure was first introduced by Deuflhard et al. (2000), where the process under considera-

tion is reversible. Here we want to extend the method so that it can be used with a Markov chain that satisfies extended detailed balance.

Analogous to the previous chapter, we will once again rely on perturbation analysis. The key idea is to view a process that exhibits metastability as the perturbation of an uncoupled Markov chain. In Subsection 4.2.1 we consider first the case of an uncoupled Markov chain and how an invariant partition can be characterized solely based on the eigenvectors of the transfer operator. In Subsection 4.2.2 we try to do the same in case of a nearly uncoupled Markov chain with perturbed transfer operator and perturbed eigenvectors. In Subsection 4.2.3 we will argue that for practical purposes it is actually better to consider a slightly changed transfer operator which is then used in Subsection 4.2.4 to formulate an algorithm for finding a metastable partition. Finally, in Subsection 4.2.5 we prove a lower bound of the metastability index which confirms theoretically that the so-obtained partition compares well to other possible partitions.

4.2.1 Metastability of an uncoupled Markov chain

Consider first an uncoupled Markov chain $X^{(0)}$ with invariant measure μ_0 satisfying Assumptions 3.3 and 3.4. Moreover, assume that the transfer operator T_0 of $X^{(0)}$ satisfies extended detailed balance with respect to an involution A and μ_0. Since $X^{(0)}$ is uncoupled, there exists a full partition $\mathfrak{S}^{(0)} = \{S_1, \ldots, S_m\}$. According to Lemma 3.6 the indicator functions $\chi_1, \ldots, \chi_m$ corresponding to the partition $\mathfrak{S}^{(0)}$ are eigenvectors of T_0 for the eigenvalue $\lambda = 1$ such that

$$P_{\mu_0}(S_i, S_i) = \frac{\langle T_0\chi_i, \chi_i\rangle_{\mu_0}}{\|\chi_i\|^2_{\mu_0}} = \frac{\langle \chi_i, \chi_i\rangle_{\mu_0}}{\|\chi_i\|^2_{\mu_0}} = 1 \tag{4.2.1}$$

for all $i = 1, \ldots, m$. In particular, in this case

$$m = M_{\mu_0}(\mathfrak{S}^{(0)}) = \sup_{\mathfrak{D}} M_{\mu_0}(\mathfrak{D})$$

is maximal when maximizing over all possible full partitions, as long as we keep m, the number of blocks, fixed. An important question is now the following: Given T_0, is it possible to characterize $\mathfrak{S}^{(0)}$ among all possible full partitions based solely on spectral properties of T_0? The key idea is to link the structure of the sets S_i via the indicator functions χ_i to the eigenvectors f of T_0 belonging to the eigenvalue 1. According to Lemma 3.6, any such eigenvector f is a linear combination of the χ_i's, i.e. there are $\alpha_i \in \mathbb{C}$ such that

$$f \;=\; \sum_{i=1}^{m} \alpha_i \chi_i.$$

Hence, any such eigenvector is constant on each invariant subset S_i. Based on this observation, we can assign a *sign structure* to every state in S as follows.

Definition 4.2. Let $F_0 = \{f_1, \ldots, f_m\}$ be a set of $\langle \cdot, \cdot \rangle_{\mu_0}$-orthonormal eigenvectors of T_0 corresponding to the eigenvalue 1. Then the sign structure of $x \in S$ with respect to F_0 is given by

$$\operatorname{sign}_{F_0}(x) \quad := \quad (\operatorname{sgn}(f_1(x)), \operatorname{sgn}(f_2(x)), \ldots, \operatorname{sgn}(f_m(x))) \in \{-1, 0, 1\}^m,$$

where

$$\operatorname{sgn}(y) \quad = \quad \begin{cases} - & \text{if } y < 0, \\ 0 & \text{if } y = 0, \\ + & \text{if } y > 0. \end{cases}$$

The sign structure is a class property of the states $x \in S$ which is shown in the next theorem.

Theorem 4.3 (Deuflhard et al. (2000))**.** *Let $x \in S_i, y \in S_j$. Then $\operatorname{sign}_{F_0}(x) = \operatorname{sign}_{F_0}(y)$ if and only if $i = j$.*

Proof. " $\Leftarrow$ " This is clear, since the f_k are constant on each invariant subset, i.e. $f_k(x) = f_k(y)$ for $k = 1, \ldots, m$. Hence, x and y have the same sign structure.

" $\Rightarrow$ " We prove the statement by contradiction. From the first part follows that all states in the same set S_i have the same sign structure. We can assume without loss of generality every invariant set has only one state. Denote by $\mathcal{D}$ the diagonal matrix with diagonal entries $\mathcal{D}_{ii} = \mu_0(x_i)$, i.e.

$$\mathcal{D} \quad = \quad \begin{pmatrix} \mu_0(x_1) & & & \\ & \mu_0(x_2) & & \\ & & \cdots & \\ & & & \mu_0(x_m) \end{pmatrix}$$

and denote by F the matrix with the vectors $f_k \in F_0$ as columns. Then $\mathcal{D}^{1/2}F$ is an orthogonal matrix. As a result, rows of $\mathcal{D}^{1/2}F$ form an orthonormal basis. This implies that no rows of $\mathcal{D}^{1/2}F$ have the same sign structure, since the scalar product between two rows would then be positive which cannot be true as different rows are orthogonal to one another. Since the sign structure of F is the same as of $\mathcal{D}^{1/2}F$, no rows of F have the same sign structure. Hence, if $x \neq y$, then $\operatorname{sign}(x) \neq \operatorname{sign}(y)$. □

This suggests that we characterize the invariant partition $\mathfrak{S}^{(0)}$ using the transfer operator T_0. Given any set F_0 of $\langle \cdot, \cdot \rangle_{\mu_0}$-orthonormal eigenvectors of T_0, calculate first the sign structures $\operatorname{sign}_{F_0}(x)$ for all $x \in S$. And second, assign all states with the same sign structure to one set, thereby yielding a partition of the state space. This partition is then indeed $\mathfrak{S}^{(0)}$. We illustrate the sign structure of an uncoupled Markov chain with a simple example.

Example 4.4. Consider a Markov chain with transition matrix P_0 such that P_0 is block diagonal with three blocks of sizes three, two, and three. Figure 4.2.1 shows in a concrete case three eigenvectors, f_1, f_2, f_3, of the transfer operator T_0 associated to the eigenvalue 1.

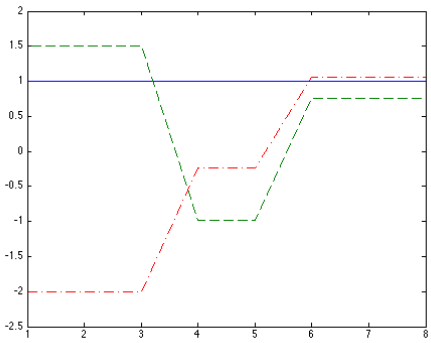

Figure 4.2.1: Largest eigenvectors: f_1 (solid line), f_2 $(-)$, f_3 $(-\cdot)$

The sign structure

	f_1	f_2	f_3
x_1	$+$	$+$	$-$
x_2	$+$	$+$	$-$
x_3	$+$	$+$	$-$
x_4	$+$	$-$	$-$
x_5	$+$	$-$	$-$
x_6	$+$	$+$	$+$
x_7	$+$	$+$	$+$
x_8	$+$	$+$	$+$

suggests that the state space can be decomposed into three invariant subsets, namely $\{x_1, x_2, x_3\}, \{x_4, x_5\}$, and $\{x_6, x_7, x_8\}$. Also observe that the eigenvectors are constant on the invariant subsets.

4.2.2 Metastability of a nearly uncoupled Markov chain

Apart from the assumptions on $X^{(0)}$, we assume now also that we have Markov chains $X^{(\varepsilon)}$, $\varepsilon > 0$, satisfying Assumption 3.7 and that the associated transfer operators satisfy extended detailed balance with respect to an involution A and the unique invariant measures μ_ε. As in the previous chapter, we think of T_ε as a linear perturbation of T_0, i.e.

$$T_\varepsilon \quad = \quad T_0 + \varepsilon L$$

with some perturbation operator L. Then for the invariant partition $\mathfrak{S}^{(0)} = \{S_1, \ldots, S_m\}$ with respect to $X^{(0)}$ we have from (4.1.4) and (4.2.1)

$$P_{\mu_\varepsilon}(S_i, S_i) = \frac{\langle T_\varepsilon \chi_i, \chi_i \rangle_{\mu_\varepsilon}}{\|\chi_i\|^2_{\mu_\varepsilon}} = \frac{\langle T_0 \chi_i, \chi_i \rangle_{\mu_\varepsilon}}{\|\chi_i\|^2_{\mu_\varepsilon}} + \varepsilon \frac{\langle L\chi_i, \chi_i \rangle_{\mu_\varepsilon}}{\|\chi_i\|^2_{\mu_\varepsilon}} = 1 + \varepsilon c_i(\varepsilon)$$

for some $c_i(\varepsilon) = \frac{\langle L\chi_i, \chi_i \rangle_{\mu_\varepsilon}}{\|\chi_i\|^2_{\mu_\varepsilon}}$. By the continuity of μ_ε (Lemma 3.8), $c_i(\varepsilon)$ converges to $c_i(0)$. So, if ε is sufficiently small, then the invariant sets S_i become metastable sets and the full partition $\mathfrak{S}^{(0)}$ is a metastable partition of the Markov chain $X^{(\varepsilon)}$. A natural question at this point is if the sign structure idea from the previous section is still applicable in this case, at least for small ε, i.e. can we still characterize the metastable partition $\mathfrak{S}^{(0)}$ among all possible full partitions based on the eigenvectors of T_ε? This is a non-trivial question, since both eigenvalues and eigenvectors of T_ε are perturbed from the ones of T_0 and it is not clear that sign-structures are still meaningful. Instead of the eigenvalue 1 in case of T_0, we are now interested in the *dominant* eigenvalues which are close to 1 and the associated eigenvectors of T_ε. Using the language of perturbation analysis, we want to study the $\lambda(0)$-group generalized eigenvectors of T_ε for $\lambda(0) = 1$ when ε is small (see also Subsection 3.2.2). As in Chapter 3, it turns out that it is useful to assume that the metastable partition we want to characterize is actually A-invariant (see Definition 3.17). We therefore assume in the following that

Assumption 4.5. *The full partition $\mathfrak{S}^{(0)} = \{S_1, \ldots, S_m\}$ with respect to $X^{(0)}$ is A-invariant.*

The next theorem then extends the result in Deuflhard et al. (2000).

