Chapter 3

Multiscale Asymptotics with Disparate Transition Scales

In this part of the thesis we return to the Fokker-Planck equation (1.3) and develop a systematic strategy to eliminate the fast degree of freedom that is mathematically rigorous in a suitable asymptotic limit. In so doing, we introduce distinguished time scales that are related to the different dynamical facets of the underlying model.

3.1 Guiding Remarks

Figure 2.1 illustrates the situation where we can apply the conditionally averaged dynamics (1.18) without doubt in order to reproduce the effective dynamics of the original system. An inspection of the picture in Fig. 3.1 shows that transitions in the original dynamics between $B^{(1)}$ and $B^{(2)}$ can additionally be caused by the slow motion due to the x dynamics. However, it is easy to observe that the reduced dynamics (1.21) do not consider the transitions along the x dynamics so that in this case the exchange between the metastable states will be underestimated. Explorating the derivation in [43] of the conditionally averaged stochastic model reveals that the averaged dynamics contained a kind of "boundary term" which was neglected in the situation where the metastable sets do not depend on x. These observations give rise to the following question, the treatment of which requires a rather lengthy technical procedure:

(Q1) If we incorporate the situation illustrated by Fig. 3.1, what is the complete representation of the effective dynamics in the asymptotic limit $\epsilon \to 0$?

To address the question, we return to system (1.1)&(1.2) and reconsider the derivation of the effective x dynamics over an order unity time scale. This time however, we do not use the approximation (1.14), but rather *almost*

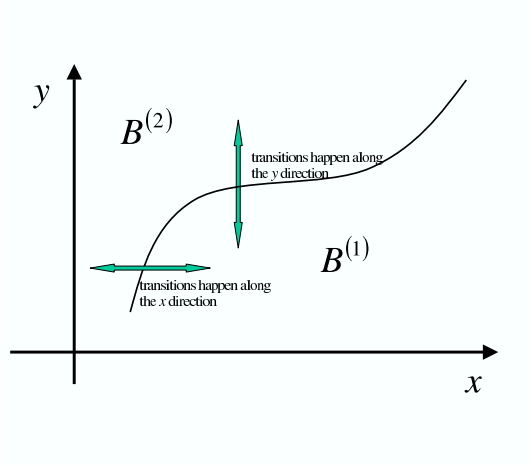

Figure 3.1: An example for the metastable decomposition in the full state space which is obtained by means of the decomposition on the fibre of the fast state space for every fixed x. We observe a decomposition that varies for different slow variable x. In contrast to the situation in Fig. 2.1, in this case transitions can also occur along the direction of the slow variable x.

constant stepfunctions that preserve equality to $u_1(x,\cdot)$. Recalling that the basis of our computation is the Fokker-Planck equation in the weighted space $L^2(\mu)$, a thorough understanding of the averaged dynamics (1.17) can only be achieved, if we can specify the space on which the generator in (1.17) is regarded to act on. This is no problem if we consider $\overline{\mathcal{L}} = \mathrm{diag}(\overline{\mathcal{L}}^{(1)}, \overline{\mathcal{L}}^{(2)})$ by itself, but the combination of $\overline{\mathcal{L}}$ and $\mathcal{Q}_x$ requires a mixed formulation which satisfies both descriptions. These examinations will answer the following question concerning the conditionally averaged dynamics (1.18):

(Q2) On which space is $\mathcal{Q}_x$ regarded to act on, and how do we have to define the space of functions and the corresponding inner product for $\overline{\mathcal{L}} + \mathcal{Q}_x$?

We carry out a detailed examination of the boundary terms that have been neglected for the Conditional Averaging scheme, which moreover requires the construction of a model potential energy landscape in the fast variable that correctly renders the scaling assumption (1.15). Therefore, we will study the following question:

(Q3) How do we have to rescale the potential energy barrier, such that the scaling assumption (1.15) is fulfilled, whereas the rest of the spectrum remains of order unity?

The various kinds of the long-time effective behaviour are then derived by more flexibly linking the time scale separation between slow and fast dynamics from the time scale of the metastable transitions, where we have

to distinguish between transitions along the x direction and those which happen due to the y dynamics. Thus, if metastable transitions (whatever direction) happen on a time scale which is longer than the scale of the slow dynamics we have to introduce a distinguished time scale which has to be considered separately in the asymptotic procedure for the derivation of the reduced dynamics. The goal of the approach 'Multiscale asymptotics with disparate transition scales' is to give a survey of the different scenarios which may appear in the modeling of complex systems. In so doing, we may concentrate on the simplest possible scenario where the metastable decomposition depends on x but only shows two metastable subsets on each fibre $\Phi(y) = \{(x, y) \mid x \in \mathbf{R}\}$; see Fig. 3.1.

Outline. We start from the notion of metastability which is crucial for the understanding of the pursued procedure. Section 3.3 gives a summary of the various kinds of long-time effective behaviour that can emerge from system (1.3). In Section 3.4 we motivate the formal asymptotic procedure. In Section 3.5 we develop the mathematical framework, and reconsider the averaged generator on an order unity time scale. The formal asymptotics follow from Section 3.6.

3.2 Dominant Spectra and Metastability

There are several recent articles on the relation between metastability and dominant eigenmodes of the transfer operator related to the considered dynamical system [11, 19, 20, 39, 41]. Within these approaches, metastability is a *set-wise* notion and conceptually defined in the following way: some dynamical system is said to exhibit metastability or to have a *metastable decomposition* if its state space can be decomposed into a finite (hopefully small) number of disjoint sets such that transitions between these sets are extremely rare [11, 41]. There are basically two different concepts to quantify the "rareness of transitions": (a) via transition probabilities w.r.t. an ensemble of systems and measured as the fraction of systems that exit the set during some fixed finite time interval [39, 41], (b) in case of a stochastic process via the expected exit probability [8], or via the decay rate of the distribution of exit times [20]. However, both concepts (a) and (b) are related to the dominant eigenvectors of the transfer operator. Accordingly, the basic insight of the transfer operator approach to metastability is [41]:

Identification of metastable decompositions. *Metastable decompositions can be detected via the discrete eigenvalues of the transfer operator P_t^ϵ close to its maximal eigenvalue $\lambda = 1$; they can be identified by exploiting structural properties of the corresponding eigenfunctions. In doing so, the number of sets in the metastable decomposition is equal to the number of*

eigenvalues close to 1, *including* $\lambda = 1$ *and counting multiplicity.*

For the diffusion processes $X^\epsilon = (x^\epsilon, y^\epsilon)$ the transfer operator P_t^ϵ is generated by the differential operator $\mathcal{L}^\epsilon$ from (1.4), i.e.,

$$P_t^\epsilon \,=\, \exp(t\mathcal{L}^\epsilon) \quad \text{ in } L^2(\mu),$$

with a suitable extension of $\mathcal{L}^\epsilon$ to $L^2(\mu)$ (cf. [20]).

3.2.1 Dominant Spectrum of the Generator in $L^2(\mu)$

Since $\mathcal{L}^\epsilon$ is self-adjoint in $L^2(\mu)$ its spectrum is real-valued. Moreover, it is non-positive with largest eigenvalue $\lambda_0 = 0$ such that eigenvalues of P_t^ϵ close to its largest eigenvalue 1 correspond to those of $\mathcal{L}^\epsilon$ close to (but smaller than) $\lambda_0 = 0$, while the eigenfunctions are the same in both cases. Consequently, we can extract metastable decompositions from the dominant eigenfunctions of the generator $\mathcal{L}^\epsilon$. The existence of a metastable decomposition into M sets is related in the following manner to the spectrum of $\mathcal{L}^\epsilon$:

Assumption 3.2.1 *There is some positive radius* $R \ll 1$ *such that the intersection of the* $L^2(\mu)$*-spectrum of* $\mathcal{L}^\epsilon$ *with the interval* $[-R, 0]$ *is discrete and contains* M *isolated eigenvalues* $0 = \lambda_0 > \lambda_1 \geq \ldots \geq \lambda_{M-1}$*, where the eigenvalues are repeated according to their multiplicity.*

Rigorous statements on the relation between the dominant spectrum in this sense and the existence of metastable decomposition can be found in [8, 12, 19, 20, 41]. Here, we only mention that whenever the process X^ϵ is geometrically ergodic then the largest eigenvalue λ_0 is an isolated, simple eigenvalue [32]; in [31] sufficient conditions for geometrical ergodicity are given in terms of smoothness and growth of the potential. The eigenfunction corresponding to the largest eigenvalue $\lambda_0 = 0$ of $\mathcal{L}^\epsilon$ is simply given by the constant function $1 \equiv \mathbf{1}(x, y)$:

$$\mathcal{L}^\epsilon \mathbf{1} \,=\, 0.$$

Let us now assume that the spectrum of $\mathcal{L}^\epsilon$ has the form described above and suppose that $M = 2$. Let us denote the eigenfunctions associated with the isolated eigenvalues $\lambda_0 = 0$ and $\lambda_1 < 0$ by u_0 and u_1, respectively. Thus we have a metastable decomposition of the state space $\mathbf{X}$ into two, disjoint sets, B and its complement $B^c = \mathbf{X} \setminus B$, which are defined by the zeros of the second eigenfunction in the following manner:

$$B \,=\, \{(x, y) :\, u_1(x, y) < 0\}, \text{ and } B^c \,=\, \{(x, y) :\, u_1(x, y) \geq 0\}. \tag{3.1}$$

Furthermore, the results of [20] tell us that the second eigenfunction u_1 can be approximated by

$$u_B \;\approx\; \sqrt{\frac{\mu(B^c)}{\mu(B)}}\,\mathbf{1}_B \,-\, \sqrt{\frac{\mu(B)}{\mu(B^c)}}\,\mathbf{1}_{B^c}\,, \tag{3.2}$$

where $\mathbf{1}_B$ denotes the indicator function of the set $B \subset \mathbf{X}$. In fact, the results of [19, 20] show that the deviation $\|u_1 - u_B\|_\mu$ decays exponentially with decreasing noise amplitude σ. The function u_B is constant on either of the two sets B and B^c, is normalized to $\|u_B\|_\mu = 1$, and satisfies $\langle \mathbf{1}_\mathbf{X}, u_B \rangle_\mu = 0$.

3.3 Summary of Effective Dynamics

We present here a categorization of the various kinds of long-time effective behaviour that can emerge from the system (1.3). The formal procedure is shown from the next section. Which scenario is appropriate for a given potential V depends on the ordering of the following three parameters:

- The small parameter ϵ which describes the time scale separation of the y and x motion; it may arise from the original potential being stiffer/steeper along the y direction than along the x direction;
- the parameter δ which describes the order of magnitude of the smallest nonzero eigenvalue of the infinitesimal generator $\mathcal{L}_x$ of the y dynamics;
- the parameter $\tilde{\epsilon}$ which describes the "size" of a certain operator $\overline{\Gamma}_\mathrm{E}$ which describes the metastable transitions induced by the effective x dynamics (on time scale $t \sim \tilde{\epsilon}^{-1}$) after averaging out the fast (but not metastable) y dynamics. The mathematical representation of the operator $\overline{\Gamma}_\mathrm{E}$, and a more precise description of its "size" will be developed in Section 3.5.4 by using an equivalent formulation for the operator; for now, we state simply that the effective x dynamics are described by dynamics within the metastable states, metastable transitions induced by the y dynamics, and metastable transitions induced by the x dynamics. Each of these three dynamical facets are represented by an infinitesimal generator, with $\overline{\Gamma}_\mathrm{E}$ representing the third.

In our ensuing discussion, we will for simplicity consider the case where the spectrum of $\mathcal{L}_x$ can be described by a simple zero eigenvalue, a finite (possibly empty) set of discrete of "small" eigenvalues, all of comparable order of magnitude (δ), and the remainder of the spectrum bounded below by an order unity constant. That is, we assume an asymptotic separation of a finite number of small eigenvalues (the *dominant spectrum* associated to metastable states) from the rest of the spectrum, and assume that the metastable component of the y dynamics can be each described by a single size parameter. We express this assumption (that is the analogue formulation of the general Assumption 3.2.1) mathematically as follows.

Assumption 3.3.1 *There is a small positive integer M and some positive radius $R \gg \delta$ such that for every x the intersection of the $L^2(\mu_x)$-spectrum of $\mathcal{L}_x$ with the interval $[-R, 0]$ is discrete and contains at most M isolated eigenvalues $0 = \lambda_0(x) > \lambda_1(x) \geq ... \geq \lambda_{m(x)}(x)$ with $m(x) < M$.*

Remark 3.3.2 *We will preliminarily ignore the problem that for some x the number of dominant eigenvalues $m(x)+1$ may be smaller than M. Instead we will assume that that there are exactly M eigenvalues in the dominant spectrum for all x. More precisely, if we really have to deal with $m(x)+1 < M$, we will assume that there are additional isolated eigenvalues $\lambda_k(x)$, $k = m(x)+1, ..., M-1$ that play the role needed here but are not contained in the dominant spectrum since $\lambda_k(x) < -R$.*

Let us consider the eigenvalue equation

$$\mathcal{L}_x u_k(x,\cdot) \;=\; \lambda_k(x) u_k(x,\cdot),$$

where $u_0 = \mathbf{1}$, $\lambda_0 = 0$. Throughout the subsequent we will assume that the eigenvectors $\{u_k(x,\cdot)\}$ of $\mathcal{L}_x$ form a complete basis in $L^2(\mu_x)$, such that any function $f(x,\cdot) \in L^2(\mu_x)$ can be expanded by means of

$$f(x,y) \;=\; \sum_k d_k(x)\, u_k(x,y). \tag{3.3}$$

We further assume that the operator $\overline{\Gamma}_{\mathrm{E}}$ describing metastable transitions induced by the x dynamics can be adequately described in terms of a single "size" $\tilde{\epsilon}$ to be defined more precisely in Section 3.5.4. With the above assumptions, the dynamics of a particle described by the equation (1.3) is governed by as many as four time scales:

- the ord(ϵ) time scale of the fast y dynamics, apart from metastable transitions,
- the ord(1) time scale of the x dynamics, apart from metastable transitions,
- the ord($\epsilon\delta^{-1}$) time scale of metastable transitions induced by dynamics along the y direction,
- the ord($\tilde{\epsilon}^{-1}$) time scale of metastable transitions induced by dynamics along the x direction.