Theorem 4.6. *Let $X^{(\varepsilon)}$ be a Markov chain satisfying Assumptions 3.3, 3.4, and 3.7. Let the transfer operator T_ε satisfy extended detailed balance with respect to an involution A and invariant measures μ_ε. Assume furthermore that the full partition $\mathfrak{S}^{(0)} = \{S_1, \ldots, S_m\}$ with respect to $X^{(0)}$ satisfies Assumption 4.5. Then for sufficiently small ε, the $\lambda(0)$-group eigenvectors $f_1(\varepsilon), \ldots, f_m(\varepsilon)$ are of the form*

$$\begin{aligned} f_i(\varepsilon) &= \Pi_{\lambda(0),0}\left(f_i(0) + \varepsilon f_i^{(1)}\right) \\ &\quad + \varepsilon \left(\sum_{j=1}^{k} \left[\frac{1}{1-\beta_j} Q_j + \sum_{l=1}^{n_j - 1} \frac{1}{(1-\beta_j)^{l+1}} D_j^l \right] L \right) f_i(0) \\ &\quad + \mathcal{O}\left(\varepsilon^2\right), \end{aligned} \tag{4.2.2}$$

for repeated eigenvalues $\beta_1, \ldots, \beta_k$ of T_0 different from 1 with multiplicities n_j, eigenprojections Q_j and eigennilpotents D_j, respectively.

Proof. This is basically an application of Theorem 2.22. The theorem shows that the total eigenprojection $\Pi_{\lambda(0),\varepsilon}$ of $\lambda(0)$-group is holomorphic at $\varepsilon = 0$

with

$$\Pi_{\lambda(0),\varepsilon} = \Pi_{\lambda(0),0} + \varepsilon\left(-\Pi_{\lambda(0),0}LH - HL\Pi_{\lambda(0),0}\right) + \mathcal{O}\left(\varepsilon^2\right), \quad (4.2.3)$$

where H is given by

$$H = -\sum_{j=1}^{k}\left[\left(1-\beta_j\right)^{-1}Q_j + \sum_{l=1}^{n_j-1}\left(1-\beta_j\right)^{-l-1}D_j^l\right]. \quad (4.2.4)$$

Theorem 3.19 and Lemma 3.12 show that for small ε the operator T_ε is self-adjoint on $\mathrm{span}\{f_1(\varepsilon),\ldots,f_m(\varepsilon)\}$ and $f_i(\varepsilon)$'s are indeed eigenvectors. Theorem 2.10 then shows that $f_i(\varepsilon)$ is not only continuous, but also holomorphic at $\varepsilon = 0$, i.e.

$$f_i(\varepsilon) = f_i(0) + f_i^{(1)}\varepsilon + f_i^{(2)}\varepsilon^2 + \cdots.$$

We then obtain

$$\begin{aligned}
f_i(\varepsilon) &= \Pi_{\lambda(0),\varepsilon}f_i(\varepsilon)\\
&= \Pi_{\lambda(0),0}\left(f_i(0) + \varepsilon f_i^{(1)}\right)\\
&\quad + \varepsilon\left(\Pi_{\lambda(0),0}L\sum_{j=1}^{k}\left[\left(1-\beta_j\right)^{-1}Q_j + \sum_{l=1}^{n_j-1}\left(1-\beta_j\right)^{-l-1}D_j^l\right]\right)f_i(0)\\
&\quad + \varepsilon\left(\sum_{j=1}^{k}\left[\left(1-\beta_j\right)^{-1}Q_j + \sum_{l=1}^{n_j-1}\left(1-\beta_j\right)^{-l-1}D_j^l\right]L\Pi_{\lambda(0),0}\right)f_i(0)\\
&\quad + \mathcal{O}\left(\varepsilon^2\right).
\end{aligned}$$

The second summand vanishes because $Q_j f_i(0) = 0$ and $D_j f_i(0) = 0$ for $i \neq j$. Hence,

$$\begin{aligned}
f_i(\varepsilon) &= \Pi_{\lambda(0),0}\left(f_i(0) + \varepsilon f_i^{(1)}\right)\\
&\quad + \varepsilon\sum_{j=1}^{k}\left[\frac{1}{1-\beta_j}Q_j + \sum_{l=1}^{n_j-1}\frac{1}{\left(1-\beta_j\right)^{l+1}}D_j^l\right]Lf_i(0) + \mathcal{O}\left(\varepsilon^2\right).
\end{aligned}$$

□

This theorem shows that the sign structure idea is still applicable when ε is small. Indeed, the first term in the expansion of the eigenvector $f_i(\varepsilon)$ in (4.2.2) is a linear combination of the indicators χ_j on each invariant set S_j, i.e.

$$f_i(0) + \varepsilon\Pi_{\lambda(0),0}f_i^{(1)} = \sum_{j=1}^{m}\alpha_{ij}\chi_j + \varepsilon\sum_{j=1}^{m}\gamma_{ij}\chi_j$$

for some coefficients α_{ij} and γ_{ij}. Hence, the structure of the sets S_i is visible in

the levels of constancy of the eigenvectors $f_i(\varepsilon)$. If we regard the second order terms as negligible, then it is only the second summand in (4.2.2) that might destroy the constancy of $f_i(\varepsilon)$. On the other hand, even for larger values of ε, the second summand is small, if the spectral gap $\sup_j \frac{1}{|1-\beta_j|}$ is small. Note that β_j can be complex-valued and/or might not be semisimple i.e. $D_j \neq 0$. This is where Theorem 4.6 differs from Deuflhard et al. (2000) where T_0 is assumed to be self-adjoint with real and semisimple eigenvalues.

Consequently, by the same steps as outlined before Example 4.4 but applied to eigenvectors of T_ε, we can find a full partition $\mathfrak{S}$ that should be a close approximation to $\mathfrak{S}^{(0)}$.

4.2.3 Metastability and A-invariance

So far we have introduced the metastability index $M_\mu(\mathfrak{S})$ for a full partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$, how it is related to the transfer operator (see (4.1.4)) and how a metastable partition $\mathfrak{S}^{(0)}$ can be characterized, at least approximately, by the sign structure of the eigenvectors of T_ε. We have already seen in Theorem 4.6 that a theoretical justification requires $\mathfrak{S}^{(0)}$ to be A-invariant. In actual applications, it may thus seem reasonable to require from an algorithm for finding metastable partitions that the returned partitions are A-invariant, as well. In the next subsection we will describe such an algorithm based on the sign structure with respect to the eigenvectors of T_ε. For sufficiently small ε Theorem 4.6 suggests that the A-invariance of the eigenvectors of T_ε remains true. In practice, however, when ε is unknown, it may happen that the eigenvectors of the transition operator are not A-invariant and thus the found partition is not, either. Instead of forcing the partition to become A-invariant manually, it turns out to be more useful to change the eigenvectors of the transfer operator to become A-invariant. For instance, we could consider the projected eigenvectors $\tilde{f} = \Pi^+ f$, where Π^+ is the orthogonal (!) projection onto $\mathcal{X}_+$ (see also Lemma 3.13). Unfortunately, in practice this leads to smaller metastability indices. A second approach is to change the transfer operator T itself to obtain directly A-invariant eigenvectors. At first this may look like a loss of information in the spectral structure of T, but the results are actually better and also lead to an easier mathematical analysis (compare e.g. Theorems 4.9 and 4.10). This idea of changing T is based on the observation that for any A-invariant partition $\mathfrak{S} = \{S_1, \ldots, S_m\}$

$$\langle T\chi_i, \chi_j \rangle_\mu = \langle T\chi_i, \chi_j \rangle_{A,\mu} = \langle AT\chi_i, \chi_j \rangle_\mu$$

and

$$\langle T\chi_i, \chi_j \rangle_\mu = \left\langle \Pi^+ T\chi_i, \chi_j \right\rangle_\mu = \left\langle \Pi^+ T \Pi^+ \chi_i, \chi_j \right\rangle_\mu ,$$

since $\Pi^+\chi_j = \chi_j$. Consequently, (4.1.4) can be written as

$$P_\mu(S_i, S_j) = \frac{\langle T\chi_i, \chi_j\rangle_\mu}{\|\chi_i\|_\mu^2} = \frac{\langle T_A\chi_i, \chi_j\rangle_\mu}{\|\chi_i\|_\mu^2} = \frac{\langle T^+\chi_i, \chi_j\rangle_\mu}{\|\chi_i\|_\mu^2} = \frac{\left\langle \hat{T}\chi_i, \chi_j\right\rangle_\mu}{\|\chi_i\|_\mu^2}, \quad (4.2.5)$$

where we denote $T_A := AT$, $T^+ := \Pi^+T$, and $\hat{T} := \Pi^+T\Pi^+$. Therefore, from the point of view of the metastability index, we can consider any of the operators T, T_A, T^+ and $\hat{T}$. Before we explain which operators perform best in practice, we discuss their mathematical properties. Note that all operators coincide, if $A = I$.

Lemma 4.7. *Let T be a transfer operator that satisfies extended detailed balance with respect to an involution A and a measure μ. Then we have:*

(i) Eigenvectors f of T^+ and $\hat{T}$ satisfy $Af = f$, i.e. $f \in \mathcal{X}_+$.

(ii) T_A is self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$.

(iii) Eigenvectors of T_A are right singular vectors of T, i.e. if $T_Af = \lambda f$, then $T^*Tf = \lambda^2 f$.

(iv) For any $f, g \in \mathcal{X}$

$$\left\langle \hat{T}f, g\right\rangle_\mu = \left\langle \hat{T}f, g\right\rangle_{A,\mu} = \left\langle f, \hat{T}g\right\rangle_{A,\mu} = \left\langle f, \hat{T}g\right\rangle_\mu .$$

In particular, $\hat{T}$ is self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$ and $\langle\cdot,\cdot\rangle_{A,\mu}$.

Proof. (i) Follows by definition, since T^+ and $\hat{T}$ are projected onto $\mathcal{X}_+$.

(ii) This is clear, since $T_A^* = T^*A^* = AT = T_A$ by Lemma 3.11.