The effective dynamics description depends on the ordering of the parameters ϵ, δ, and $\tilde{\epsilon}$, or equivalently, of these four time scales. We always assume $\epsilon \ll 1$ (so that there is a time scale separation of the two coordinates), but allow δ and $\tilde{\epsilon}$ to be small or of order unity, and now summarize the effective dynamics under the various possible orderings of these parameters. We define the effective equations in terms of the function $\rho^0(t,x,y)$ which represents the limiting form of the (weighted) probability density in the asymptotic limit $\epsilon \to 0$ along with the special asymptotics defining the regime under consideration (so for example $\delta \gg \epsilon$ implies a distinguished limit in which $\epsilon\delta^{-1} \to 0$ in addition to $\epsilon \to 0$).

Remark 3.3.3 *For later use it seems necessary to shortly comment on the usage of the relation symbols as defined in the introduction. In order to compare smallness parameters that are of the same order, we can make use of the symbol* 'ord' *as well as* '$\sim$' *and* '$=$'*. The reason for the equivalence is that the smallness parameters δ and $\tilde{\epsilon}$ are connected to a quantity that is of order one. For example, if we assume the second eigenvalue $\lambda_1(x)$ to scale with δ we will write $\lambda_1(x) = \delta\tilde{\lambda}_1(x)$ with $\tilde{\lambda}_1(x) = \mathrm{ord}(1)$. If we want to indicate that δ is comparable to ϵ, we can write $\delta = \mathrm{ord}(\epsilon)$, $\delta \sim \epsilon$, or $\delta = \epsilon$. To give an explicit example: Assuming $\lambda_1(x) = (C\epsilon + \epsilon^2)\tilde{\lambda}_1(x)$, we obtain three different possibilities to denote δ: First, we can establish $\delta = C\epsilon+\epsilon^2 = \mathrm{ord}(\epsilon)$ with $\tilde{\lambda}_1(x) = \mathrm{ord}(1)$; second, we determine $\delta = C\epsilon \sim \epsilon$ with $(1+\epsilon/C)\tilde{\lambda}_1(x) = \mathrm{ord}(1)$; third, we arrange $\delta = \epsilon$ with $(C+\epsilon)\tilde{\lambda}_1(x) = \mathrm{ord}(1)$. The important point is that δ is chosen in such a way that $\lambda_1(x)/\delta = \mathrm{ord}(1)$, which is fulfilled for each of the three relation symbols whenever it applies to one of them. The same consideration will apply in cases where we relate $\tilde{\epsilon}$ to ϵ.*

3.3.1 Standard Averaging: $\delta \gg \epsilon$

In this regime, the y variable relaxes to its invariant distribution on a time scale faster than the x dynamics, so the latter can be described by the standard averaging principle

$$\begin{aligned} \partial_t \rho^0 &= \Pi\mathcal{L}_y\Pi\rho^0, \\ \rho^0(t=0,x) &= f(x), \end{aligned}$$

with Π defined in (1.11), and $\overline{\mathcal{L}}$ is the operator $\mathcal{L}^\epsilon$ averaged against the invariant measure of the y dynamics:

$$\overline{\mathcal{L}} = \Pi\mathcal{L}^\epsilon\Pi = \Pi\mathcal{L}_y\Pi. \tag{3.4}$$

For the Smoluchowski dynamics (1.1)&(1.2), this implies that the motion of the particle along x has effective dynamics governed by an averaged potential related to the usual free energy:

$$\dot{x}^0 = -D_x\overline{V}(x^0) + \sigma\,\dot{W}_1,$$

where

$$\overline{V}(x) = -\frac{1}{\beta}\ln\int \exp(-\beta V(x,y))\,\mathrm{d}y. \tag{3.5}$$

3.3.2 Slow Variable Dynamics Coupled to Metastable Relaxation: $\delta = \mathrm{ord}(\epsilon)$

Here, we suppose that Assumption 3.3.1 is satisfied with $\delta = \mathrm{ord}(\epsilon)$.In this case, the fast variable y evolves into a metastable configuration, which relaxes to its final stationary distribution on the same ord(1) time scale as the

slow x dynamics, so the metastable transitions are coupled to the dynamics in x. In this situation there is only one possibility to obtain the effective dynamics, for the metastable transitions are necessarily dominated by the y dynamics, whereas the x dynamics contribute to metastable transitions on longer time scales $t \gg 1$.

Without loss of generality we can assume $\tilde{\epsilon} \ll 1$ here. In the examples studied in [43], the x dynamics were found to make negligible contribution to the metastable transitions. The effective dynamics on the $t = \mathrm{ord}(1)$ time scale were then found to be well described by the coarse-grained Fokker-Planck equation, which actually must be written as a system:

$$\begin{aligned} \rho^0(t,x,y) &= \sum_{k=1}^{M} c_k(t,x)\chi_k(x,y), \\ \partial_t \vec{c} &= \overline{\mathcal{L}}\,\vec{c} + \mathcal{Q}\,\vec{c}, \end{aligned} \tag{3.6}$$

where $\chi_k(x,\cdot)$ here are approximate indicator functions of the metastable sets $B_x^{(k)}$ (for fixed x) that span the dominant subspace of $\mathcal{L}_x$,

$$\vec{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_M \end{pmatrix},$$

$\overline{\mathcal{L}}$ is a diagonal matrix with operators

$$\overline{\mathcal{L}}^{(k)} = \frac{1}{\mu_x(B_x^{(k)})}\big\langle \chi_k, \chi_k \mathcal{L}_y \cdot \big\rangle_{\mu_x} + \frac{\sigma^2}{\mu_x(B_x^{(k)})}\big\langle \chi_k, D_x\chi_k \big\rangle_{\mu_x}, \tag{3.7}$$

and $\mathcal{Q}$ is the infinitesimal generator of a Markov chain describing jumps between metastable sets $B^{(k)} = \cup_x B_x^{(k)}$ along fibres of constant x. That is, metastable transitions are induced solely by the y dynamics. The inclusion of the indices $k \in \{1,\ldots,M\}$ is needed to track the metastable transitions that are occurring simultaneously with the dynamics of the x variable. The dynamics of the x variable is itself dependent on the metastable set in which the particle is located. The effective equation (3.6) is established rigorously in Section 3.6 for the case $M = 2$, and corresponds to the conditionally averaged system (1.18) as derived in [43].

For Smoluchowski dynamics, the effective x dynamics can be characterized as follows:

$$\dot{x}^0 = -D_x \overline{V}^{(I(t,x))}(x) + \sigma\,\dot{W}, \tag{3.8}$$

where $I(t,x) \in \{1,...,M\}$ evolves according to a Markov chain dynamics with infinitesimal generator (transition rate matrix) depending on the variable x:

$$\mathcal{Q} = \mathcal{Q}_x = \frac{|\lambda_1(x)|}{\epsilon}\begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix}$$

and the potential governing the x dynamics can be considered as asymptotically conditionally averaged over the metastable set in which the particle is momentarily located:

$$\overline{V}^{(i)}(x) = -\frac{1}{\beta} \ln \int \exp(-\beta V(x,y)) \chi_i^2(x,y)\, \mathrm{d}y.$$

A similar conditionally averaged representation of the effective dynamics would appear to be valid for $M > 2$, but has not been established.

3.3.3 Slow Variable Dynamics Followed by Metastable Relaxation: $\delta \ll \epsilon$

Here, Assumption 3.3.1 applies to $\delta = o(\epsilon)$, and we can assume $\tilde{\epsilon} \ll 1$. In this regime, the rate at which the metastable transitions are induced by the y dynamics is much smaller than the rate at which the x dynamics proceed, and the stochastic dynamics will manifest three distinct time scales: the ord(ϵ) time scale over which the y dynamics achieve a metastable configuration, the ord(1) time scale over which the x dynamics proceed and induce the relaxation to the invariant probability density *conditioned upon remaining within one metastable set*, and finally a longer time scale over which the transitions between metastable sets occur and the probability density of the system relaxes to its invariant distribution. To quantify the evolution of the weighted probability density, we then a need a two time-scale description: $\rho^\epsilon = \rho^\epsilon(t, \tau, x, y)$ where τ is a slow time scale on which the metastable relaxation occurs. (A fast time scale t/ϵ would also enter if $\rho^\epsilon|_{t=0}$ were also to depend on y.)

The evolution of the weighted probability density over ord(1) time scales in t is described by the Fokker-Planck equation written as a system:

$$\begin{aligned} \rho^0(t,\tau,x,y) &= \sum_{k=1}^{M} c_k(t,\tau,x)\chi_k(x,y), \\ \vec{c} &= \begin{pmatrix} c_1(t,\tau,x) \\ c_2(t,\tau,x) \\ \vdots \\ c_M(t,\tau,x) \end{pmatrix}, \\ \partial_t \vec{c} &= \overline{\mathcal{L}}\, \vec{c}, \end{aligned} \tag{3.9}$$

where $\overline{\mathcal{L}}$ is the diagonal matrix with the operators $\overline{\mathcal{L}}^{(k)}$ defined in (3.7). For long times, the weighted probability density converges to an M dimensional simplex face:

$$\lim_{t\to\infty} \rho^0(t,\tau,x,y) = \sum_{k=1}^{M} b_k(\tau)\vec{\xi}_k(x)$$

with $\sum_{k=1}^{M} b_k(\tau) = 1$ and the vector functions $\vec{\xi}_k(x)$ span the null space of $\overline{\mathcal{L}}$ and thus are independent of x. The coordinates $b_k(\tau)$ parameterize the metastable configuration of the system, intuitively a linear combination of probabilities for being located within each of the M metastable sets. We made this concrete for the case $M = 2$. The dynamics of these probabilities evolve on a longer time scale (over which metastable transitions occur) according to the system:

$$\vec{b} = \begin{pmatrix} b_1 \\ b_1 \\ \vdots \\ b_M \end{pmatrix}, \qquad \partial_\tau \vec{b} = \Xi \cdot \vec{b} \tag{3.10}$$

with the time scale τ and the (constant) entries in the matrix Ξ depending on the relative ease with which the metastable transitions are induced by the x and y dynamics. We consider in turn the three possible cases.

Final Metastable Relaxation Through Transitions Along Fast Variable Direction: $\tilde{\epsilon} \ll \delta/\epsilon$

When the metastable transitions are dominated by the y dynamics, then the amplitudes appearing in the probability density evolve on the time scale $t \sim \epsilon\delta^{-1}$ (with slow time variable $\tau = \epsilon^{-1}\delta t$), and for $M = 2$ the matrix Ξ is expressed as

$$\Xi = \overline{\mathcal{Q}} = \frac{1}{\delta}\left\langle |\lambda_1|, (\gamma_x)^2 \right\rangle_{\bar{\mu}} \begin{pmatrix} -1/\mu(B^{(1)}) & 1/\mu(B^{(1)}) \\ 1/\mu(B^{(2)}) & -1/\mu(B^{(2)}) \end{pmatrix}, \tag{3.11}$$

where γ_x is given by

$$\gamma_x = \sqrt{\mu_x(B_x^{(1)})\mu_x(B_x^{(2)})}.$$

This metastable relaxation is fairly easy to understand, if we rewrite the entries in $\overline{\mathcal{Q}}$ according to

$$\begin{aligned} \frac{1}{\delta}\left\langle |\lambda_1|, (\gamma_x)^2 \right\rangle_{\bar{\mu}} \frac{1}{\mu(B^{(1)})} &= \int \frac{|\lambda_1(x)|}{\delta} \mu_x(B_x^{(2)})\, \bar{\mu}^{(1)}(x)\, \mathrm{d}x, \\ \frac{1}{\delta}\left\langle |\lambda_1|, (\gamma_x)^2 \right\rangle_{\bar{\mu}} \frac{1}{\mu(B^{(2)})} &= \int \frac{|\lambda_1(x)|}{\delta} \mu_x(B_x^{(1)})\, \bar{\mu}^{(2)}(x)\, \mathrm{d}x. \end{aligned}$$

The rates of transition are now constants, the x-dependence of the transition rates induced by the y dynamics along a fibre of constant x are now averaged with respect to the invariant probability distribution of the conditionally averaged x dynamics:

$$\bar{\mu}^{(i)}(x) \sim \exp(-\beta \overline{V}^{(i)}(x)), \qquad i = 1, 2.$$

These equations are derived in Section 3.7.1 for the case $\delta = \epsilon^2$.

Final Metastable Relaxation Through Transitions along Both Fast and Slow Variable Directions: $\tilde{\epsilon} = \mathrm{ord}(\delta/\epsilon)$

When metastable transitions are induced by both the x and y dynamics, the transition rates describing the metastable relaxation on time scale $t \sim \tilde{\epsilon}^{-1} \sim \epsilon\delta^{-1}$ (with time variable $\tau = \epsilon^{-1}\delta t = \tilde{\epsilon}\, t$) include now some more complicated contributions arising from the x dynamics. For the case $M = 2$ the matrix Ξ is now given by

$$\Xi = \overline{\mathcal{Q}} + |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix}, \tag{3.12}$$

where the matrix $\overline{\mathcal{Q}}$ is taken from (3.11) and $\bar{\lambda}_1^{(1)}$ is the eigenvalue of the matrix containing some 'exchange' terms and restricted to the nullspace of the generator $\overline{\mathcal{L}}$. The value is given explicitly by

$$\bar{\lambda}_1^{(1)} = \frac{1}{\tilde{\epsilon}} \big\langle (\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2) \big\rangle_\mu$$

with

$$\alpha_1 = \sqrt{\frac{\mu(B^{(2)})}{\mu(B^{(1)})}}, \qquad \alpha_2 = -\sqrt{\frac{\mu(B^{(1)})}{\mu(B^{(2)})}}.$$

These equations are derived for the case $\delta = \epsilon^2$ in Section 3.7.2.

Final Metastable Relaxation Through Transitions Along Slow Variable Direction: $\delta \ll \epsilon\tilde{\epsilon} \ll \epsilon$

If the x dynamics induce metastable transitions faster than the y dynamics do, then the metastable relaxation occurs on time scale $t \sim \tilde{\epsilon}^{-1}$, and the effective dynamics for the (weighted) probability density reads with the slow time scale $\tau = \tilde{\epsilon}\, t$. The equation for the effective dynamics is the same as in Section 3.3.3 except the terms representing the metastable transitions arising from the y dynamics are omitted (and the equation is set on a longer time scale). These are derived for the case $\delta = \epsilon^2$ in Subsection 3.7.3 and have for $M = 2$ the following form:

$$\begin{aligned} \partial_\tau \vec{b} &= \overline{\mathcal{E}}\, \vec{b}, \\ \overline{\mathcal{E}} &= |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix}. \end{aligned}$$

3.3.4 Interpretation for the Case $\delta = \mathcal{O}(\epsilon)$

For ease of presentation, we summarize the averaged dynamics in Figure 3.2, where we have assumed that the fast dynamics exhibit metastability being expressed by $\delta = \mathcal{O}(\epsilon)$. In this situation, we have $\tilde{\epsilon} \ll 1$.

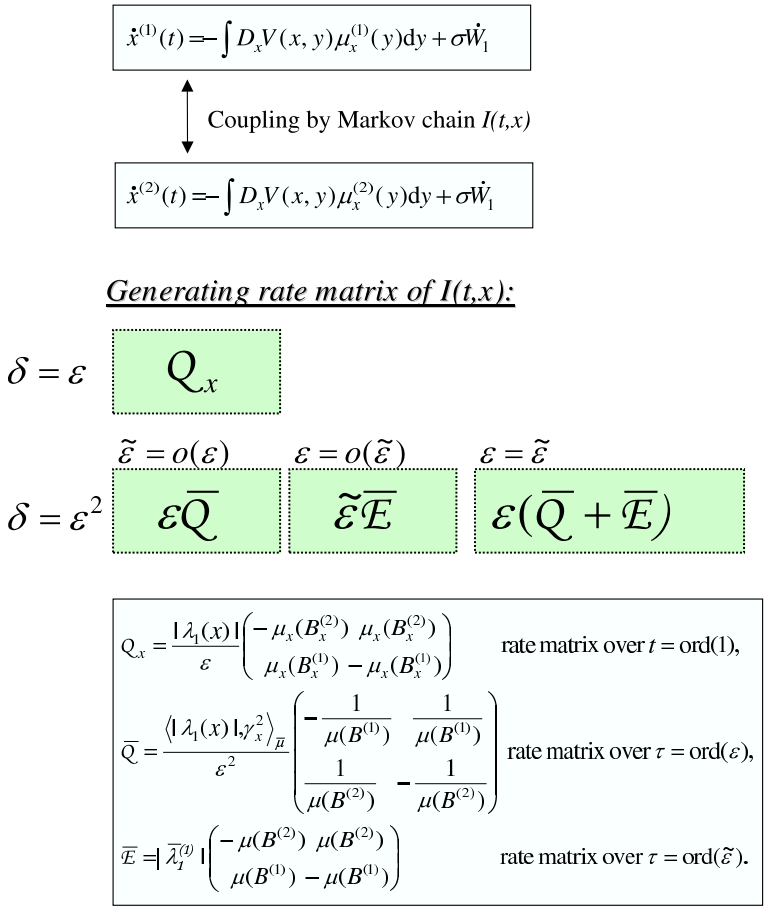

Figure 3.2: Graphical illustration of the averaged models. The various kinds of effective long-time behaviour vary solely in the exchange term that controls the switches between the two averaged Smoluchowski dynamics over time t =ord(1). The matrices $\overline{\mathcal{Q}}$ and $\overline{\mathcal{E}}$ have to be considered on longer time scales with time variables $\tau = \epsilon\, t$ and $\tau = \tilde{\epsilon}\, t$, respectively. A discretizeable scheme is obtained by switching to the equivalent picture $\epsilon\,\overline{\mathcal{Q}}$ and $\tilde{\epsilon}\,\overline{\mathcal{E}}$ which then have to be considered over time t. The same applies to $\overline{\mathcal{Q}} + \overline{\mathcal{E}}$.

3.3.5 Arising Problems

The problems that aim directly for the numerical feasibility, such as the construction of examples tailored to the different cases, will not be considered here. In this direction the main problem will be to decide whether the exchange term for the metastable x transitions accounts adequately for the effective x dynamics or not. A qualitative possibility in which the metastable transitions induced by the x dynamics may be of most importance is illustrated in the right picture of Fig. 3.3. Moreover, as schematically illustrated in the left panel of Fig. 3.3, it is not so clear what it means to talk about metastable transitions along x or y (should going across at a significant diagonal count as an x transition?).

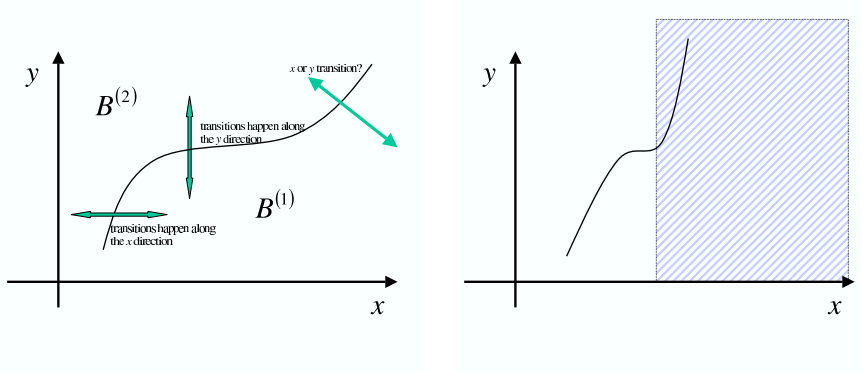

Figure 3.3: Metastable subsets $B^{(1)}$ and $B^{(2)}$ can also depend on x. The regime to the right shows a qualitative possibility in which the metastable transitions may be dominated by the x dynamics. In particular, for the marked region we observe that the decomposition does *almost* not depend on y.

The pursued approach can only be seen as a first effort to develop an asymptotic strategy that combines averaging techniques with the ensemble approach to metastability. There are a number of directions for future development of this subject. Even the easiest scenario with a decomposition into exactly two metastable subsets on every fibre of the fast state space gives rise to some obscurities. In the situation illustrated in the left panel of Fig. 3.3 we may apply the methodology of the approach for sure, but one could also contemplate a situation, such as that schematically indicated at the left-hand side of Fig. 3.4. We observe that for fixed fast variable y there

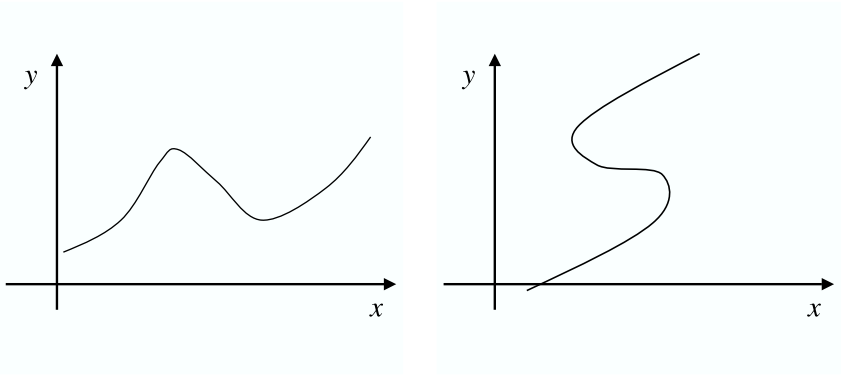

Figure 3.4: Left: For fixed y, there could be as many as 4 metastable regimes for the x variable. Right: For fixed x, there could be as many as $M = 4$ metastable regimes for the y variable.

could be as many as 4 metastable regimes for the x variable. In this situation it is not so clear if the exchange term for the metastable x transitions effectively recovers what is going on, and a possible interpretation of the origin of the term will be complicated, for the generator $\mathcal{L}_y$ could have four

dominant eigenvalues in this case.

In a more general setting we could assume the decomposition considered within the full state space to consist of two metastable subsets. A possible example is illustrated at the right-hand side of Fig. 3.4, where we observe as many as $M = 4$ metastable regimes for the y variable for a fixed value of x. Here, the metastability can be relaxed not only by transitions over the ridge induced by the y dynamics, but by moving around the ridge through joint x and y motion. We have established the effective equations for the case $M = 2$, and one of the directions for future development is to generalize the approach to $M > 2$ metastable subsets (Fig. 3.5).

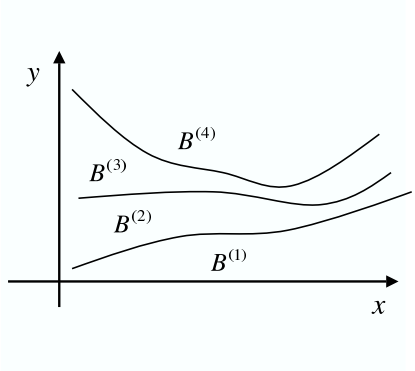

Figure 3.5: Metastable decomposition into $M = 4$ metastable subsets $B^{(1)}, ..., B^{(4)}$.

3.4 Multiscale Aymptotics and Averaging

We illustrate the method of averaging by using multiscale asymptotics of the solution of the Fokker-Planck equation (1.3). This is the major tool that we use to derive stochastic model equations for the slow variable alone in the limit $\epsilon \to 0$.

3.4.1 Standard Averaging

Here, we consider the situation with no temporal fast scale effects, i.e., the fast DOF sample the accessible state space entirely before the slow ones effectively change. In this case, the averaged system for timescale t is obtained by applying the original theorem of Kurtz [25].