(iii) Let f be an eigenvector of T_A for the eigenvalue λ. Then by Lemma 3.11

$$T^*Tf = ATATf = T_AT_Af = \lambda^2 f.$$

(iv) By Lemma 3.13, $\Pi^+ = \frac{I+A}{2}$ such that for any $f, g \in \mathcal{X}$

$$\left\langle \Pi^+f, g\right\rangle_\mu \quad = \quad \left\langle f, \Pi^+g\right\rangle_\mu .$$

Since $\Pi^+A = \Pi^+ = A\Pi^+$, we have

$$\Pi^+T^*\Pi^+ = \Pi^+ATA\Pi^+ = \Pi^+T\Pi^+.$$

Consequently,

$$\begin{aligned}\left\langle \hat{T}f, g\right\rangle_\mu &= \left\langle \Pi^+ T \Pi^+ f, g\right\rangle_\mu \\ &= \left\langle f, \Pi^+ T^* \Pi^+ g\right\rangle_\mu \\ &= \left\langle f, \hat{T}g\right\rangle_\mu .\end{aligned}$$

Moreover,

$$\left\langle \hat{T}f, g\right\rangle_\mu = \left\langle A\hat{T}f, g\right\rangle_\mu = \left\langle \hat{T}f, g\right\rangle_{A,\mu}$$

and

$$\left\langle f, \hat{T}g\right\rangle_\mu = \left\langle A^2 f, \hat{T}g\right\rangle_\mu = \left\langle Af, A\hat{T}g\right\rangle_\mu = \left\langle f, \hat{T}g\right\rangle_{A,\mu}.$$

□

The lemma shows that T_A and $\hat{T}$ are always self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$ which means that we can immediately apply the previous theory from the literature by Huisinga and Schmidt (2006). We also see that the eigenvectors of T^+ and $\hat{T}$ always lie in $\mathcal{X}_+$, while eigenvectors of T_A may not (see examples in Section 4.4). In all, $\hat{T}$ seems more natural and closer to T than T_A or T^+, since it is also self-adjoint with respect to $\langle\cdot,\cdot\rangle_{A,\mu}$ (note that $\langle\cdot,\cdot\rangle_{A,\mu}$ is actually a scalar product on $\mathcal{X}_+$). In the perturbation setting, the operators $T_{A,\varepsilon} = AT_\varepsilon$, $T_\varepsilon^+ = \Pi^+ T_\varepsilon$, and $\hat{T}_\varepsilon = \Pi^+ T_\varepsilon \Pi^+$ all coincide at $\varepsilon = 0$ when restricted to the $\mathcal{E}_{\lambda(0)}(0)$-eigenspace. We will show now that Theorem 4.6 also holds for $\hat{T}_\varepsilon$ and thus the sign structure approach is justified when using $\hat{T}_\varepsilon$ instead of T_ε.

Theorem 4.8. *Under the assumptions of Theorem 4.6, the $\lambda(0)$-group eigenvectors $f_1(\varepsilon), \ldots, f_m(\varepsilon)$ of $\hat{T}_\varepsilon = \hat{T}_0 + \varepsilon\hat{L}$ are of the form*

$$f_i(\varepsilon) = \Pi_{\lambda(0),0}\left(f_i(0) + \varepsilon f_i^{(1)}\right) + \varepsilon \sum_{j=1}^{k} \frac{1}{1-\beta_j} Q_j \hat{L} f_i(0) + \mathcal{O}\left(\varepsilon^2\right)$$

for repeated eigenvalues $\beta_1, \ldots, \beta_k$ of $\hat{T}_0$ different from 1 with eigenprojection $Q_1, \ldots, Q_k$, and $\Pi_{\lambda(0),0}$ is the eigenprojection belonging to $\lambda(0)$.

Proof. The proof of Theorem 4.6 follows analogously and is actually simpler, as $\hat{T}_\varepsilon$ is self-adjoint on all of $\mathcal{X}$. □

This essentially justifies the use of $\hat{T}$ in practice, when ε is not known. The numerical examples in Section 4.4 will demonstrate that the sign structure algorithm always leads to a better identification of metastable partitions and higher metastability indices when applied to $\hat{T}$ as compared to T, T_A or T^+. While the metastability indices of T, T_A, T^+ and $\hat{T}$ all coincide according to (4.2.5), we want to emphasize that there is in general to relation between the spectral properties of these operators, except for the ones mentioned in Lemma 4.7.

4.2.4 Algorithm

Based on the last three subsections we suggest the following algorithm for identifying metastable sets of a Markov chain X that satisfies an extended detailed balance condition. We assume that we are given a Markov chain with a matrix $\tilde{T}$ representing the associated transfer operator T and unique invariant measure μ which is the unique normalized left eigenvector of $\tilde{T}$. After that we form a second matrix

$$\tilde{\hat{T}} = \left(\frac{I+\tilde{A}}{2}\right)\tilde{T}\left(\frac{I+\tilde{A}}{2}\right),$$

where I is the $N \times N$ identity matrix and where $\tilde{A}(x,y) = \delta_{a(x)}(y)$ is the matrix representation of A. Consequently, $\tilde{\hat{T}}$ is the matrix representation of the operator $\hat{T}$. We then compute the eigenvalues of $\tilde{\hat{T}}$ and determine heuristically the number m of dominant eigenvalues that cluster around 1. The eigenvalues of $\hat{T}$ (and thus of $\tilde{\hat{T}}$) are always real. Denote the chosen dominant eigenvalues by $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_m$ and the corresponding $\langle\cdot,\cdot\rangle_{A,\mu}$-orthonormal dominant eigenvectors by $f_1, f_2, \ldots, f_m$. We then compute the sign structure of $f_1, f_2, \ldots, f_m$ for all $x \in S$ with respect to some threshold value $\theta > 0$, i.e.

$$\operatorname{sgn}(f_i(x)) \quad = \quad \begin{cases} + & \text{if } f_i(x) > \theta, \\ - & \text{if } f_i(x) < -\theta, \\ 0 & \text{else.} \end{cases}$$

The threshold value θ can be chosen from the procedure described in Deuflhard et al. (2000). Finally, all states $x \in S$ with the same sign structure $\operatorname{sign}(x)$ are added to the same set S_j. We then obtain at most m sets S_j, which are the alleged metastable sets.

4.2.5 Lower bounds of the metastability index

Theorem 4.8 verifies that the algorithm above is reasonable, under the assumption of a perturbation model and in first order. Since finding the optimal partition with the highest metastability index is intractable in practice (see also Huisinga and Schmidt (2006)), we will prove a lower bound on the metastability index for arbitrary (A-invariant) partitions. The lower bound is an extension of the results in Huisinga and Schmidt (2006) in order to deal with a transfer operator that satisfies extended detailed balance.

Theorem 4.9. *Let X be a Markov chain with unique invariant measure μ. Assume that the associated transfer operator T satisfies extended detailed balance with respect to an involution A and μ. Denote by $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_m$ the m largest eigenvalues of $\hat{T} = \Pi^+ T \Pi^+$ and by $f_1, \ldots, f_m$ the corresponding $\langle\cdot,\cdot\rangle_\mu$-orthonormal eigenvectors. Let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be an arbitrary partition of the state space S chosen such that it is A-invariant. Moreover, let Q be the*

orthogonal projection with respect to $\langle\cdot,\cdot\rangle_\mu$ *onto* $\mathrm{span}\{\chi_1,\ldots,\chi_m\}$. *Then the metastability index of the decomposition* $\mathfrak{S}$ *has the lower bound*

$$M_\mu(\mathfrak{S}) \geq \sum_{j=1}^m \lambda_j\kappa_j + \alpha\sum_{j=1}^m (1-\kappa_j).$$

where $\kappa_j = \|Qf_j\|_\mu^2$, $\alpha \in (-1,1)$ *is the smallest eigenvalue of the operator* $\hat{T}$.

Proof. Let $\chi_i, i=1,\ldots,m$ be the indicator functions of S_i's in the partition $\mathfrak{S}$. Since $A\chi_i = \chi_i$, we have

$$\begin{aligned} M_\mu(\mathfrak{S}) &= \sum_{i=1}^m P_\mu(S_i,S_i) \\ &= \sum_{i=1}^m \frac{\langle T\chi_i,\chi_i\rangle_\mu}{\|\chi_i\|_\mu^2} = \sum_{i=1}^m \frac{\left\langle \hat{T}\chi_i,\chi_i\right\rangle_\mu}{\|\chi_i\|_\mu^2}. \end{aligned}$$

Let Π be the orthogonal projection onto $\mathrm{span}\{f_1,\ldots,f_m\}$ with respect to $\langle\cdot,\cdot\rangle_\mu$ such that for all $i=1,\ldots,m$

$$\Pi\chi_i = \sum_{k=1}^m \langle\chi_i,f_k\rangle_\mu f_k. \tag{4.2.6}$$

Denote furthermore the projection on the complement of $\mathrm{span}\{f_1,\ldots,f_m\}$ by $\Pi^\perp$, i.e. $\Pi^\perp = I-\Pi$. Let α be the smallest eigenvalue of $\hat{T}$ on $\Pi^\perp(\mathcal{X})$. Note that clearly $|\alpha|<1$. Then $\hat{T}-\alpha I$ is invariant on $\Pi(\mathcal{X})$ and on $\Pi^\perp(\mathcal{X})$, i.e.

$$\begin{aligned} \left(\hat{T}-\alpha I\right)\Pi(\mathcal{X}) &= \Pi(\mathcal{X}), \\ \left(\hat{T}-\alpha I\right)\Pi^\perp(\mathcal{X}) &= \Pi^\perp(\mathcal{X}). \end{aligned}$$