We study the case where the initial condition $\rho^\epsilon(t = 0, x, y) = f(x)$ depends on x only. We now make the following ansatz for the solution of the Fokker-Planck equation (1.3) with the initial conditions described above:

$$\rho^\epsilon = \rho^0 + \epsilon\,\rho^1 + \epsilon^2\,\rho^2 + ... \tag{3.13}$$

This ansatz is inserted into the Fokker-Planck equation and then, by comparison of coefficients of different powers of ϵ we get:

$$\epsilon^{-1} \; : \quad \mathcal{L}_x \rho^0 = 0 \tag{3.14}$$

$$\epsilon^{0} \; : \quad \mathcal{L}_x \rho^1 + \mathcal{L}_y \rho^0 = \partial_t \rho^0 \tag{3.15}$$

$$\epsilon^{1} \; : \quad \mathcal{L}_x \rho^2 + \mathcal{L}_y \rho^1 = \partial_t \rho^1 \tag{3.16}$$

1. step: (3.14) immediately yields that ρ^0 does not depend on y, i.e, with the help of the projection operator Π from (1.11) we obtain

$$\Pi \rho^0 = \rho^0.$$

2. step: Let Π act on (3.15) and use $\Pi \mathcal{L}_x = 0$. This time

$$\partial_t \rho^0 = \Pi \mathcal{L}_y \rho^0 = \Pi \mathcal{L}_y \Pi \rho^0.$$

Let us abbreviate

$$\overline{\mathcal{L}} = \Pi \mathcal{L}_y \Pi.$$

Since $\mathcal{L}_y$ contains derivatives wrt. x only, we immediately see that

$$\overline{\mathcal{L}} = \frac{\sigma^2}{2} \Delta_x - (\Pi D_x V) \cdot D_x, \quad \text{acting on } L^2(\bar{\mu}).$$

One easily computes that $\Pi D_x V$ can again be expressed as the gradient of the averaged potential, i.e., $\Pi D_x V = D_x \overline{V}$ with $\overline{V}$ defined in (3.5). Thus, ρ^0 is determined by a Fokker-Planck equation with averaged potential, and its solution gives us ρ^ϵ up to error $\mathcal{O}(\epsilon)$. The associated SDE

$$\dot{x}^0 \;\; = \;\; -D_x \overline{V}(x^0) + \sigma \dot{W}_1 \tag{3.17}$$

thus describes the limit dynamics of (1.1)&(1.2) in the sense that its solution satisfies $x^\epsilon \to x^0$ as $\epsilon \to 0$ either pathwise [15], or in the distributional sense [25, 29]. Obviously, the invariant measure of the averaged dynamics (3.17) is given by $\bar{\mu}$ as given in (1.10). We additionally can represent $\bar{\mu}$ via

$$\bar{\mu}(x) = \frac{1}{Z} \exp(-\beta \overline{V}(x)).$$

3.4.2 Strategy under Consideration of Fast Scale Effects

In this section, we generalize the result of the last section by incorporating temporal fast scale effects into the multiscale asymptotics of (1.3). These effects are reflected in the dominant spectrum of the infinitesimal generator $\mathcal{L}_x$ corresponding to the second equation of (1.2). As shown in [43], the spectral gap $\delta_x = |\lambda_1(x)|$ of $\mathcal{L}_x$ wrt. its lowest eigenvalue $\lambda_0 = 0$ may serve as an indicator for the inappropriateness of the asymptotic procedure

introduced in Section 3.4.1: If the inequality $\epsilon \ll \delta_x$, which establishes a relation between the time scale of the fast motion and the exit rate/time from metastable subsets in the fast DOF, does not hold, deviations from the averaged dynamics (3.17) have to be anticipated[1]. If we want to study the effect of δ_x being comparable or smaller than ϵ by means of multiscale asymptotics, the averaging method must be modified by an explicit coupling of δ_x to ϵ, i.e., $\delta_x \sim \epsilon^r$, $r \geq 1$. In order to account for the fast scale effects, we have to decompose the operator $\mathcal{L}_x$ into a part $\mathcal{R}_x$ (which then is the only one entering the equation (3.14)) and a finite-dimensional part $\epsilon^r \mathcal{L}_x^{\text{act}}$ accounting for the fast scale effects. However, we will distinguish between the situation where $\delta_x \sim \epsilon$ and the situation where $\delta_x \ll \epsilon$. The reason for this distinction is that the situation with $\delta \ll \epsilon$ requires an additional timescale $\tau = \text{ord}(\delta)/\epsilon$ representing the metastable transitions along the y-direction. However, in this case we will restrict the formal asymptotic derivation of the averaged equations to $\delta \sim \epsilon^2$. The case of $\delta \sim \epsilon$ is considered in Section 3.6 and the case of $\delta \sim \epsilon^2$ in Section 3.7. The key step in both situations is to exploit the basic approach for the identification of metastable conformations which justifies the expression of the dominant eigenfunctions in terms of approximate step functions which are almost constant on the metastable subsets. In Section 3.5.1 we establish the necessary background and notation tailored to the situation where the metastable decomposition of the fast state space depends on the slow variable x.

Motivation

The key assumption which we utilize here is that the dominant spectrum of $\mathcal{L}_x$ scales with δ for $\delta = \mathcal{O}(\epsilon)$, that is, we assume $\lambda_k(x) = \delta\tilde{\lambda}_k(x)$, $k = 0, ..., M-1$, with $\tilde{\lambda}_k = \text{ord}(1)$, while the remainder of the spectrum is left unchanged, i.e., contributes to order ord(1) only. Explicitly:

$$\sigma(\mathcal{L}_x) \quad \subset \quad \{0, \delta\tilde{\lambda}_1(x), ..., \delta\tilde{\lambda}_{M-1}(x)\} \cup [-R, -\infty). \tag{3.18}$$

As a consequence we can express $\mathcal{L}_x$ in the following form:

$$\mathcal{L}_x \quad = \quad \delta \sum_{k=0}^{M-1} \tilde{\lambda}_k(x) \langle \cdot, u_k(x, \cdot) \rangle_{\mu_x} u_k \, + \, \mathcal{R}_x \, = \, \delta \mathcal{L}_x^{\text{act}} \, + \, \mathcal{R}_x, \tag{3.19}$$

with $\mathcal{R}(\mathcal{R}_x) \subset \mathcal{N}(\mathcal{L}_x^{\text{act}})$ and $\mathcal{R}(\mathcal{L}_x^{\text{act}}) \subset \mathcal{N}(\mathcal{R}_x) = \{u_k(x, \cdot) \,|\, k = 0, ..., M-1\}$ with $\mathcal{N}(A)$ and $\mathcal{R}(A)$ denoting the nullspace and range of an operator A, respectively.

[1] This result is easily obtained by replacing $\partial_t \rho^0$ in equation (3.15) by $\overline{\mathcal{L}}\rho^0$ and resolving the equation wrt. $(\text{Id} - \Pi)\rho^1$.

With the decomposition of $\mathcal{L}_x$ according to (3.19) the infinitesimal generator $\mathcal{L}^\epsilon$ in the Fokker-Planck equation (1.3) is given by

$$\mathcal{L}^\epsilon \;=\; \frac{1}{\epsilon}\mathcal{R}_x \,+\, \mathcal{L}_y \,+\, \epsilon^{r-1}\mathcal{L}_x^{\rm act}, \qquad \delta = \epsilon^r, \tag{3.20}$$

which nicely illustrates that for $r > 1$ we need a two time scale description $\rho^\epsilon = \rho^\epsilon(t, \tau, x, y)$ with $\tau = \epsilon^{r-1}t$. To motivate our further approach let us assume $\delta = \epsilon^2$ and expand $\rho^\epsilon = \rho^\epsilon(t, \tau, x, y)$ wrt. powers of ϵ. As before, we will assume that $\rho^\epsilon(t = 0, \tau = 0, x, y) = f(x)$, i.e., the initial density depends only on the slow variable x. Thus, we seek for a formal asymptotic solution of (1.3) with to distinguished timescales

$$\rho^\epsilon(t, \tau, x, y) \;=\; \rho^0(t, \tau, x, y) + \epsilon\,\rho^1(t, \tau, x, y) + \epsilon^2\,\rho^2(t, \tau, x, y) + ..., \quad \tau \;=\; \epsilon\, t.$$

We treat these two times scales as if they were independent which is consistent to the separation of scales between t and τ. Thus, we set

$$\frac{\partial}{\partial t} \;\mapsto\; \frac{\partial}{\partial t} \,+\, \epsilon\frac{\partial}{\partial \tau}.$$

If we repeat the procedure of Section 3.4.1, we observe that we have to replace $\mathcal{L}_x$ by $\mathcal{R}_x$ in equation (3.14) to get the solvability condition for ρ^0: $\rho^0 \in \mathcal{N}(\mathcal{R}_x)$. Thus, the simple idea here is to project the dynamics onto the subspace spanned by the dominant spectrum of the generator $\mathcal{L}_x$, which we make rigorous by introducing the projection operator $\tilde{\Pi}$:

$$(\tilde{\Pi} f)(x, \cdot) \;=\; \sum_{k=0}^{M-1} \big\langle f, u_k(x, \cdot)\big\rangle_{\mu_x}\, u_k(x, \cdot). \tag{3.21}$$

Considering $\tilde{\Pi}$ in $L^2(\mu_x)$, it is the orthogonal projection onto the nullspace of $\mathcal{R}_x$, i.e., $\mathcal{R}(\tilde{\Pi}) = \mathcal{N}(\mathcal{R}_x)$, such that the next order of comparison of coefficients yields (after applying $\tilde{\Pi}$):

$$\partial_t \rho^0 \;=\; \tilde{\Pi}\mathcal{L}_y\tilde{\Pi}\rho^0, \qquad \text{for } \rho^0 \in \mathcal{R}(\tilde{\Pi}).$$

If we express ρ^0 by means of the orthonormal basis $\{u_0, u_1, ..., u_{M-1}\} \subset L^2(\mu_x)$ of $\mathcal{R}(\tilde{\Pi})$, the above evolution equation for ρ^0 results in a system of equations for the coefficients $A_i(t, \tau, x) := \langle \rho^0(t, \tau, x, \cdot), u_i(x, \cdot)\rangle_{\mu_x}$, $i = 0, ..., M-1$:

$$\begin{pmatrix} \partial_t A_0 \\ \partial_t A_1 \\ \vdots \\ \partial_t A_{M-1} \end{pmatrix} \;=\; \Gamma \begin{pmatrix} A_0 \\ A_1 \\ \vdots \\ A_{M-1} \end{pmatrix}, \tag{3.22}$$

with $\Gamma = (\Gamma_{ij})$ being an M-dimensional matrix with entries

$$\Gamma_{ij} \;=\; \big\langle u_{i-1}, \mathcal{L}_y(\cdot\, u_{j-1})\big\rangle_{\mu_x}, \qquad i, j = 1, ..., M. \tag{3.23}$$

If we assume Γ to be dissipative (this is shown below in Section 3.5.1), the solution $\vec{A} = (A_0, ..., A_{M-1})^T$ of (3.22) is then expressed as

$$\vec{A}(t, \tau, x) \;=\; \exp(t\Gamma)\vec{A}(t = 0, \tau, x),$$

where Γ generates a stationary process such that

$$\exp(t\Gamma)\cdot \;\to\; P\cdot, \qquad \text{as } t \to \infty.$$

This already tells us that the solution on the longest timescale τ has to be in the range of the projection operator P.

Further Development. The previous motivation tells us that the projection onto the dominant subspace yields a reduced dynamical model for the time scale of the slow variable dynamics that will have a rigorous justification under the scaling assumption (3.19) with $\delta = \epsilon^2$. Before evaluating the motion on the longest time scale τ or considering different scenarios such as $\delta \sim \epsilon$, it is of most importance for us to obtain a physical understanding of the evolution equation $\partial_t \vec{A} = \Gamma \vec{A}$. Unfortunately, a simple evaluation of the involved terms $\Gamma_{ij} A_j$ in (3.23) will not allow for a lucid interpretation or for some simple discretization scheme. However, using the fact that the dominant eigenfunctions u_i (for fixed x) as a collectivity define the metastable decomposition, allows us to switch from the orthonormal basis $\{u_0, ..., u_{M-1}\}$ to an orthogonal basis $\{\chi_1, ..., \chi_M\}$ that approximates the characteristic functions on the metastable states. With some patience it is then possible to construct an equivalent formulation of system (3.22) that models the evolution of the coefficients wrt. $\{\chi_i \mid i = 1, ..., M\}$, and allows for an intriguing interpretation.

3.5 Averaged Generator over ord(1) Time Scale

Throughout the subsequent we will assume $M = 2$, such that for every x we do have two metastable subsets along the y direction. In a first step, we substitute the dominant eigenfunctions $u_0(x, \cdot) = \mathbf{1}$ and $u_1(x, \cdot)$ for *almost* characteristic functions $\chi_1, \chi_2 \in \text{span}\{\mathbf{1}, u_1(x, \cdot)\}$, approximately assembling the metastable decomposition of the fast dynamics. This allows us to reformulate the evolution equations (3.22) for the coefficients A_0, A_1 by an equivalent formulation $\partial_t \vec{c} = \Upsilon \vec{c}$ for the coefficients c_1, c_2 wrt. the basis $\{\chi_1, \chi_2\}$. Evaluating the operator Υ will admit for a decomposition of Υ reflecting the different dynamical facets of the x dynamics: One term represents $M = 2$ independent Fokker-Planck generators where each describes the averaged dynamics *within* one metastable set; the other term represents the interplay between these generators ascribing to transitions *between* the metastable subsets which happen (in the full dynamics) along the x direction.

In Section 3.5.1 we develop the mathematical framework that will allow us to derive an interpretable system from (3.22). In so doing, we define the transformation from $\{\mathbf{1} = u_0, u_1\}$ to the orthogonal basis $\{\chi_1, \chi_2\}$, which then allows us to optionally switch between the corresponding coefficients A_0, A_1 and c_1, c_2. We derive the evolution equation $\partial_t \vec{c} = \Upsilon \vec{c}$ that is equivalent to $\partial_t \vec{A} = \Gamma \vec{A}$. In Section 3.5.2 we show how to decompose the generator $\Upsilon = \overline{\mathcal{L}} + \overline{\mathcal{L}}_{\mathrm{B}} + \overline{\mathcal{L}}_{\mathrm{E}}$, where $\overline{\mathcal{L}}$ denotes a Fokker-Planck generator of order one. The extra terms $\overline{\mathcal{L}}_{\mathrm{B}}$ and $\overline{\mathcal{L}}_{\mathrm{E}}$ go far beyond the order one scale, which is shown in Section 3.5.3. The term $\overline{\mathcal{L}}_{\mathrm{B}}$ can be skipped , whereas $\overline{\mathcal{L}}_{\mathrm{E}}$ contributes to higher order terms. According to $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$, in Section 3.5.4 we introduce a smallness parameter $\tilde{\epsilon}$ describing the size of $\overline{\mathcal{L}}_{\mathrm{E}} = \tilde{\epsilon}\widehat{\mathcal{L}}_{\mathrm{E}}$. For $\overline{\mathcal{L}} + \tilde{\epsilon}\widehat{\mathcal{L}}_{\mathrm{E}}$ we then use perturbation methods to obtain the relevant part of $\overline{\mathcal{L}}_{\mathrm{E}}$ that will be used to explicitly derive the dynamics evolving on the longest time scale $t \gg 1$. In Section 3.5.5 we give a short summary of the main results and show how to assign them to the formulation with coefficients A_0, A_1.