Since $\hat{T}$ is self-adjoint with respect to $\langle\cdot,\cdot\rangle_\mu$, we thus have

$$\begin{aligned} \left\langle \hat{T}\chi_i,\chi_i\right\rangle_\mu &= \left\langle \left(\hat{T}-\alpha I\right)\left(\Pi+\Pi^\perp\right)\chi_i, \left(\Pi+\Pi^\perp\right)\chi_i\right\rangle_\mu + \alpha\|\chi_i\|_\mu^2 \\ &= \left\langle \left(\hat{T}-\alpha I\right)\Pi\chi_i,\Pi\chi_i\right\rangle_\mu + \left\langle \left(\hat{T}-\alpha I\right)\Pi^\perp\chi_i,\Pi^\perp\chi_i\right\rangle_\mu + \alpha\|\chi_i\|_\mu^2 \\ &\geq \left\langle \left(\hat{T}-\alpha I\right)\Pi\chi_i,\Pi\chi_i\right\rangle_\mu + \alpha\|\chi_i\|_\mu^2 \\ &= \left\langle \hat{T}\Pi\chi_i,\Pi\chi_i\right\rangle_\mu + \alpha\left(\|\chi_i\|_\mu^2 - \|\Pi\chi_i\|_\mu^2\right), \end{aligned}$$

where the inequality in the third line is due to the fact that $\hat{T}-\alpha I$ is positive

definite. For the first summand we have by (4.2.6)

$$\begin{aligned}\left\langle \hat{T}\Pi\chi_i, \Pi\chi_i \right\rangle_\mu &= \left\langle \hat{T}\sum_{j=1}^m \langle \chi_i, f_j\rangle_\mu f_j, \sum_{j=1}^m \langle \chi_i, f_j\rangle_\mu f_j \right\rangle_\mu \\ &= \sum_{j=1}^m \lambda_j \left|\langle \chi_i, f_j\rangle_\mu\right|^2.\end{aligned}$$

Since

$$\|Qf_j\|_\mu^2 = \sum_{i=1}^m \frac{\left|\langle \chi_i, f_j\rangle_\mu\right|^2}{\|\chi_i\|_\mu^2},$$

we thus obtain

$$\begin{aligned}M_\mu(\mathfrak{S}) &= \sum_{i=1}^m \frac{\left\langle \hat{T}\chi_i, \chi_i\right\rangle_\mu}{\|\chi_i\|_\mu^2} \\ &= \sum_{i=1}^m \frac{1}{\|\chi_i\|_\mu^2}\left(\sum_{j=1}^m \left(\lambda_j \left|\langle \chi_i, f_j\rangle_\mu\right|^2\right) + \alpha\left(\|\chi_i\|_\mu^2 - \|\Pi\chi_i\|_\mu^2\right)\right) \\ &= \sum_{i=1}^m \frac{1}{\|\chi_i\|_\mu^2}\left(\sum_{j=1}^m (\lambda_j - \alpha)\left|\langle \chi_i, f_j\rangle_\mu\right|^2\right) + \alpha m \\ &= \sum_{j=1}^m (\lambda_j - \alpha)\|Qf_j\|_\mu^2 + \alpha m \\ &= \sum_{j=1}^m \lambda_j\kappa_j + \alpha\sum_{j=1}^m (1-\kappa_j).\end{aligned}$$

□

This theorem shows that a high metastability index is achieved, if we consider dominant eigenvalues close to 1 and if the partition is chosen such that the m eigenvectors, associated to the m dominant eigenvalues, are almost constant on the sets of the partition. Indeed, $\kappa_j = \|Qf_j\|_\mu^2$ is close to 1, if f_j lies *almost* in the linear span of the indicators $\chi_1, \ldots, \chi_m$, i.e. if f_j is almost constant on the sets $S_1, \ldots, S_m$. This is exactly what is achieved by the sign-structure algorithm.

For completeness we also prove a lower bound for the metastability index when we choose sets according to the eigenvectors of T. The lower bound differs from the one for $\hat{T}$, since it is harder to deal with the action of T on the eigenspaces different from $\mathcal{E}_{\lambda(0)}$. Moreover, the eigenvectors are orthogonal with respect to $\langle\cdot,\cdot\rangle_{A,\mu}$, but not with respect to $\langle\cdot,\cdot\rangle_\mu$. Note again that the eigenvalues and eigenvectors of T and $\hat{T}$ are in general not related, and it is thus not possible to

answer in advance which lower bound is better. However, the structure of the lower bounds is very similar, and, up to first order, the crucial quantities κ_j are the same (see below). However, compared to the first lower bound, in case of T we have to assume that the dominant eigenvalues are actually real, while in case of $\hat{T}$ all eigenvalues are real, since it is self-adjoint. This is however not a problem, as in the perturbation setting for small ε (see Theorem 3.19) and in practice (see examples in Section 4.4) the dominant eigenvalues are always real.

Theorem 4.10. *Let X be a Markov chain with unique invariant measure μ. Assume that the associated transfer operator T satisfies extended detailed balance with respect to an involution A and μ. Denote by $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_m$ the m largest eigenvalues of T and by $f_1, \ldots, f_m$ the corresponding $\langle \cdot, \cdot \rangle_{A,\mu}$-orthonormal eigenvectors. Let $\mathfrak{S} = \{S_1, \ldots, S_m\}$ be an arbitrary partition of the state space S chosen such that it is A-invariant. Moreover, let Q be the orthogonal projection with respect to $\langle \cdot, \cdot \rangle_\mu$ onto $\operatorname{span}\{\chi_1, \ldots, \chi_m\}$. Then the metastability index of the decomposition $\mathfrak{S}$ has the lower bound*

$$M_\mu(\mathfrak{S}) \geq \sum_{j=1}^{m} \lambda_j \kappa_j + \alpha \sum_{j=1}^{m} (1 - \kappa_j) + (\alpha \wedge 0) \left(\sum_{k,j=1}^{m} \langle Q f_k, f_j \rangle_\mu \langle f_j, f_k \rangle_\mu - \sum_{j=1}^{m} \kappa_j \right)$$

where $\kappa_j = \|Q f_j\|_\mu^2$, $\alpha \in (-1, 1)$ is the smallest eigenvalue of the operator T_A.

Proof. Since $A\chi_i = \chi_i$, we have

$$\begin{aligned} M_\mu(\mathfrak{S}) &= \sum_{i=1}^{m} P_\mu(S_i, S_i) \\ &= \sum_{i=1}^{m} \frac{\langle T\chi_i, \chi_i \rangle_\mu}{\|\chi_i\|_\mu^2} = \sum_{i=1}^{m} \frac{\langle T\chi_i, \chi_i \rangle_{A,\mu}}{\|\chi_i\|_\mu^2}. \end{aligned}$$

Let Π be the orthogonal projection onto $\operatorname{span}\{f_1, \ldots, f_m\}$ with respect to $\langle \cdot, \cdot \rangle_{A,\mu}$ such that for all $i = 1, \ldots, m$

$$\Pi \chi_i = \sum_{k=1}^{m} \langle \chi_i, f_k \rangle_{A,\mu} f_k.$$

Denote furthermore the projection on the complement of $\operatorname{span}\{f_1, \ldots, f_m\}$ by $\Pi^\perp$, i.e. $\Pi^\perp = I - \Pi$. $\Pi^\perp(\mathcal{X})$ is a closed subspace of $\mathcal{X}$ with respect to $\|\cdot\|_\mu$ on which T is invariant, i.e. $T\Pi^\perp(\mathcal{X}) = \Pi^\perp(\mathcal{X})$. This is clear, since we can find a basis of generalized eigenvectors of T for $\Pi^\perp(\mathcal{X})$. Note that $\Pi^\perp$ is in general *not* an orthogonal projection with respect to $\langle \cdot, \cdot \rangle_{A,\mu}$, since the Hermitian form does not yield a scalar product on all of $\mathcal{X}$ (see Lemma 3.13). Nevertheless, since Π is spanned by $f_1, \ldots, f_m$ where every f_i belongs to a real eigenvalue, and $\Pi^\perp$ is spanned by some generalized eigenvectors belonging to some other eigenvalues which are different from the ones associated with f_i, then from Lemma 3.12 it

follows immediately that

$$\begin{aligned}\langle T\chi_i,\chi_i\rangle_{A,\mu} &= \left\langle T\left(\Pi+\Pi^{\perp}\right)\chi_i,\left(\Pi+\Pi^{\perp}\right)\chi_i\right\rangle_{A,\mu}\\ &= \langle T\Pi\chi_i,\Pi\chi_i\rangle_{A,\mu}+\left\langle T\Pi^{\perp}\chi_i,\Pi^{\perp}\chi_i\right\rangle_{A,\mu}.\end{aligned}$$

We first deal with the second term. Consider the operator $T_A = AT$. On $\Pi^{\perp}(\mathcal{X})$ the operator T_A has only eigenvalues in the open interval $(-1,1)$. Let α be the smallest such eigenvalue of T_A. Since T_A is self-adjoint (Lemma (4.7)) with respect to $\langle\cdot,\cdot\rangle_{\mu}$ we have

$$\begin{aligned}\left\langle T\Pi^{\perp}\chi_i,\Pi^{\perp}\chi_i\right\rangle_{A,\mu} &= \left\langle AT-\alpha\Pi^{\perp}\chi_i,\Pi^{\perp}\chi_i\right\rangle_{\mu}+\alpha\|\Pi^{\perp}\chi_i\|_{\mu}^2\\ &= \left\langle\left(T_A-\alpha I\right)\Pi^{\perp}\chi_i,\Pi^{\perp}\chi_i\right\rangle_{\mu}+\alpha\|\Pi^{\perp}\chi_i\|_{\mu}^2\\ &\geq \alpha\|\Pi^{\perp}\chi_i\|_{\mu}^2,\end{aligned}$$

where we use positive definiteness of $T_A-\alpha I$ in the last inequality. Then

$$\begin{aligned}\alpha\|\Pi^{\perp}\chi_i\|_{\mu}^2 &= \alpha\|\chi_i-\Pi\chi_i\|_{\mu}^2\\ &= \alpha\left(\|\chi_i\|_{\mu}^2-2\left\langle\chi_i,\Pi\chi_i\right\rangle_{\mu}+\|\Pi\chi_i\|_{\mu}^2\right)\\ &= \alpha\left(\|\chi_i\|_{\mu}^2-2\|\Pi\chi_i\|_{A,\mu}^2+\|\Pi\chi_i\|_{\mu}^2\right)\\ &= \alpha\left(\|\chi_i\|_{\mu}^2-\|\Pi\chi_i\|_{A,\mu}^2\right)+\alpha\left(\|\Pi\chi_i\|_{\mu}^2-\|\Pi\chi_i\|_{A,\mu}^2\right)\\ &= \alpha\left(\|\chi_i\|_{\mu}^2-\|\Pi\chi_i\|_{A,\mu}^2\right)+\alpha\left\langle\left(I-A\right)\Pi\chi_i,\Pi\chi_i\right\rangle_{\mu},\end{aligned}\tag{4.2.7}$$

where the third equality comes from $\langle\chi_i,\Pi\chi_i\rangle_{\mu}=\langle A\chi_i,\Pi\chi_i\rangle_{\mu}=\langle\chi_i,\Pi\chi_i\rangle_{A,\mu}=\left\langle\chi_i,\Pi^2\chi_i\right\rangle_{A,\mu}=\langle\Pi\chi_i,\Pi\chi_i\rangle_{A,\mu}$. Consider first the case that $\alpha\geq 0$. Note that $\frac{1}{2}(I-A)$ is idempotent, since

$$\frac{1}{4}\left(I-A\right)\left(I-A\right)=\frac{1}{4}(I-A-A+A^2)=\frac{1}{4}\left(I-A-A+I\right)=\frac{1}{2}(I-A).$$