3.5.1 Preparatory Work

We suppose that Assumption 3.3.1 is satisfied for $M = 2$. Then, for each fixed x, the zero of the second eigenvector $u_1(x, \cdot)$ of $\mathcal{L}_x$ in $L^2(\mu_x)$ decomposes the fibre $\Phi(x) = \{(x, y) \mid y \in \mathbf{R}\}$ according to:

$$B_x^{(1)} = B_x = \{y \mid u_1(x, y) < 0\}, \qquad B_x^{(2)} = B_x^c = \{y \mid u_1(x, y) \geq 0\}.$$

Therefore, the metastable decomposition in the entire state space of the (x, y) dynamics is

$$B^{(1)} = \{(x, y) \mid u_1(x, y) < 0\}, \qquad B^{(2)} = \{(x, y) \mid u_1(x, y) \geq 0\}.$$

Let us denote the indicator functions of $B_x^{(1)}$ and $B_x^{(2)}$ by $\mathbf{1}_{B_x^{(1)}}$ and $\mathbf{1}_{B_x^{(2)}}$ such that $\mathbf{1}_{B_x^{(1)}} + \mathbf{1}_{B_x^{(2)}} = \mathbf{1}(x, \cdot)$. Now, remember that due to (3.2) u_1 is an approximate stepfunction:

$$u_1(x, \cdot) \approx \sqrt{\frac{\mu_x(B_x^{(2)})}{\mu_x(B_x^{(1)})}}\mathbf{1}_{B_x^{(1)}} - \sqrt{\frac{\mu_x(B_x^{(1)})}{\mu_x(B_x^{(2)})}}\mathbf{1}_{B_x^{(2)}}. \tag{3.24}$$

For abbreviation we set

$$\alpha_1^x = \sqrt{\frac{\mu_x(B_x^{(2)})}{\mu_x(B_x^{(1)})}}, \quad \alpha_2^x = -\sqrt{\frac{\mu_x(B_x^{(1)})}{\mu_x(B_x^{(2)})}} \quad \Rightarrow \quad \alpha_2^x = -\frac{1}{\alpha_1^x}. \tag{3.25}$$

Resolving (3.24) wrt. $\mathbf{1}_{B_x^{(i)}}$ for $i = 1, 2$ yields

$$\begin{aligned} \mathbf{1}_{B_x^{(1)}} &\approx \mu_x(B_x^{(1)})\mathbf{1} + \gamma_x\, u_1(x, \cdot), \\ \mathbf{1}_{B_x^{(2)}} &\approx \mu_x(B_x^{(2)})\mathbf{1} - \gamma_x\, u_1(x, \cdot), \end{aligned}$$

where

$$\gamma_x \;=\; \langle u_1, \mathbf{1}_{B_x^{(1)}} \rangle_{\mu_x} \;=\; -\langle u_1, \mathbf{1}_{B_x^{(2)}} \rangle_{\mu_x} \;=\; \sqrt{\mu_x(B_x^{(1)})\mu_x(B_x^{(2)})}. \quad (3.26)$$

For the next steps we replace $\mathbf{1}_{B_x^{(i)}}$, $i = 1, 2$ by functions $\chi_1(x,\cdot)$, $\chi_2(x,\cdot)$ such that we get equality in (3.24):

$$\chi_1 \;=\; \mu_x(B_x^{(1)})\mathbf{1} \,+\, \gamma_x\, u_1, \quad (3.27)$$

$$\chi_2 \;=\; \mu_x(B_x^{(2)})\mathbf{1} \,-\, \gamma_x\, u_1. \quad (3.28)$$

Then, $\{\chi_1(x,\cdot), \chi_2(x,\cdot)\}$ is an orthogonal basis of $\mathrm{span}\{u_0(x,\cdot), u_1(x,\cdot)\}$ in $L^2(\mu_x)$. Thus, we can reformulate our ansatz $\rho^0 = A_0 u_0 + A_1 u_1$ in the following form:

$$\rho^0(t,x,y) \;=\; c_1(t,x)\chi_1(x,y) \,+\, c_2(t,x)\chi_2(x,y).$$

This allows us to reformulate the evolution system (3.22) by equivalent equations for the coefficients $c_1(t,x)$, $c_2(t,x)$ instead, where we have to carefully distinguish between the different spaces for the coefficients. To this end, it is reasonable to define additional measures $\mu^{(i)}(\mathrm{d}x, \mathrm{d}y)$, $\mu_x^{(i)}(\mathrm{d}y)$, $\bar{\mu}^{(i)}(\mathrm{d}x)$ for $i = 1, 2$ which correspond to the probability densities

$$\mu^{(i)}(x,y) \;=\; \frac{1}{\mu(B^i)}\,\mu(x,y)\,\chi_i^2(x,y), \quad (3.29)$$

$$\bar{\mu}^{(i)}(x) \;=\; \int \mu^{(i)}(x,y)\,\mathrm{d}y, \quad (3.30)$$

$$\mu_x^{(i)}(y) \;=\; \frac{1}{\bar{\mu}^{(i)}(x)}\,\mu^{(i)}(x,y). \quad (3.31)$$

The relation $\chi_i(x,\cdot) \approx \mathbf{1}_{B_x^{(i)}}$ allows us to interpret $\mu^{(i)}$ as the (approximate) restriction of the 'full' measure μ to the set $B^{(i)}$. Hence, the analogy of $\mu_x^{(i)}$, $\bar{\mu}^{(i)}$ to the definitions of μ_x, $\bar{\mu}$ is obvious. For the definition of $\mu^{(i)}$ we used χ_i^2 instead of χ_i to guarantee positivity of the density. Squaring of χ_i has no effect on the density $\bar{\mu}^{(i)}$ due to

$$\int \mu(x,y)\,\chi_i^2(x,y)\,\mathrm{d}y \;=\; \int \mu(x,y)\,\chi_i(x,y)\,\mathrm{d}y \;=\; \mu_x(B_x^{(1)})\,\bar{\mu}(x). \quad (3.32)$$

Now, the transformation from $\vec{A} = (A_0(x), A_1(x))^T$ to $\vec{c} = (c_1(x), c_2(x))^T$ (and vice versa) is described by matrices $\mathcal{S}$ and $\tilde{\mathcal{S}}$ which are given by

$$\mathcal{S} \;=\; \begin{pmatrix} \mathbf{1}(x) & \alpha_1^x \\ \mathbf{1}(x) & \alpha_2^x \end{pmatrix} \qquad \Rightarrow \quad \mathcal{S}\begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \quad (3.33)$$

$$\tilde{\mathcal{S}} \;=\; \begin{pmatrix} \mu_x(B_x^{(1)}) & \mu_x(B_x^{(2)}) \\ \gamma_x & -\gamma_x \end{pmatrix} \quad \Rightarrow \quad \tilde{\mathcal{S}}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} A_0 \\ A_1 \end{pmatrix}. \quad (3.34)$$

Considering $\mathcal{S}$ and $\tilde{\mathcal{S}}$ as operators acting on functions of x requires the specification of domain and range. The implications

$$A_i\, u_i \,\in\, L^2(\mu) \quad \text{for } i=0,1 \quad\Longleftrightarrow\quad c_j\,\chi_j \,\in\, L^2(\mu^{(j)}) \quad \text{for } j=1,2,$$

suggest to define the spaces

$$\mathbf{L} := L^2(\bar{\mu}) \times L^2(\bar{\mu}), \qquad\qquad \mathbf{H} := L^2(\bar{\mu}^{(1)}) \times L^2(\bar{\mu}^{(2)}), \tag{3.35}$$

such that we obtain

$$\mathcal{S} : \mathbf{L} \,\to\, \mathbf{H}, \qquad\qquad \tilde{\mathcal{S}} : \mathbf{H} \,\to\, \mathbf{L}.$$

We easily verify this by using Hoelder's inequality, the fact that $L^2(\bar{\mu}) \subset L^2(\bar{\mu}^{(i)})$, and

$$\mu_x(B_x^{(i)}) \cdot c_i \in L^2(\bar{\mu}) \quad \text{ for } c_i \in L^2(\bar{\mu}^{(i)}).$$

The inner products of $L^2(\bar{\mu})$ and $L^2(\bar{\mu}^{(i)})$ for $i=1,2$ are given by

$$\begin{aligned} \langle f,g\rangle_{\bar{\mu}} &= \int f(x)\, g(x)\, \bar{\mu}(x)\, \mathrm{d}x, \qquad f,g \in L^2(\bar{\mu}), \\ \langle f,g\rangle_{\bar{\mu}^{(i)}} &= \int f(x)\, g(x)\, \bar{\mu}^{(i)}(x)\, \mathrm{d}x, \qquad f,g \in L^2(\bar{\mu}^{(i)}). \end{aligned}$$

Then, $\mathbf{L}$ and $\mathbf{H}$, endowed with the inner products

$$\left\langle \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle_{\mathbf{L}} = \sum_{i=1}^{2} \langle f_i, g_i\rangle_{\bar{\mu}}, \tag{3.36}$$

$$\left\langle \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle_{\mathbf{H}} = \sum_{i=1}^{2} \mu(B^i)\, \langle f_i, g_i\rangle_{\bar{\mu}^{(i)}}, \tag{3.37}$$

are Hilbert spaces. It follows that $\mathcal{S}$ and $\tilde{\mathcal{S}}$ are adjoint to each other:

$$\langle \mathcal{S}\vec{A}, \vec{c}\rangle_{\mathbf{H}} = \langle \vec{A}, \tilde{\mathcal{S}}\vec{c}\rangle_{\mathbf{L}} \quad \text{ for } \vec{A} \in \mathbf{L},\ \vec{c} \in \mathbf{H}. \tag{3.38}$$

As $\tilde{\mathcal{S}}$ is the inverse of $\mathcal{S}$, we find that $\mathcal{S}$ is unitary, i.e., $\tilde{\mathcal{S}} = \mathcal{S}^{-1} = \mathcal{S}^*$.

With these preliminaries we return to the evolution of $\vec{A}$ being described by (3.22). Applying the operators $\mathcal{S}$, $\mathcal{S}^{-1}$, we easily arrive at the evolution of the coefficients $\vec{c} = (c_1, c_2)^T$ over time scale t which is governed by $\partial_t \vec{c} = \Upsilon \vec{c}$ with $\Upsilon = \mathcal{S}\Gamma\mathcal{S}^{-1}$. This yields

$$\partial_t c_1 = \frac{1}{\mu_x(B_x^{(1)})} \left\langle \chi_1, \mathcal{L}_y(c_1\chi_1 + c_2\chi_2)\right\rangle_{\mu_x}, \tag{3.39}$$

$$\partial_t c_2 = \frac{1}{\mu_x(B_x^{(2)})} \left\langle \chi_2, \mathcal{L}_y(c_1\chi_1 + c_2\chi_2)\right\rangle_{\mu_x}, \tag{3.40}$$

such that Υ is defined by

$$\Upsilon \;=\; \begin{pmatrix} \frac{1}{\mu_x(B_x^{(1)})}\big\langle \chi_1, \mathcal{L}_y(\cdot\,\chi_1)\big\rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(1)})}\big\langle \chi_1, \mathcal{L}_y(\cdot\,\chi_2)\big\rangle_{\mu_x} \\ \frac{1}{\mu_x(B_x^{(2)})}\big\langle \chi_2, \mathcal{L}_y(\cdot\,\chi_1)\big\rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(2)})}\big\langle \chi_2, \mathcal{L}_y(\cdot\,\chi_2)\big\rangle_{\mu_x} \end{pmatrix}. \quad (3.41)$$

Note that Υ is acting as a differential operator on a suitable subspace of $\mathbf{H}$ and actually generates a semigroup of operators on $\mathbf{H}$. To this end, one has to verify that Υ is dissipative and self-adjoint. This allows to express Υ by its spectral decomposition with non-positive eigenvalues. We easily compute

$$\left\langle \Upsilon \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \right\rangle_{\mathbf{H}} = \big\langle \mathcal{L}_y(c_1\chi_1 + c_2\chi_2), (c_1\chi_1 + c_2\chi_2)\big\rangle_{\mu},$$

such that dissipativity and self-adjointness[2] of $\mathcal{L}_y$ in $L^2(\mu)$ implies the same properties for Υ in $\mathbf{H}$. The above equality also shows that the nullspace of Υ is given by c_1, c_2 such that $(c_1\chi_1 + c_2\chi_2) \in \mathcal{N}(\mathcal{L}_y) = \{f \in L^2(\mu) : f(x,y) = g(y)\}$. Thus, we have to distinguish between

$$(1) \qquad \chi_i \text{ indep. of } x \implies \mathcal{N}(\Upsilon) = \operatorname{span}\left\{ \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \mathbf{1}(x) \end{pmatrix} \right\}, \quad (3.42)$$

$$(2) \qquad \chi_i \text{ depends on } x \implies \mathcal{N}(\Upsilon) = \operatorname{span}\left\{ \begin{pmatrix} \mathbf{1}(x) \\ \mathbf{1}(x) \end{pmatrix} \right\}. \quad (3.43)$$

The first situation with χ_i, $i = 1, 2$ independent of x is strongly related to a model system where the metastable decomposition $B^{(1)} \cup B^{(2)}$ does not depend on x. However, in this case we only can assume to obtain χ_i, $i = 1, 2$ independent of x in the asymptotic limit $\epsilon \to 0$. Then it can be shown that Υ is decomposed into a main term $\overline{\mathcal{L}}$ with two-dimensional nullspace according to (3.42) and an extra term that asymptotically vanishes. In what follows we show how to decompose Υ into different operators illustrating the dynamical facets over which the x dynamics proceed.