Therefore $\sigma(\frac{1}{2}\left(I-A\right))\subset\{0,1\}$ such that in the case where $\alpha\geq 0$

$$\left\langle T\Pi^{\perp}\chi_i,\Pi^{\perp}\chi_i\right\rangle_{A,\mu} \geq \alpha\left(\|\chi_i\|_{\mu}^2-\|\Pi\chi_i\|_{A,\mu}^2\right).$$

Observe that

$$\|Qf_j\|_{\mu}^2 = \sum_{i=1}^{m}\frac{\left|\langle\chi_i,f_j\rangle_{\mu}\right|^2}{\|\chi_i\|_{\mu}^2}.$$

This yields

$$\begin{aligned}
M_\mu(\mathfrak{S}) &= \sum_{i=1}^m \frac{1}{\|\chi_i\|_\mu^2}\left(\langle T\Pi\chi_i,\Pi\chi_i\rangle_{A,\mu}+\left\langle T\Pi^\perp\chi_i,\Pi^\perp\chi_i\right\rangle_{A,\mu}\right)\\
&\geq \sum_{i=1}^m \frac{1}{\|\chi_i\|_\mu^2}\left(\sum_{j=1}^m\left(\lambda_j\left|\langle\chi_i,f_j\rangle_{A,\mu}\right|^2\right)+\alpha\left(\|\chi_i\|_\mu^2-\|\Pi\chi_i\|_{A,\mu}^2\right)\right)\\
&= \sum_{j=1}^m(\lambda_j-\alpha)\left(\sum_{i=1}^m\frac{\left|\langle\chi_i,f_j\rangle_{A,\mu}\right|^2}{\|\chi_i\|_\mu^2}\right)+\alpha m\\
&= \sum_{j=1}^m(\lambda_j-\alpha)\|Qf_j\|_\mu^2+\alpha m\\
&= \sum_{j=1}^m\lambda_j\kappa_j+\alpha\sum_{j=1}^m(1-\kappa_j).
\end{aligned}$$

On the other hand, if $\alpha<0$, then we have

$$\begin{aligned}
&\sum_{i=1}^m\frac{1}{\|\chi_i\|_\mu^2}\langle(I-A)\Pi\chi_i,\Pi\chi_i\rangle_\mu\\
&\quad=\sum_{k,j=1}^m\left(\sum_{i=1}^m\frac{1}{\|\chi_i\|_\mu^2}\langle\chi_i,f_j\rangle_{A,\mu}\overline{\langle\chi_i,f_k\rangle}_{A,\mu}\right)\langle(I-A)f_j,f_k\rangle_\mu\\
&\quad=\sum_{k,j=1}^m\left(\sum_{i=1}^m\frac{1}{\|\chi_i\|_\mu^2}\langle f_k,\chi_i\rangle_\mu\langle\chi_i,f_j\rangle_\mu\right)\langle(I-A)f_j,f_k\rangle_\mu\\
&\quad=\sum_{k,j=1}^m\left(\left\langle\sum_{i=1}^m\frac{1}{\|\chi_i\|_\mu^2}\langle f_k,\chi_i\rangle_\mu\chi_i,f_j\right\rangle_\mu\right)\langle(I-A)f_j,f_k\rangle_\mu\\
&\quad=\sum_{k,j=1}^m\langle Qf_k,f_j\rangle_\mu\langle(I-A)f_j,f_k\rangle_\mu\\
&\quad=\sum_{k,j=1}^m\langle Qf_k,f_j\rangle_\mu\langle f_j,f_k\rangle_\mu-\sum_{j=1}^m\langle Qf_j,f_j\rangle_\mu,
\end{aligned}\tag{4.2.8}$$

where we use $\langle\cdot,\cdot\rangle_{A,\mu}$-orthogonality of f_j's in the last line. Note that

$$\langle Qf_j,f_j\rangle_\mu=\sum_{i=1}^m\frac{1}{\|\chi_i\|_\mu^2}\langle\chi_i,f_j\rangle_\mu\overline{\langle\chi_i,f_j\rangle}_\mu=\sum_{i=1}^m\|Qf_j\|_\mu^2.$$

The first term in (4.2.8), however, cannot be estimated in a meaningful way, since the f_j are not necessarily orthogonal with respect to $\langle\cdot,\cdot\rangle_\mu$. Hence, for

$\alpha < 0$ we have the lower bound

$$M_\mu(\mathfrak{S}) \geq \sum_{j=1}^{m} \lambda_j \kappa_j + \alpha \sum_{j=1}^{m} (1 - \kappa_j) + \alpha \left(\sum_{k,j=1}^{m} \langle Q f_k, f_j \rangle_\mu \langle f_j, f_k \rangle_\mu - \sum_{j=1}^{m} \kappa_j \right).$$

Combining this with the lower bound for $\alpha \geq 0$ yields the statement. □

4.3 Related work for non-reversible processes

In this section we shortly comment on related works on dominant structures of non-reversible processes. We focus here only on the spectral approaches. For non-spectral approaches on non-reversible processes, see for example Sarich and Schütte (2014).

4.3.1 Related approach for identifying metastable sets

The main structural assumption of our work is the extended detailed balance condition with respect to an involution A. Without this we can not assume in general that the transfer operator behaves in any way similar to a self-adjoint operator which is useful in the analysis. Instead of working with eigenvalues it is then more appropriate to work with singular values. This approach was studied by Fritzsche et al. (2007). It is based on the singular value decomposition with a bisectioning iterative procedure. That means in each iteration the method computes the left or right singular vector corresponding to the second largest singular value and determines where the Markov chain is bisectioned into two metastable sets according to the sign structure, here either $+$ or $-$, of the second singular vector. However, recall from Lemma 4.7 that for a Markov chain with extended detailed balance, the right singular vectors are just the eigenvectors of T_A, which do not perform in practice as well as the eigenvectors of $\hat{T}$, as will be seen in the examples in the following section.

4.3.2 Identification of dominant cycles

Metastability is not the only structural property of molecular dynamics studied in the literature. Another interesting phenomenon exhibited by dynamical systems are *dominant cycles*. The states within a metastable set are grouped together, because the system rarely moves out of the set when starting from it. In case of a dominant cycle, on the other hand, states are clustered together into sets, because the system tends to move between these sets in a cyclic fashion. We give two small examples to motivate the concept of a cycle.

Example 4.11.

(a) Consider a permutation matrix

$$T_0 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

In this matrix there are four sets $\{1\}, \{3\}$, $\{2\}$ and $\{4\}$ which form a 4-cycle $\{1\} \to \{3\} \to \{2\} \to \{4\} \to \{1\}$. Note that the spectrum of T_0 is $\{1, \mathrm{i}, -\mathrm{i}, -1\}$. Now let

$$L = \begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

such that for $\varepsilon = 0.01$ we have

$$T_\varepsilon = T_\varepsilon = T_0 + \varepsilon L = \begin{pmatrix} 0 & 0.01 & 0.99 & 0 \\ 0 & 0 & 0.01 & 0.99 \\ 0.01 & 0.99 & 0 & 0 \\ 0.99 & 0 & 0 & 0.01 \end{pmatrix},$$

which we say to have one dominant cycle.

(b) For the second example consider

$$T_\varepsilon = \begin{pmatrix} 0 & 0.01 & 0.49 & 0.50 & 0 & 0 \\ 0 & 0 & 0.50 & 0.50 & 0 & 0 \\ 0.50 & 0.48 & 0.01 & 0 & 0 & 0.01 \\ 0.50 & 0.50 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.50 & 0.50 \\ 0 & 0.01 & 0 & 0 & 0.50 & 0.49 \end{pmatrix},$$

with spectrum

$$\sigma = \{1, 0.9851, 0.0083, -0.0068 + 0.0096\mathrm{i}, -0.0068 - 0.0096\mathrm{i}, -0.9873\}.$$

We can identify two metastable sets, namely $\{1, 2, 3, 4\}$ and $\{5, 6\}$, which is consistent with the number of dominant eigenvalues close to 1. However, T_ε not only has metastable sets, but also has a dominant cycle, namely $\{1, 2\} \to \{3, 4\} \to \{1, 2\}$.

The detection of dominant cycles for non-reversible processes has been studied by Djurdjevac-Conrad et al. (2015). Their approach of detecting of dominant cycles has been successfully applied to Langevin dynamics. The method in-

volves Schur decomposition of the transition matrix. Similar to the SVD approach from the previous subsection, this is another way to work with spectral methods without assuming any reversibility condition. The clustering into sets between which the process moves in a cyclic fashion is achieved by the PCCA+ algorithm (see Weber and Fackeldey (2015); Deuflhard and Weber (2005)) using *dominant* Schur vectors. In contrast to the concept of metastability, the dominant vectors do not correspond to eigenvalues close to 1, but rather to the eigenvalues close to the unit circle. This is due to the observation that permutation matrices, which exhibit the "perfect" cycle structure as seen in the first example above, have eigenvalues on the unit circle. In other words, the number of eigenvalues with absolute value close to 1 determines how many Schur vectors will be used in the algorithm. Take, for example, the second example above, there are three dominant Schur vectors of T_ε, corresponding to the Schur values $1, 0.9851, -0.9873$.

4.4 Numerical examples

4.4.1 Illustrative example I

A simple example is presented here to illustrate the algorithm proposed in Section 4.2.4. We construct a 90×90 stochastic matrix T according to the Generalized Metropolis-Hastings algorithm (see Section 4.4.4) for a given random invariant measure μ, random proposition transition kernel Q and an involution matrix A such that the related involution function is given by

$$a(x) \quad = \quad 30 \left\lceil \frac{x}{30} \right\rceil - \left(x - 30 \left\lfloor \frac{x-1}{30} \right\rfloor \right) + 1.$$

We thus obtain T that satisfies extended detailed balance condition with respect to the given involution A and the unique invariant measure μ.