We close this section with a remark about the mathematical model used to describe the averaged dynamics.

Remark 3.5.1 *Recall that the Fokker-Planck equation (1.3) describes the evolution of measures $\rho^\epsilon(t)$ normalized relative to the invariant density μ. Therefore, the physical density that describes the possibility of finding a single system in a certain state is given by $\rho^\epsilon(t,x,y)\mu(x,y)$. This level of awareness leads to a better understanding of the weighted space $\mathbf{H}$ that is used for the averaged dynamics: If we multiply ρ^0 by μ, that is,*

$$\rho^0(t,x,y)\,\mu(x,y) \;=\; c_1(t,x)\chi_1(x,y)\,\mu(x,y) \,+\, c_2(t,x)\chi_2(x,y)\,\mu(x,y),$$

[2]For a complex Hilbert space H with inner product $\langle\cdot,\cdot\rangle_H : H \times H \to \mathbf{C}$ we have:

$$\text{The linear operator } T \text{ is self-adjoint and dissipative} \iff \langle Tx, x\rangle_H \le 0.$$

we obtain the zeroth order approximation of the 'probability density' at time t. Averaging both sides of the equation over the fast variable yields

$$\begin{aligned}\int \rho^0(t,x,y)\,\mu(x,y)\,\mathrm{d}y &= c_1(t,x)\,\mu_x(B_x^{(1)})\bar{\mu}(x) + c_2(t,x)\,\mu_x(B_x^{(2)})\bar{\mu}(x)\\ &= c_1(t,x)\,\mu(B^{(1)})\bar{\mu}^{(1)}(x) + c_2(t,x)\,\mu(B^{(2)})\bar{\mu}^{(2)}(x).\end{aligned}$$

The RHS at the top nicely illustrates the relation of $c_1(t,x)$ and $c_2(t,x)$ for fixed x*, that is, whenever we consider for fixed x some exchange process between c_1 and c_2, the corresponding invariant density will be given by the scalar-valued vector $\psi_x = (\mu_x(B_x^{(1)}), \mu_x(B_x^{(2)}))^T$. A more comprehensive information is detected at the bottom of the RHS. We observe that the evolution of $c_1(t,x)$ is performed in the weighted space $L^2(\bar{\mu}^{(1)})$, whereas $c_2 \in L^2(\bar{\mu}^{(2)})$. The two spaces $L^2(\bar{\mu}^{(1)})$ and $L^2(\bar{\mu}^{(2)})$ are correlated by the invariant probability vector $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$. This perfectly explains the weighting in the definition (3.37) of the inner product in* $\mathbf{H}$.

3.5.2 Reduced Generator in Explicit Form

So far, the operator Υ in (3.41) does not allow for efficiently computing the slow variable dynamics on time scale $t = \mathrm{ord}(1)$. On the way to a discretized system, in this section we demonstrate that Υ is basically split into two terms where the main term appears on the order one scale and represents the dynamics of the slow variable x alone conditioned upon remaining within the metastable subsets. The second term goes beyond the time scale of the slow motion and will have contribution to a higher order.

In a first step, we formally derive the decomposition of Υ according to $\Upsilon = \overline{\mathcal{L}} + \overline{\mathcal{L}}_{\mathrm{B}} + \overline{\mathcal{L}}_{\mathrm{E}}$, see (3.49). Here, $\overline{\mathcal{L}}$ denotes a Fokker-Planck generator of order one that is associated to the averaged potentials $\overline{V}^{(i)}$ in (3.44) for $i = 1, 2$. In Section 3.5.3 we show that the extra terms $\overline{\mathcal{L}}_{\mathrm{B}}$ and $\overline{\mathcal{L}}_{\mathrm{E}}$ account for higher order equations. As a consequence, we can neglect $\overline{\mathcal{L}}_{\mathrm{B}}$, for it has no contribution in the nullspace of $\overline{\mathcal{L}}$. The operator $\overline{\mathcal{L}}_{\mathrm{E}}$ can be interpreted as an exchange term mimicking the transitions between the metastable sets $B^{(1)}$ and $B^{(2)}$ that are created by the x dynamics. It appears on a time scale that is longer than the order one over which the x dynamics takes place.

We decompose Υ into three matrices:

$$\Upsilon = \Upsilon_1 + \Upsilon_2 + \Upsilon_3,$$

with

$$\Upsilon_1 = \begin{pmatrix} \frac{1}{\mu_x(B_x^{(1)})}\langle \chi_1, \chi_1 \mathcal{L}_y \cdot \rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(1)})}\langle \chi_1, \chi_2 \mathcal{L}_y \cdot \rangle_{\mu_x} \\ \frac{1}{\mu_x(B_x^{(2)})}\langle \chi_2, \chi_1 \mathcal{L}_y \cdot \rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(2)})}\langle \chi_2, \chi_2 \mathcal{L}_y \cdot \rangle_{\mu_x} \end{pmatrix},$$

$$\Upsilon_2 = \begin{pmatrix} \frac{\sigma^2}{\mu_x(B_x^{(1)})}\langle \chi_1, D_x\chi_1\rangle_{\mu_x} D_x\cdot & \frac{\sigma^2}{\mu_x(B_x^{(1)})}\langle \chi_1, D_x\chi_2\rangle_{\mu_x} D_x\cdot \\ \frac{\sigma^2}{\mu_x(B_x^{(2)})}\langle \chi_2, D_x\chi_1\rangle_{\mu_x} D_x\cdot & \frac{\sigma^2}{\mu_x(B_x^{(2)})}\langle \chi_2, D_x\chi_2\rangle_{\mu_x} D_x\cdot \end{pmatrix},$$

$$\Upsilon_3 = \begin{pmatrix} \frac{1}{\mu_x(B_x^{(1)})}\langle \chi_1, \mathcal{L}_y\chi_1\rangle_{\mu_x}\cdot & \frac{1}{\mu_x(B_x^{(1)})}\langle \chi_1, \mathcal{L}_y\chi_2\rangle_{\mu_x}\cdot \\ \frac{1}{\mu_x(B_x^{(2)})}\langle \chi_2, \mathcal{L}_y\chi_1\rangle_{\mu_x}\cdot & \frac{1}{\mu_x(B_x^{(2)})}\langle \chi_2, \mathcal{L}_y\chi_2\rangle_{\mu_x}\cdot \end{pmatrix}.$$

A straightforward calculation will reveal that the diagonal entries of Υ_1 and Υ_2 sum up to Fokker-Planck generators. Therefore, from a formal point of view it is natural to add the diagonal entries of Υ_1 and Υ_2 on the one hand and the off-diagonal entries on the other. We thus define

$$\begin{aligned} \overline{\mathcal{L}} &= \operatorname{diag}(\Upsilon_1) + \operatorname{diag}(\Upsilon_2), \\ \overline{\mathcal{L}}_{\mathrm{B}} &= \Upsilon_1 + \Upsilon_2 - \overline{\mathcal{L}}, \end{aligned}$$

and compute the entries[3]. To this end, we define the averaged potentials $\overline{V}^{(i)}$, $i = 1, 2$ that correspond to the invariant densities $\bar{\mu}^{(i)}$, $i = 1, 2$ defined in (3.30):

$$\overline{V}^{(i)}(x) = -\frac{1}{\beta} \ln \bar{\mu}^{(i)}(x). \tag{3.44}$$

Using (3.32) together with the relation

$$\mu(B^{(i)})\, \bar{\mu}^{(i)}(x) = \mu_x(B_x^{(1)})\, \bar{\mu}(x), \tag{3.45}$$

we then obtain

$$\begin{aligned} D_x\overline{V}^{(i)} &= \frac{1}{\mu_x(B_x^{(i)})} \int D_x V(x,y) \chi_i^2(x,y) \mu_x(y) \mathrm{d}y - \frac{\sigma^2}{\mu_x(B_x^{(i)})} \langle \chi_i, D_x\chi_i\rangle_{\mu_x} \\ &= \frac{1}{\mu_x(B_x^{(i)})} \int D_x V(x,y) \chi_i(x,y) \mu_x(y) \mathrm{d}y - \frac{\sigma^2}{2\mu_x(B_x^{(i)})} \langle \mathbf{1}, D_x\chi_i\rangle_{\mu_x}. \end{aligned}$$

This enables us to rewrite $\overline{\mathcal{L}}$ and $\overline{\mathcal{L}}_{\mathrm{B}}$ according to

$$\overline{\mathcal{L}} = \begin{pmatrix} \overline{\mathcal{L}}^{(1)} & 0 \\ 0 & \overline{\mathcal{L}}^{(2)} \end{pmatrix}, \tag{3.46}$$

$$\overline{\mathcal{L}}_{\mathrm{B}} = \frac{\sigma^2}{2} \begin{pmatrix} 0 & \frac{1}{\mu_x(B_x^{(1)})}\langle \mathbf{1}, D_x\chi_2\rangle_{\mu_x} D_x\cdot \\ \frac{1}{\mu_x(B_x^{(2)})}\langle \mathbf{1}, D_x\chi_1\rangle_{\mu_x} D_x\cdot & 0 \end{pmatrix}, \tag{3.47}$$

[3] We have indexed the second operator with a B to indicate that it is has to be considered as a Boundary term. This will become clear below.

where $\overline{\mathcal{L}}^{(i)}$ for $i = 1, 2$ is the Fokker-Planck operator corresponding to the potential $\overline{V}^{(i)}$, that is, $\overline{\mathcal{L}}^{(i)} : L^2(\bar{\mu}^{(i)}) \to L^2(\bar{\mu}^{(i)})$ with

$$\overline{\mathcal{L}}^{(i)} \;=\; \big\langle \mathbf{1}, \mathcal{L}_y \cdot \big\rangle_{\mu_x^{(i)}} + \frac{\sigma^2}{\mu_x(B_x^{(i)})} \big\langle \chi_i, D_x \chi_i \big\rangle_{\mu_x} \;=\; \frac{\sigma^2}{2}\Delta_x \;-\; D_x \overline{V}^{(i)}\, D_x \;.$$

In contrast to the operators $\overline{\mathcal{L}}^{(i)}$, the matrix $\overline{\mathcal{L}}_{\mathrm{B}}$ seems to be a serious problem for the interpretation of the slow dynamics as a Markov process. To obtain a possible explanation for the existence of these terms, we recall the scaling assumption (3.18) with $\delta \ll 1$ that represents a modeling step: The dominant eigenvalues of $\mathcal{L}_x$ scale like $\exp(-\beta \Delta V_x)$ with ΔV_x denoting the energy barrier for fixed x which will have its highest point at the boundary of the metastable sets $B_x^{(1)}$, $B_x^{(2)}$. A situation like (3.18) can explicitly be realized only if these barriers scale like $\Delta V_x \sim -\ln \delta$. However, in this case the corresponding eigenvectors and the invariant density μ_x will also depend on $\delta \sim \epsilon^r$, $r \geq 1$, and thus on ϵ. Now, recall that $\partial_t \vec{c} = \Upsilon \vec{c}$ is an equivalent formulation of $\partial_t \rho^0 = \tilde{\Pi} \mathcal{L}_y \tilde{\Pi} \rho^0$ for the evolution of the zeroth order term $\rho^0 = \tilde{\Pi} \rho^0$. But according to (3.21), the ϵ-dependence of μ_x and $u_1(x, \cdot)$ implies that $\tilde{\Pi}$ as well as ρ^0 will depend on ϵ. It is the authors conjecture that this dependence is reflected in the term $\overline{\mathcal{L}}_{\mathrm{B}}$ in such a way that $\overline{\mathcal{L}}_{\mathrm{B}}$ asymptotically will vanish. The consideration is confirmed by the following consequences of (3.18): The dominant eigenfunction will have constant parts outside a neighbourhood of the potentials' saddle point and there is an internal layer with vanishing measure that glues these parts together. Therefore, the evaluation of the derivative can be restricted to this internal layer, where the eigenfunction shows an asymptotically sharp decline. However, the invariant density will have exponentially small values in that region, such that averaging leads to an 'overcompensation' of the ascending derivatives. In Section 3.5.3 we validate the speculation by constructing a potential energy surface that correctly renders the consequences of (3.18). For now, we simply state $\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$ and continue by considering Υ_3.

In accordance with the notation $\overline{\mathcal{L}}$, $\overline{\mathcal{L}}_{\mathrm{B}}$ we set $\overline{\mathcal{L}}_{\mathrm{E}} := \Upsilon_3$, that is,

$$\overline{\mathcal{L}}_{\mathrm{E}} \;=\; \begin{pmatrix} \frac{1}{\mu_x(B_x^{(1)})} \big\langle \chi_1, \mathcal{L}_y \chi_1 \big\rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(1)})} \big\langle \chi_1, \mathcal{L}_y \chi_2 \big\rangle_{\mu_x} \\ \frac{1}{\mu_x(B_x^{(2)})} \big\langle \chi_2, \mathcal{L}_y \chi_1 \big\rangle_{\mu_x} & \frac{1}{\mu_x(B_x^{(2)})} \big\langle \chi_2, \mathcal{L}_y \chi_2 \big\rangle_{\mu_x} \end{pmatrix}. \tag{3.48}$$

The index will be used to indicate the interpretation of the operator as an Exchange term between the two levels $i = 1$ and $i = 2$. We come back to this issue later on, where we indicate that the interpretation as rate matrix only is valid on a longer time scale $t \gg 1$. Therefore it is natural to hope $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$. Let us consider the entries of $\overline{\mathcal{L}}_{\mathrm{E}}$. For y fixed, $\mathcal{L}_y$ is acting as a differential operator on functions of the slow variable x. Therefore the components of $\overline{\mathcal{L}}_{\mathrm{E}}$ contain derivatives of χ_i wrt. x that are averaged against the invariant density μ_x. Thus, it is natural to relate the order of $\overline{\mathcal{L}}_{\mathrm{E}}$ to

the order of $\overline{\mathcal{L}}_{\mathrm{B}}$ and infer $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$ from $\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$. We verify $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$ in Section 3.5.3.

Then the evolution system for the coefficients $\vec{c} = (c_1, c_2)$ on time scale $t = \mathrm{ord}(1)$ reads

$$\partial_t \vec{c} \;=\; \big(\overline{\mathcal{L}} + \overline{\mathcal{L}}_{\mathrm{B}} + \overline{\mathcal{L}}_{\mathrm{E}}\big)\,\vec{c}, \qquad \overline{\mathcal{L}}_{\mathrm{B}} \ll 1, \quad \overline{\mathcal{L}}_{\mathrm{E}} \ll 1. \tag{3.49}$$

Consequently, the solution $\vec{c}$ of the above equation is expressed as

$$\vec{c}(t,\tau,x) \;=\; \exp(t\overline{\mathcal{L}})\,\vec{c}(t=0,\tau,x),$$

whereas the operators $\overline{\mathcal{L}}_{\mathrm{B}}$ and $\overline{\mathcal{L}}_{\mathrm{E}}$ contribute to higher order terms. A simple consideration may allow to neglect $\overline{\mathcal{L}}_{\mathrm{B}}$ in any case: $\overline{\mathcal{L}}$ generates a stationary process such that

$$\exp(t\overline{\mathcal{L}})\,\vec{c}(t=0,\tau,x) \;\longrightarrow\; \mathbf{P}\,\vec{c}(t=0,\tau,x), \qquad \text{as } t \to \infty,$$

which tells us that the solution on longer time scales has to be in the range of $\mathbf{P}$. As $\mathbf{P}$ equals the orthogonal projection onto the nullspace of $\overline{\mathcal{L}}$, we have $\mathcal{R}(\mathbf{P}) = \mathrm{span}\{(\mathbf{1},0)^T, (0,\mathbf{1})^T\}$, which is the space of vector-valued functions being independent of x. Therefore, for every $\vec{b} \in \mathcal{R}(\mathbf{P})$ we obtain $\overline{\mathcal{L}}_{\mathrm{B}}\vec{b} = 0$, such that $\overline{\mathcal{L}}_{\mathrm{B}}$ does not contribute to the dynamics on a longer time scale $t \gg 1$.

Comments on $\overline{\mathcal{L}}_{\mathbf{E}}$

Suppose for the moment that for every x

$$\big\langle \chi_i, \mathcal{L}_y \chi_i \big\rangle_{\mu_x} \;<\; 0, \qquad i = 1,2, \tag{3.50}$$

and abbreviate $a(x) = \big\langle \chi_1, \mathcal{L}_y \chi_2 \big\rangle_{\mu_x} > 0$ and $b(x) = \big\langle \chi_2, \mathcal{L}_y \chi_1 \big\rangle_{\mu_x} > 0$. With this we rewrite $\overline{\mathcal{L}}_{\mathrm{E}}$ according to

$$\overline{\mathcal{L}}_{\mathrm{E}} \;=\; \begin{pmatrix} -a(x)/\mu_x(B_x^{(1)}) & a(x)/\mu_x(B_x^{(1)}) \\ b(x)/\mu_x(B_x^{(2)}) & -b(x)/\mu_x(B_x^{(2)}) \end{pmatrix}.$$

This representation could lead us to interpret $\overline{\mathcal{L}}_{\mathrm{E}}$ as a rate matrix that generates a transition process between the levels $i = 1$ and $i = 2$ for fixed x. However, the fact that we are working in a weighted space requires to carefully inspect the matrix before drawing any conclusion in this direction.

Following the considerations in Remark 3.5.1, the invariant density for fixed x is $\psi_x = (\mu_x(B_x^{(1)}), \mu_x(B_x^{(2)}))^T$, such that $\overline{\mathcal{L}}_{\mathrm{E}}$ is considered to act on the ψ_x-weighted space $l^2(\psi_x)$. As outlined in Remark 2.2.3, we can interpret $\overline{\mathcal{L}}_{\mathrm{E}}$ as the generator of a transition chain on state space $\mathbf{S} = \{1,2\}$ only if $(\overline{\mathcal{L}}_{\mathrm{E}})^T\psi_x = 0$. This immediately implies the condition

$$a(x) \;=\; \big\langle \chi_1, \mathcal{L}_y \chi_2 \big\rangle_{\mu_x} \;=\; \big\langle \chi_2, \mathcal{L}_y \chi_1 \big\rangle_{\mu_x} \;=\; b(x).$$

Using $\langle \chi_1, \mathcal{L}_y \chi_2 \rangle_{\mu_x} = -\langle \chi_1, \mathcal{L}_y \chi_1 \rangle_{\mu_x}$ results in

$$\langle \mathbf{1}, \mathcal{L}_y \chi_1 \rangle_{\mu_x} = 0 \implies \langle \chi_i, \mathcal{L}_y \chi_j \rangle_{\mu_x} = 0, \qquad i = 1, 2.$$

The last statement follows from $\chi_i \in L^\infty$ for $i = 1, 2$, and we obtain $\overline{\mathcal{L}}_{\mathrm{E}} = 0$. This shows that the effort to interpret $\overline{\mathcal{L}}_{\mathrm{E}}$ as an order one term actually makes no sense, and therefore, we can refrain from verifying (3.50). As a consequence, we expect $\overline{\mathcal{L}}_{\mathrm{E}}$ to contribute to higher order terms. It becomes apparent in Section 3.5.4 that the only remaining part of the operator on longer time scales is given by $\mathbf{P}\overline{\mathcal{L}}_{\mathrm{E}}\mathbf{P}$ with $\mathbf{P}$ denoting the nullspace of the order one generator $\overline{\mathcal{L}}$.

To conclude the considerations we illustrate that the order of $\overline{\mathcal{L}}_{\mathrm{E}}$ must be somehow connected to the order of $\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$. To this end, let us assume $\overline{\mathcal{L}}_{\mathrm{E}} \gg \overline{\mathcal{L}}_{\mathrm{B}}$. Above, we addressed the problem that $\overline{\mathcal{L}}_{\mathrm{E}}$ is not self-adjoint in $l^2(\psi_x)$ with $\psi_x = (\mu_x(B_x^{(1)}), \mu_x(B_x^{(2)}))^T$. However, if we consider $\overline{\mathcal{L}}_{\mathrm{E}} + \overline{\mathcal{L}}_{\mathrm{B}}$, the operator becomes self-adjoint in $\mathbf{H}$. To this end, note that $\overline{\mathcal{L}}$ is self-adjoint as well as Υ. As $\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$ (which implies $\overline{\mathcal{L}}_{\mathrm{B}}^* \ll 1$ for the adjoint), we deduce that $\overline{\mathcal{L}}_{\mathrm{E}}$ must approximately be self-adjoint in the asymptotic limit $\epsilon \to 0$, that is, for ϵ small we have

$$\overline{\mathcal{L}}_{\mathrm{E}} \simeq \overline{\mathcal{L}}_{\mathrm{E}}^*, \qquad \text{in } \mathbf{H},$$

and, consequently,

$$\langle \mathbf{1}, \mathcal{L}_y \chi_i \rangle_{\mu_x} \simeq 0 \implies \overline{\mathcal{L}}_{\mathrm{E}} \ll 1.$$

Non-Rigorous Approach to Interpret the Origin of $\overline{\mathcal{L}}_{\mathbf{E}}$. Let us inspect the diagonal entries of $\overline{\mathcal{L}}_{\mathrm{E}}$ being less mathematically rigorous. We assume δ to be very small. Then, we can approximate $\chi_i(x, \cdot)$, $i = 1, 2$ by the characteristic functions $\mathbf{1}_{B_x^{(i)}}$ which can equivalently be defined by the stepfunctions on the metastable sets of the entire state space:

$$\chi_1 \approx \mathbf{1}_{B^{(1)}}, \qquad \chi_2 \approx \mathbf{1}_{B^{(2)}},$$

and, consequently,

$$\chi_1(\cdot, y) \approx \mathbf{1}_{B_y^{(1)}}, \qquad \chi_2(\cdot, y) \approx \mathbf{1}_{B_y^{(2)}},$$

for fixed y, where $B_y^{(i)}$ denotes the restriction of $B^{(i)}$ to the fibre $\Phi(y) = \{(x, y) \mid x \in \mathbf{R}\}$, i.e., $B_y^{(i)} = B^{(i)} \cap \Phi(y)$. Now, remember that the scaling assumption (3.18) entails the dominant eigenvalue of $\mathcal{L}_x$ to scale like $\exp(-\beta \Delta V_x)$ with ΔV_x denoting the most important energy barrier in the system for fixed x. This is explicitly realized only if $\Delta V_x \sim -\ln \delta$. The consequences on the operator $\mathcal{L}_y$ for fixed y are obvious: If $\chi_i(\cdot, y) \not\approx \mathbf{1}$, we

find a point $x = x(y)$ such that $\Delta V_{x(y)}$ asymptotically becomes the highest barrier on the fibre $\Phi(y)$. But this entails the most dominant eigenvalue $\lambda_1(y) \neq 0$ of $\mathcal{L}_y$ to scale with $\exp(-\beta\Delta V_{x(y)}) \sim \delta$. Note that the dominant eigenvector $v_1(\cdot, y)$ of $\mathcal{L}_y$ is approximated by

$$\begin{aligned} v_1(x,y) &\approx \sqrt{\frac{\mu_y(B_y^{(2)})}{\mu_y(B_y^{(1)})}}\mathbf{1}_{B_y^{(1)}}(x) - \sqrt{\frac{\mu_y(B_y^{(2)})}{\mu_y(B_y^{(1)})}}\mathbf{1}_{B_y^{(2)}}(x), \\ \mu_y(x) &= \frac{\mu(x,y)}{\int \mu(x,y)\,\mathrm{d}x}. \end{aligned}$$

Thus we have

$$\begin{aligned} \mathbf{1}_{B_y^{(1)}}(x) &\approx \mu_y(B_y^{(1)})\mathbf{1} + \sqrt{\mu_y(B_y^{(1)})\mu_y(B_y^{(2)})}v_1(x,y), \\ \mathbf{1}_{B_y^{(2)}}(x) &\approx \mu_y(B_y^{(2)})\mathbf{1} - \sqrt{\mu_y(B_y^{(1)})\mu_y(B_y^{(2)})}v_1(x,y), \end{aligned}$$

which instantly provides us with

$$\begin{aligned} \mathcal{L}_y\mathbf{1}_{B_y^{(1)}} &\approx \lambda_1(y)\left(\mu_y(B_y^{(2)})\mathbf{1}_{B_y^{(1)}} - \mu_y(B_y^{(1)})\mathbf{1}_{B_y^{(2)}}\right), \\ \mathcal{L}_y\mathbf{1}_{B_y^{(2)}} &\approx \lambda_1(y)\left(\mu_y(B_y^{(1)})\mathbf{1}_{B_y^{(2)}} - \mu_y(B_y^{(2)})\mathbf{1}_{B_y^{(1)}}\right). \end{aligned}$$

Replacing $\chi_i(x,y)$ by $\mathbf{1}_{B_y^{(i)}}(x)$ allows to explicitly evaluate the entries of $\overline{\mathcal{L}}_{\mathrm{E}}$:

$$\begin{aligned} \frac{1}{\mu_x(B_x^{(1)})}\langle\chi_1, \mathcal{L}_y\chi_1\rangle_{\mu_x} &\approx \int \lambda_1(y)\mu_y(B_y^{(2)})\,\mu_x^{(1)}(y)\,\mathrm{d}x, \\ \frac{1}{\mu_x(B_x^{(2)})}\langle\chi_2, \mathcal{L}_y\chi_2\rangle_{\mu_x} &\approx \int \lambda_1(y)\mu_y(B_y^{(1)})\,\mu_x^{(2)}(y)\,\mathrm{d}x. \end{aligned}$$

As is known, $\lambda_1(y)\mu_y(B_y^{(i)})$ is the transition rate for a particle evolving according to $\mathcal{L}_y$ to jump from the metastable subset $B_y^{(j)}$ to $B_y^{(i)}$ (with $j \neq i$). If we consider the particle in the full system evolving according to $\mathcal{L}^\epsilon$ and keep in mind that the fast state space restricted to $B^{(j)}$ is entirely sampled before the position of the slow variable effectively changes, the rate for a particle in x to jump from $B^{(j)}$ to $B^{(i)}$ (for $i \neq j$) along the x direction will asymptotically be given by $\lambda_1(y)\mu_y(B_y^{(i)})$ averaged against the restricted invariant density $\mu_x^{(j)}$. However, this has to be considered as a very rough approach of the asymptotic behaviour that does not have the demand of being mathematically rigorous. But it provides an insightful interpretation of the origin of the term.