Now set

$$\hat{T} = \left(\frac{I + A}{2} \right) T \left(\frac{I + A}{2} \right)$$

and compute the first seven eigenvalues of $\hat{T}$ which are

λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7
1	0.9161	0.9113	0.7070	0.6699	0.6456	0.6054.

Observe that there is a big gap between the third and fourth eigenvalues, so we heuristically choose $m = 3$, i.e. we expect three metastable sets. The corresponding $\langle \cdot, \cdot \rangle_\mu$- orthonormal dominant eigenvectors f_1, f_2, f_3 of $\hat{T}$ are shown in Figure 4.4.1.

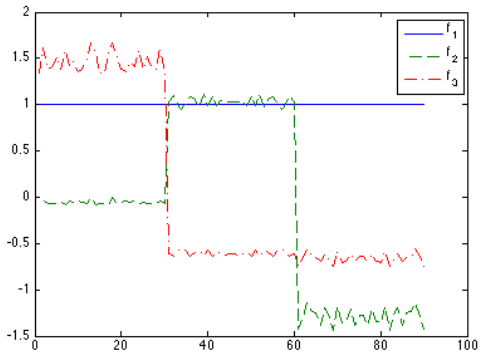

Figure 4.4.1: Dominant eigenvectors f_1, f_2, f_3 of $\hat{T}$.

Next, we compute the sign structures with respect to f_1, f_2, f_3 with threshold $\theta = 0.1$ and decompose the state space into three partitions according to the sign structures. This yields the partition $\mathfrak{S}^* = \{[1, 30], (30, 60], (60, 90]\}$ which has the metastability index $M(\mathfrak{S}^*) = 2.8252$. In fact, this is the maximal metastability index possible for partitions with three sets of the form $\mathfrak{S} = \{[1, R_1], (R_1, R_2], (R_2, 90]\}$. This can be seen in Figure 4.4.2 which shows the metastability index $M(\mathfrak{S})$ for $1 \leq R_1 < R_2 \leq 90$. Note also that $\mathfrak{S}^*$ is A-invariant.

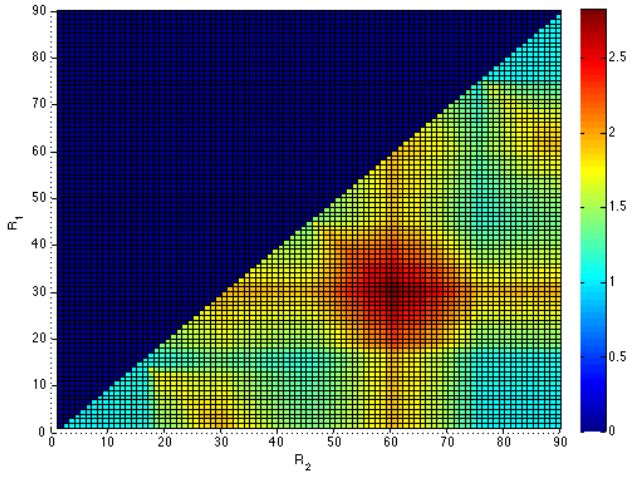

Figure 4.4.2: Metastability index $M(\mathfrak{S})$ with $\mathfrak{S} = \{[1, R_1], (R_1, R_2], (R_2, 90]\}$.

4.4.2 Illustrative example II

The previous example shows that the sign structure of dominant eigenvectors of $\hat{T}$ gives a good result. In this example, we want to compare the results obtained from eigenvectors of different operators, namely T, T_A and $\hat{T}$. We generate a 12×12 stochastic matrix T, again, by the Generalized Metropolis-Hastings algorithm, for a random invariant measure μ and random proposition transition kernel Q. Let furthermore A be an involution matrix such that the related involution function is given by

$$a(x) \quad = \quad 4\left\lceil \frac{x}{4} \right\rceil - \left(x - 4\left\lfloor \frac{x-1}{4} \right\rfloor \right) + 1.$$

The first five eigenvalues of T are

λ_1	λ_2	λ_3	λ_4	λ_5
1	0.8363	0.7750	0.3313	0.2469

We choose again $m = 3$. Figure 4.4.3 below shows the first three dominant eigenvectors f_1, f_2, f_3 of T, T_A, and $\hat{T}$. Observe that the eigenvectors of T_A vary more, as compared to the eigenvectors of T and $\hat{T}$. The sign structures with respect to eigenvectors of T and $\hat{T}$ with threshold $\theta = 0.1$ suggest the same metastable partition

$$\mathfrak{S}^1 = \{\{1,2,3,4\},\{5,6,7,8\},\{9,10,11,12\}\},$$

where we obtain as metastability index $M(\mathfrak{S}^1) = 2.6132$. The sign structures with respect to eigenvectors of T_A with the same threshold value $\theta = 0.1$, on the other hand, result in the decomposition

$$\mathfrak{S}^2 \quad = \quad \{\{1,2,3,4\},\{5,7,8\},\{6,9,10,11,12\}\}$$

with metastability index $M\left(\mathfrak{S}^2\right) = 1.5510$.

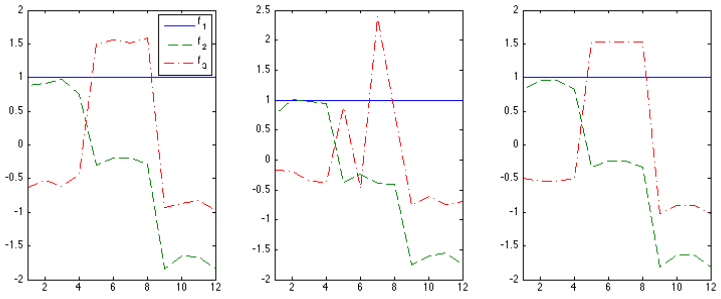

Figure 4.4.3: Dominant eigenvectors of T (left), T_A (middle), $\hat{T}$ (right).

We see that eigenvectors of T and $\hat{T}$ gives better result than of T_A in this example. Recall that eigenvectors of T_A are nothing but right singular vectors of T by Lemma 4.7. Thus, our algorithm to identify metastable sets via eigenvectors of $\hat{T}$ outperforms the algorithm proposed in Fritzsche et al. (2007) where they use the sign structure of singular vectors of T.

4.4.3 Example III : Langevin dynamics

Consider the Langevin dynamics

$$\begin{aligned} \mathrm{d}q_t &= p_t \mathrm{d}t, \\ \mathrm{d}p_t &= -\nabla V(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}W_t, \end{aligned}$$

with the given friction coefficient $\gamma = 1$ and the inverse temperature $\beta = 5$. The potential given by

$$V(q) = \left(q^2 - 1\right)^2 + 0.1q$$

is illustrated in Figure 4.4.4. Note that for Langevin dynamics, the T_0-invariant partition is decomposed according to the geometric position. This means that how the state space is divided depends only on q, i.e.

$$\chi_i\left((q,p)\right) = \chi_i\left((q,p')\right)$$

Hence, the assumption that the T_0-invariant partition is also A-invariant is automatically fulfilled because for A being the momentum reversal

$$A\chi_i\left((q,p)\right) = \chi_i\left(a\left(q,p\right)\right) = \chi_i\left((q,-p)\right) = \chi_i\left((q,p)\right).$$

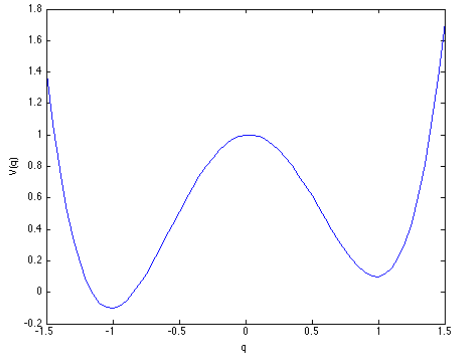

Figure 4.4.4: Potential V

The discretized transfer operator T related to the Langevin dynamics was com-

puted from discretizing the state space with $\Delta q = 0.1$ and $\Delta p = 0.15$, resulting in a 961×961 matrix. The eigenvalues of T are shown in Figure 4.4.5. The first five eigenvalues of T, ordered with respect to absolute value, are

λ_1	λ_2	λ_3	λ_4	λ_5
1.0000	0.9995	$0.8887 + 0.2396\mathrm{i}$	$0.8887 - 0.2396\mathrm{i}$.	$0.8895 + 0.2260\mathrm{i}$.

There is a significant gap between λ_2 and λ_3 and therefore we choose $m = 2$. Note that the dominant eigenvalues λ_1 and λ_2 are real-valued.

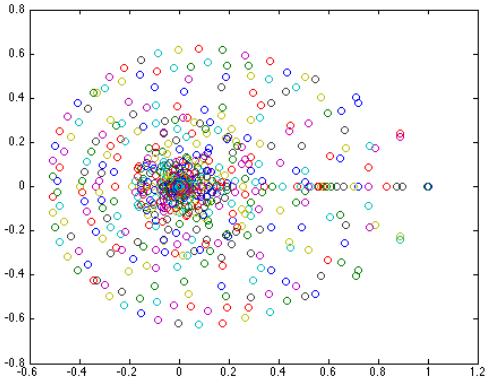

Figure 4.4.5: Eigenvalues in the complex plane of Langevin transfer operator.

The first eigenvector $f_1 = \mathbf{1}$ of T is constant while the second eigenvector f_2 of T shows two almost constant levels in a "twisted" fashion, compared to the second eigenvector of T_A and $\hat{T}$ which are almost constant in the momentum p axis. This is shown in the left Figure 4.4.6.

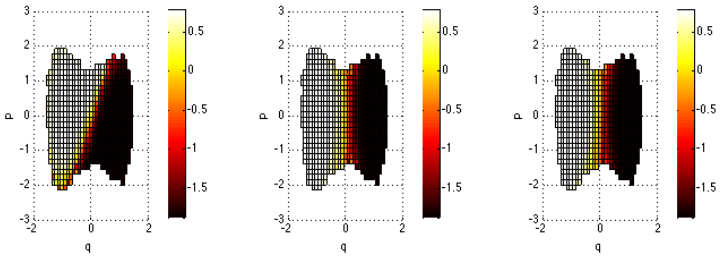

Figure 4.4.6: Second eigenvector of T (left), T_A (middle), and $\hat{T}$ (right).

Figure 4.4.7 shows the partitions $\mathfrak{S}^1, \mathfrak{S}^2, \mathfrak{S}^3$ with metastability indices of 1.9980, 1.9993, 1.9994 determined via the sign structures with respect to the dominant eigenvectors of T, T_A, and $\hat{T}$, respectively. Observe that the sign structures

with respect to the dominant eigenvectors of $\hat{T}$ suggest that a partition which is very similar to the one of T_A. Moreover, the partition $\mathfrak{S}^3$ is A-invariant where A is the momentum reversal with

$$a(x) \quad = \quad (q, -p), \quad x = (q, p),$$

which is typical for Langevin dynamics. On the other hand, $\mathfrak{S}^1$ is clearly not A-invariant as for $-1 < q < 0.5$, (q, p) and $(q, -p)$ are in two different subsets.

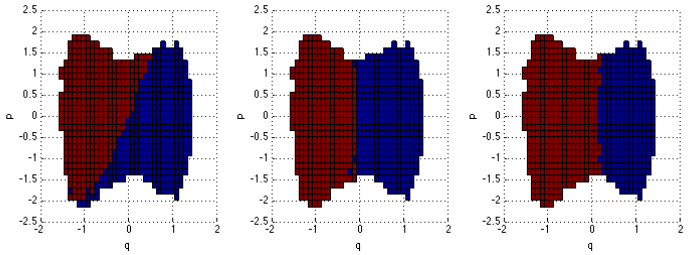

Figure 4.4.7: Metastable partitions from sign structures with respect to dominant eigenvectors of T (left), T_A (middle), and $\hat{T}$ (right).

4.4.4 Construction of transfer operators with extended detailed balance

For simulation purposes, we are interested in constructing a Markov chain with transition probability P that satisfies the extended detailed balance condition with respect to an involution A and a given measure μ, i.e.

$$\mu(x)P(x, y) \quad = \quad \mu(a(y))P(a(y), a(x)), \tag{4.4.1}$$

where a is the involution function related to A by $Af(x) = f(a(x)), f \in \mathcal{X}$. This section consists of two parts. The first part involves construction of a Markov chain that satisfies (4.4.1) using generalized Metropolis-Hastings algorithm, while the second part extends the construction to not only any Markov chain that satisfies (4.4.1), but also ones that have metastable structure.

Generalized Metropolis-Hastings algorithm

Here we present the generalized Metropolis-Hastings algorithm in Bou-Rabee and Vanden-Eijnden (2010) which is more general than the well-known Metropolis-Hastings algorithm, an approach to generate a reversible Markov chain, given an invariant measure μ (see for example Brooks et al. (2011)). Recall that the steps in the classical Metropolis-Hastings algorithm consists of proposing a next move according to the proposition transition kernel Q, computing a ratio, then

accepting or rejecting the proposed move according to the computed ratio. The generalized Metropolis-Hastings algorithm carries the same steps but with the different ratio computation and the rejection move. This yields instead a chain that satisfy extended detailed balance (4.4.1). We first present the algorithm and then discuss it in more detail later.

Algorithm 4.12. *Suppose a is a given involution function and μ is a probability measure that is invariant under a. With a proposition transition kernel Q, compute the ratio*

$$r(x,y) \quad = \quad \frac{Q(a(y), a(x))\mu(a(y))}{Q(x,y)\mu(x)},$$

which is assumed to be well-defined. Consider an initial point x_0, then for each iteration n:

1) Generate x'_{n+1} according to $Q(x_n, \cdot)$.

2) Accept the proposed x'_{n+1} with probability $\min\{1, r(x_n, x_{n+1})\}$ and set $x_{n+1} = x'_{n+1}$. Otherwise, reject the proposal move and set $x_{n+1} = a(x_n)$.

From Algorithm 4.12, it can be easily derived that the probability transition function of the generated Markov chain is

$$P(x,y) \quad = \quad \begin{cases} min\{1, r(x,y)\} Q(x,y) & , y \neq a(x); \\ 1 - \sum_{y \neq a(x)} min\{1, r(x,y)\} Q(x,y) & , else, \end{cases}$$

and it was shown in Lelièvre et al. (2010) that the transition function P satisfy extended detailed balance (3.3.2) with μ as its invariant measure.

Remark 4.13. As all of our analysis is based on transfer operators, instead of generating a transition matrix P, we are rather interested in building the matrix representation of a transfer operator. In particular, we can form a matrix T representing the transfer operator via

$$T_{x,y} = \frac{\mu(y)}{\mu(x)} P_{y,x}.$$

Then any vector $v \in \mathbb{R}^N$ satisfies

$$\begin{aligned} (Tv)(y) \quad &= \quad \sum_x v_x (Te_x)(y) = \sum_x v_x T_{y,x} \\ &= \quad \frac{1}{\mu(y)} \sum_x P(x,y) v_x \mu(x), \end{aligned}$$

where $(e_x)_{x \in S}$ is the standard basis, i.e. T has the form of a transfer operator according to 2.2.1. And it can be easily shown that the transfer operator satisfies extended detailed balance.

Construction of nearly uncoupled Markov chain

In the first part of this section, we discuss about how to generate a transfer operator that satisfies the extended detailed balance condition. In metastability applications, we are rather interested in generating a transfer operator satisfying the extended detailed balance condition that is also metastable. In particular, the question now extends to the family of transfer operators $\{T_\varepsilon\}_{\varepsilon\geq 0}$ that comes from perturbation. How can we construct T_ε satisfying extended detailed balance for all ε? The difficulty comes from the unknown μ_ε that keeps changing according to ε.

To answer this question, let us first denote for a vector $\mu \in \mathbb{R}^N$ by D_μ the diagonal matrix with the elements of μ on the diagonal and, without loss of generality, let T_0 be block diagonal. Additionally, we assume that the T_0-invariant partition is also A-invariant, i.e. if $x \in S_i$ then $a(x) \in S_i$ for all $x \in S, j = 1, \ldots, m$. This will allow us to rewrite the extended balance condition. Then (4.4.1) can be written as

$$D_\mu T \quad = \quad A T^\top D_\mu A. \tag{4.4.2}$$

Suppose μ_ε, the unique invariant measure of T_ε, are holomorphic and of the form

$$\mu_\varepsilon = \sum_{i=0}^{n} \mu^{(i)} \varepsilon^i + O\left(\varepsilon^{n+1}\right),$$

where $\mu^{(0)} = \mu_0$. The extended detailed balance (4.4.2) is thus equivalent to

$$D_{\mu_\varepsilon} T_\varepsilon \quad = \quad A T_\varepsilon^\top D_{\mu_\varepsilon} A.$$

That is

$$\begin{aligned}\left(\sum_{i=0}^{n} \varepsilon^i D_{\mu^{(i)}} + \mathcal{O}\left(\varepsilon^{n+1}\right)\right)(T_0 + \varepsilon L) \\ = \quad A\left(T_0^\top + \varepsilon L^\top\right)\left(\sum_{i=0}^{n} \varepsilon^i D_{\mu^{(i)}} + \mathcal{O}\left(\varepsilon^{n+1}\right)\right) A,\end{aligned}$$

which yields the following after spreading out the terms

$$\begin{aligned}D_{\mu_0} T_0 + \sum_{i=1}^{n} \varepsilon^i \left(D_{\mu^{(i)}} T_0 + D_{\mu^{(i-1)}} L\right) + \mathcal{O}\left(\varepsilon^{n+1}\right) \\ = \quad A\left(T_0^\top D_{\mu_0} + \sum_{i=1}^{n} \varepsilon^i \left(T_0^\top D_{\mu^{(i)}} + L^\top D_{\mu^{(i-1)}}\right) + \mathcal{O}\left(\varepsilon^{n+1}\right)\right) A.\end{aligned}$$

Comparing the coefficients for each order of ε we see that satisfying

$$\begin{aligned} D_{\mu_0} T_0 &= A T_0^\top D_{\mu_0} A, \\ D_{\mu^{(i)}} T_0 + D_{\mu^{(i-1)}} L &= A T_0^\top D_{\mu^{(i)}} A + A L^\top D_{\mu^{(i-1)}} A, i = 1, \dots, n \end{aligned}$$

makes sure that T_ε satisfies extended detailed balance with respect to μ_ε up to the order ε^{n+1}. An obvious way to satisfy these equations is to require that

i) T_0 satisfies extended detailed balance with respect to μ_0,

ii) L satisfies extended detailed balance with respect to $\mu^{(i-1)}$ for $i = 1, \dots, n$,

iii) T_0 satisfies extended detailed balance with respect to $\mu^{(i)}$ for $i = 1, \dots, n$.

However, it turns out that we only need the first two conditions, as the third one is then automatically satisfied.

Theorem 4.14. *Assume that T_0 satisfies extended detailed balance with respect to A and μ_0 and L satisfies extended detailed balance with respect to A and $\mu^{(i)}$ for $i = 0, \dots, n-1$. Then*

(i) $\left(\mu^{(i)}\right)^\top L = 0^\top$ *for* $i = 0, \dots, n-1$.

(ii) $\left(\mu^{(i)}\right)^\top T_\varepsilon = \left(\mu^{(i)}\right)^\top$ *for* $i = 1, \dots, n$.

(iii) T_0 *satisfies extended detailed balance with respect to* $\mu^{(i)}$ *for* $i = 1, \dots, n$.

Proof. *(i)* Let $\mathbf{1}^\top = (1, \dots, 1)$. Then the assumptions give for $i = 0, \dots, n-1$

$$\begin{aligned} \left(\mu^{(i)}\right)^\top L &= \mathbf{1}^\top D_{\mu^{(i)}} L \\ &= \mathbf{1}^\top A L^\top D_{\mu^{(i)}} A. \end{aligned}$$

Because $\mathbf{1}^\top A = \mathbf{1}^\top$ and $\mathbf{1}^\top L^\top = 0^\top$, it follows that $\left(\mu^{(i)}\right)^\top L = 0^\top$.

(ii) We differentiate $\mu_\varepsilon^\top T_\varepsilon = \mu_\varepsilon^\top$ to get

$$\left(\mu^{(i)}\right)^\top T_\varepsilon + \left(\mu^{(i-1)}\right)^\top L = \left(\mu^{(i)}\right)^\top$$

Then the first part immediately gives $\left(\mu^{(i)}\right)^\top T_\varepsilon = \left(\mu^{(i)}\right)^\top$.

(iii) The second part shows that $\mu^{(i)}$ for $i = 1, \dots, n$ is a left eigenvector of T_0 for eigenvalue 1. Because T_0 is block-diagonal and on each block $k = 1, \dots, m$ with unique invariant measure η_k which is also the unique left eigenvector for the eigenvalue 1 for this block, all left eigenvectors of T_0 are linear combinations of the block-invariant measures η_k (considered as vectors in the space $\mathbb{C}^N$). In

particular,

$$\begin{aligned} D_{\mu_0} &= \sum_{k=1}^{m} a_k D_{\eta_k}, a_k \in \mathbb{R}, \\ D_{\mu^{(i)}} &= \sum_{k=1}^{m} a_k^{(i)} D_{\eta_k}, a_k^{(i)} \in \mathbb{R}, \ \ i = 1, .., n. \end{aligned}$$

Define the vector $d_k^{(i)} \in \mathbb{R}^N$ such that $d_k^{(i)} = \frac{a_k^{(i)}}{a_k}$. Then

$$D_{\mu^{(i)}} = D_{d^{(i)}} D_{\mu_0}.$$

Therefore

$$\begin{aligned} D_{\mu^{(i)}} T_0 &= D_{d^{(i)}} D_{\mu_0} T_0 \\ &= D_{d^{(i)}} A T_0^\top D_{\mu_0} A, \end{aligned}$$

and because $D_{d^{(i)}}$ is constant on each block, it commutes with block diagonal matrices. By the assumption that T_0 is block diagonal and that A preserves invariance of S_k, we have $AT_0^\top$ is a block diagonal matrix. That is $D_{\mu^{(i)}} T_0 = AT_0^\top D_{d^{(i)}} D_{\mu_0} A = AT_0^\top D_{\mu^{(i)}} A$. □

What the above theorem is saying is even though we do not know how to construct $T_\varepsilon = T_0 + \varepsilon L$ that satisfies the extended detailed balance exactly with respect to μ_ε, for all ε, because μ_ε's are unknown , it is possible to construct T_ε such that it satisfies the extended detailed balance up to the first order because we only need to construct T_0 and L that satisfy the extended detailed balance with respect to μ_0, which can be done easily using the generalized Metropolis-Hastings algorithm. Of course, for L some steps in Algorithm 4.12 need to be adjusted accordingly, i.e. L can be generated from

$$L(x,y) = \begin{cases} min\left\{1, r_l\left(x,y\right)\right\} K(x,y) & , y \neq a\left(x\right); \\ -\sum_{y \neq a(x)} min\left\{1, r_l(x,y)\right\} K(x,y) & , else, \end{cases}$$

where K is a proposal matrix whose rows sum to 0 and elements in off-diagonal blocks are non-negative, and well-defined $r_l(x,y) = \frac{K(a(y),a(x))\mu_0(a(y))}{K(x,y)\mu_0(x)}$.

In fact, we can do better than the first order approximation. We say a matrix M is A-symmetric if

$$M = AM^\top A.$$

which is actually equivalent to having $M(x,y) = M(a\left(y\right), a\left(x\right))$ for all x, y. Then consider a non-negative block-diagonal A-symmetric matrix S_0 and an A-symmetric matrix R whose off-diagonal blocks are non-negative. These two matrices can be constructed, again, using the generalized Metropolis-Hastings

algorithm, with the ratio

$$r(x,y) \quad = \quad \frac{Q(a(y),a(x))}{Q(x,y)},$$

where Q is some proposition matrix. Additionally, assume that for all x, $\sum_y S_0(x,y) = \sum_y S_0(a(x),y)$ and $\sum_y R(x,y) = \sum_y R(a(x),y)$. Then the matrix $S_\varepsilon = S_0 + \varepsilon R$ is A-symmetric and satisfies

$$\sum_y S_\varepsilon(x,y) \quad = \quad \sum_y S_\varepsilon(a(x),y), \tag{4.4.3}$$

for all ε. Define the matrix U_ε with

$$U_\varepsilon(x,y) \quad = \quad \frac{S_\varepsilon(x,y)}{S_\varepsilon^{(x)}}, \tag{4.4.4}$$

where $S_\varepsilon^{(x)} = \sum_y S_\varepsilon(x,y)$. Then U_ε is a stochastic matrix for small enough ε. Let

$$\mu_\varepsilon(x) \quad = \quad \frac{S_\varepsilon^{(x)}}{\sum_x S_\varepsilon^{(x)}}, \tag{4.4.5}$$

we thus have

Theorem 4.15. *Let U_ε and μ_ε be defined as in (4.4.4) and (4.4.5), respectively. It holds*

(i) μ_ε is an invariant measure of U_ε.

(ii) U_ε satisfies extended detailed balance with respect to μ_ε.

Proof. (i) Obviously, μ_ε is a probability measure. It remains to show the stationarity of μ_ε. We have

$$\begin{aligned}
\mu_\varepsilon^\top U_\varepsilon(y) &= \frac{1}{\sum_x S_\varepsilon^{(x)}} \sum_x S_\varepsilon(x,y) \\
&= \frac{1}{\sum_x S_\varepsilon^{(x)}} \sum_x S_\varepsilon(a(y),a(x)) \\
&= \frac{1}{\sum_x S_\varepsilon^{(x)}} \sum_x S_\varepsilon(y,x) \\
&= \mu_\varepsilon^\top(y),
\end{aligned}$$

where we use the A-symmetry of S_ε and (4.4.3).

(ii) The extended detailed balance follows immediately from the A-symmetry

of S_ε as

$$\begin{aligned}\mu_\varepsilon(x)U_\varepsilon(x,y) &= \frac{1}{\sum_x S_\varepsilon^{(x)}} S_\varepsilon(x,y) \\ &= \frac{1}{\sum_x S_\varepsilon^{(x)}} S_\varepsilon(a(y), a(x)) \\ &= \mu_\varepsilon(a(y))U_\varepsilon(a(y), a(x)).\end{aligned}$$

This finishes the proof. □

Observe that even though U_ε cannot be written as a linear perturbation, U_ε satisfies the extended detailed balance with respect to μ_ε for all ε.

Summary

In this thesis we study the metastable dynamics exhibited by Markov processes. Metastability refers to a property of a process that is likely to stay within some sets of a state space for a long period of time, as compared to the time it spends to transit between these sets. The main approach to identify metastable sets is based on dominant spectral elements of the transfer operator of a Markov process. Much work in the past has been done with the assumption that the Markov process is reversible because, with this condition, the spectral objects have nice properties, e.g. the transfer operator is diagonalizable with respect to an orthonormal basis of eigenvectors and the eigenvalues are real. On the other hand, many interesting processes are not reversible. One important example are the so-called Langevin dynamics, which are often commonly used to describe the dynamics of molecular systems. However, it is found that a Langevin process admits one form of generalized reversibility, namely the *extended detailed balance* (EDB) condition.

Motivated by the spectral approach to metastability, we extended the study to non-reversible processes with EDB. First, we showed that for a Markov chain on a finite state space satisfying the EDB condition with respect to some involution, the associated transfer operator has real dominant eigenvalues and orthogonal dominant eigenvectors with respect to some scalar product defined by the involution. In the spectral analysis we use perturbation theory for linear operators. Based on these dominant spectral properties, we proposed an algorithm to identify metastable sets. The main idea is to use the eigenvalues to determine the number of metastable sets and to use the sign structure of the dominant eigenvectors to determine states that belong to the same metastable set. However, instead of using the eigenvectors of the transfer operator itself, we discovered that using the eigenvectors of the projected transfer operator onto the subspace that is invariant under the involution yields a better yet result. Along with the proposed algorithm, we have established mathematical justifications and numerical examples, including the discretized Langevin dynamics, for illustration.

Zusammenfassung

In dieser Arbeit beschäftigen wir uns mit der Metastabilität von Markovprozessen. Eine Partition von Teilmengen des Zustandsraums heißt metastabil, wenn der Prozess wesentlich mehr Zeit innerhalb der einzelnen Teilmengen verbringt und eher selten zwischen ihnen hin- und herwechselt. Ein wichtiger Ansatz um solche metastabilen Partitionen zu finden basiert auf den dominierenden spektralen Eigenschaften des Transferoperators. Ein großer Teil der bisher erzielten Resultate in der Literatur bezieht sich auf reversible Markovprozesse, da diese wesentlich leichter zu analysieren sind. Beispielsweise ist der Transferoperator dann stets diagonalisierbar bezüglich einer Orthonormalbasis aus Eigenvektoren und hat reelle Eigenwerte. Allerdings sind viele wichtige Prozesse nicht reversibel. Dazu gehören auch Prozesse, die durch Langevin-Gleichungen beschrieben werden, welche oft zur Modellierung von Moleküldynamik verwendet werden. Auch wenn solche Prozesse im Allgemeinen nicht reversibel sind, d.h. der Transferoperator des Prozesses erfüllt nicht die Bedingung der detaillierten Balance, so verfügen sie dennoch über eine verallgemeinerte Form von Reversibilität. Denn der Transferoperator erfüllt die sogenannte erweiterte detaillierte Balance-Bedingung (EDB).

Aufbauend auf dem spektralen Ansatz zur Analyse von Metastabilität, haben wir die zentralen Ideen und Algorithmen erweitert, um auch nicht-reversible Prozesse behandeln zu können, die die EDB-Bedingung erfüllen. Wir haben zunächst Markovketten auf endlichen Zustandsräumen betrachtet, die die EDB-Bedingung erfüllen bezüglich einer Involution, und gezeigt, dass die Eigenwerte des zugehörigen Transferoperators reell sind. Darüberhinaus sind die entsprechenden Eigenvektoren orthogonal bezüglich einem speziellen Skalarprodukt, das über die Involution definiert wird. Unsere Analyse basiert auf der Störungstheorie für lineare Operatoren und dient als Grundlage für einen Algorithmus zur Identifikation von metastabilen Partitionen. Die Hauptideen des Algorithmus bestehen einerseits darin die Anzahl der Teilmengen in der Partition über die Anzahl der dominanten Eigenwerte zu bestimmen, und andererseits darin die Teilmengen selber über die Vorzeichenstruktur der dazugehörigen Eigenvektoren zu berechnen. Eine wichtige Erkenntnis ist, dass wir wesentlich bessere Resultate erzielen, wenn wir den Transferoperator zuvor auf den Unterraum projizieren, der bezüglich der Involution invariant ist. Darüberhinaus haben wir unsere Ergebnisse durch zahlreiche numerische Beispiele illustriert, insbesondere im Bezug auf diskretisierte Langevin-Prozesse, und mathematisch rigoros begründet.

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