3.5.3 Boundary Terms $\overline{\mathcal{L}}_{\mathrm{B}}$ and $\overline{\mathcal{L}}_{\mathrm{E}}$ Contribute to Higher Order

In this section our goal is to mathematically verify the assertion $\overline{\mathcal{L}}_{\mathrm{B}}, \overline{\mathcal{L}}_{\mathrm{E}} \ll 1$ in (3.49). In so doing, we asymptotically evaluate the entries in the matrices, which necessitates some knowledge of the heuristic derivation of the dominant eigenvalue $\lambda_1(x)$ of $\mathcal{L}_x$ and the corresponding eigenvector $u_1(x,\cdot)$. The key step for the procedure is to design a potential energy surface on the fast fibre that correctly renders the consequences of the scaling assumption (3.18). As $\chi_2(x,y) = \mathbf{1} - \chi_1(x,y)$, we can restrict to the evaluation of terms containing $\chi_1(x,y)$.

Construction of Potential Energy Surface

To simplify the approach, we make the following basic assumption about the potential $V = V(x,y)$:

Assumption 3.5.2 *(i)* $V \in \mathcal{C}^\infty(\mathbf{R}^2)$*;*

(i) $V(x,\cdot)$ *is a double-well potential for all* $x \in \mathbf{R}$ *with two local minima at* $y = m^{(1)}(x), m^{(2)}(x)$ *and one local maximum at* $y = y_0(x)$ *where we establish* $m^{(1)}(x) < y_0(x) < m^{(2)}(x)$*;*

(ii) the extrema are non-degenerate, i.e., for $i = 1, 2$

$$D_{yy}V(x, y_i(x)) \,=\, \omega^{(i)}(x) \,>\, 0, \qquad D_{yy}V(x, y_0) \,=\, -\omega_0(x) \,<\, 0.$$

As the spectrum of $\mathcal{L}_x$ is supposed to consist of $M = 2$ dominant eigenvalues, the double-well structure of $V(x,\cdot)$ is a reasonable presumption. The left and right potential barriers are denoted $V^{(1)}_{\mathrm{bar}}(x) = V(x,y_0) - V(x,m^{(1)}(x))$ and $V^{(2)}_{\mathrm{bar}}(x) = V(x,y_0) - V(x,m^{(2)}(x))$, and let

$$V_{\mathrm{bar}}(x) \,=\, \min\{V^{(1)}_{\mathrm{bar}}(x), V^{(2)}_{\mathrm{bar}}(x)\}.$$

Without loss of generality we assume $V_{\mathrm{bar}}(x) = V^{(1)}_{\mathrm{bar}}(x)$, that is, the shallow well is at the left side and the deep well at the right.

We first investigate the first eigenvalue $\lambda_1(x)$ of $\mathcal{L}_x$ and the consequences of the situation (3.18) on the potential barrier for small values of δ. The informations about the behaviour of λ_1 are based on the results of Pavlyukevich in [36] who derived the asymptotic formula of $\lambda_1(x)$ in the small noise limit by expanding λ_1 into a power series. The refinement for a double-well potential gives the accurate asymptotics in terms of quantities concerning the *shallow* well of the potential:

$$\lambda_1(x)\mu_x(B^{(2)}_x) \;\doteq\; \frac{\sqrt{\omega^{(1)}(x)\omega_0(x)}}{2\pi}\,\exp\big(-\frac{2}{\sigma^2}V_{\mathrm{bar}}(x)\big), \qquad (3.51)$$

where $\mu_x(B_x^{(2)})$ is the weight over the deep well. Thus, for asymmetric double well potentials we have $\mu_x(B_x^{(2)}) \doteq 1$ in the limit of vanishing noise intensity σ. With the estimate (3.51) we are in position to examine the asymptotic effects of the scaling assumption $\lambda_1(x) = \delta\,\tilde{\lambda}_1(x) = \mathrm{ord}(\delta)$ where $\delta \to 0$:

$$\frac{\sqrt{\omega^{(1)}(x)\omega_0(x)}}{\mu_x(B_x^{(2)})2\pi}\,\exp\big(-\frac{2}{\sigma^2}V_{\mathrm{bar}}(x)\big) \;=\; \mathrm{ord}(\delta).$$

We observe that we basically have two possibilities to derive the asymptotic equality: First, we can change the curvature in the minima and/or in the saddle point of the potential $V(x,\cdot)$; second, and this is more feasible, we logarithmically couple $V_{\mathrm{bar}}(x)$ to the smallness parameter δ. Let us for the moment forget about $\omega^{(1)}$, ω_0, and the weight $\mu_x(B_x^{(2)})$, and simply demand

$$\exp\big(-\frac{2}{\sigma^2}(V_{\mathrm{bar}}(x)+\xi_\delta)\big) \;\sim\; \delta,$$

where the actual barrier height for fixed δ is now given by $V_{\mathrm{bar}}(x)+\xi_\delta$ such that ξ_δ represents the increase of the original potential barrier $V_{\mathrm{bar}}(x)$. Resolving the (proportional) equality wrt. ξ_δ reveals that $\xi_\delta = -(\sigma^2/2)\,\ln\delta$ performs the desired relation.

In a next step we reconsider how to incorporate the increase ξ_δ of the potential barrier into a new potential $\tilde{V}(x,y)$ still satisfying Assumption 3.5.2. A natural way for the derivation is to define $\tilde{V}$ by the sum of V and a correction potential V_{corr} with

$$\max\{V_{\mathrm{corr}}(x,y):\, y\in\mathbf{R}\} \;=\; V_{\mathrm{corr}}(x,y_0(x)) \;=\; \xi_\delta.$$

In order to asymptotically preserve the minima $m^{(1)}(x)$ and $m^{(2)}(x)$, it is convenient to suppose an exponential decrease of V_{corr}, which immediately brings about

$$\begin{aligned} V_{\mathrm{corr}}(x,y) &= \frac{1}{g}\exp\Big(-\frac{1}{2}\Big(\frac{y-y_0(x)}{g}\Big)^2\Big), \qquad (3.52)\\ g &= \frac{1}{\xi_\delta} = -\frac{2}{\sigma^2\ln\delta}. \end{aligned}$$

An illustrative example of the thus defined potential $V(x,\cdot)+V_{\mathrm{corr}}(x,\cdot)$ for fixed x is shown in Fig. 3.6, where we have chosen $g = 0.5, 0.1, 0.05$.

The invariant density of the fast process for fixed x is no longer given by $\mu_x \sim \exp(-\beta V(x,\cdot))$ but by

$$\begin{aligned} \tilde{\mu}_x(y) &= \frac{1}{\tilde{Z}(x)}\exp\big(-\beta V(x,y)\big)\exp\Big(-\frac{\beta}{g}\exp\Big(-\frac{1}{2}\big(\frac{y-y_0(x)}{g}\big)^2\Big)\Big),\\ \tilde{Z}(x) &= \int\exp\Big(-\beta\big(V(x,y)+V_{\mathrm{corr}}(x,y)\big)\Big)\,\mathrm{d}y. \end{aligned}$$

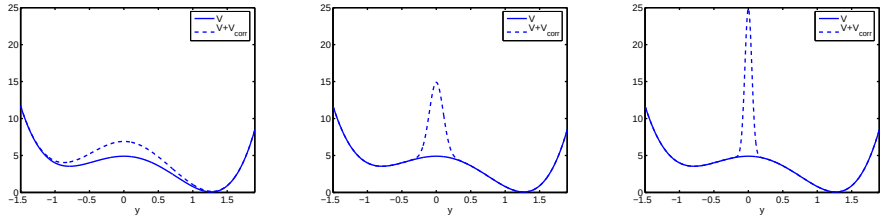

Figure 3.6: Illustrative example to visualize the correction term V_{corr} for decreasing values of g. The full line shows the original potential $V(y)$, and the dashed line the new potential $V + V_{\mathrm{corr}}$.

Using Lebesgue's dominated convergence theorem we easily observe

$$\lim_{\delta\to 0} \tilde{Z}(x) \;=\; \int \exp\big(-\beta V(x,y)\big)\,\mathrm{d}y,$$

for pointwise everywhere

$$\lim_{\delta\to 0} \exp\big(-\beta V_{\mathrm{corr}}(x,y)\big) \;=\; \begin{cases} 0, & y = y_0(x) \\ 1, & y \neq y_0(x) \end{cases}.$$

Thus, for fixed x we pointwise almost everywhere obtain $\lim_{\delta\to 0} \tilde{\mu}_x = \mu_x$.

With this preparatives we reconsider the dominant spectrum of $\mathcal{L}_x$. In the asymptotic limit $\sigma \to 0$, the first eigenvalue $\lambda_1(x) \neq 0$ is now given by

$$\lambda_1(x)\tilde{\mu}_x(B_x^{(2)}) \;\doteq\; \frac{\sqrt{\tilde{\omega}^{(1)}(x)\tilde{\omega}_0(x)}}{2\pi}\,\delta\,\exp\big(-\frac{2}{\sigma^2}V_{\mathrm{bar}}(x)\big),$$

where $\tilde{\omega}^{(1)}(x)$ and $\tilde{\omega}_0(x)$ denote the curvature of the potential $\tilde{V}(x,\cdot)$ in the extrema $m^{(1)}(x)$, $y_0(x)$, i.e,

$$\begin{aligned} D_{yy}\tilde{V}(x, y_0(x)) &= -\tilde{\omega}_0(x), \\ D_{yy}\tilde{V}(x, m^{(1)}(x)) &= \tilde{\omega}^{(1)}(x), \end{aligned}$$

where

$$\begin{aligned} \tilde{\omega}_0(x) &= \omega_0(x) + \frac{1}{g^3}, \\ \tilde{\omega}^{(1)}(x) &= \omega^{(1)}(x) \\ &+ \frac{1}{g^3}\left(\Big(\frac{m^{(1)}(x) - y_0(x)}{g}\Big)^2 - 1\right)\exp\left(-\frac{1}{2}\Big(\frac{m^{(1)}(x) - y_0(x)}{g}\Big)^2\right). \end{aligned}$$

Considering the asymptotic behaviour of $\tilde{\omega}_0(x)$ and $\tilde{\omega}^{(1)}(x)$ as $\delta \to 0$ (use $1/g = -(\sigma^2/2)\ln\delta$), the first eigenvalue $\lambda_1(x)$ satisfies

$$\lambda_1(x) \;=\; \mathrm{ord}(\tilde{\delta}), \qquad \tilde{\delta} \;=\; \delta\,(\ln\delta)^{3/2}.$$

Thus, the scaling assumption (3.18) now is fulfilled with $\tilde{\delta}$ instead of δ. This means that we have to relate the smallness parameter ϵ in (1.3) to $\delta(\ln\delta)^{3/2}$.

Zeroth Order Approximation of Dominant Eigenfunction. For the derivation of χ_1 we follow the line of PAVLYUKEVICH in [36]. As outlined in Section 2.2.6, the solution of $\mathcal{L}_x u_1(x,y) = \lambda_1(x)\, u_1(x,y)$ can be expanded into a power series wrt. the parameter $\lambda_1(x)$, which is formally given in (2.52). Using (3.27) we obtain an analogue power series for χ_1:

$$\chi_1(x,y) = \chi_1^{(0)}(x,y) + \lambda_1(x)\chi_1^{(1)}(x,y) + (\lambda_1(x))^2\chi_1^{(2)}(x,y) + ...$$

If we use the results from Section 2.2.6, and carry them over to the power series of χ_1, we obtain the zeroth order approximation $\chi_1^{(0)}$ which is continuous and lies in $L^2(\tilde{\mu}_x)$:

$$\begin{aligned}\chi_1^{(0)}(x,\cdot) &= h_0(x,\cdot)\mathbf{1}_{(-\infty,m^{(1)}(x)]}(y)\\ &+ f_0(x,\cdot)\mathbf{1}_{[m^{(1)}(x),m^{(2)}(x)]}(y) + g_0(x,\cdot)\mathbf{1}_{[m^{(2)}(x),\infty)}(y), \quad (3.53)\end{aligned}$$

where the functions h_0, f_0 and g_0 are defined by

$$\begin{aligned}h_0(x,y) &= 1, \quad x \in \mathbf{R},\, y \in (-\infty, m^{(1)}(x)],\\ f_0(x,y) &= 1 - \frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}},\ x \in \mathbf{R},\, y \in [m^{(1)}(x), m^{(2)}(x)], \quad (3.54)\\ g_0(x,y) &= 0, \quad x \in \mathbf{R},\, y \in [m^{(2)}(x), \infty).\end{aligned}$$

Thus, $\chi_1^{(0)}(x,\cdot)$ takes constant values outside of $[m^{(1)}(x), m^{(2)}(x)]$ and $f_0(x,\cdot)$ glues the constant parts together. We can easily show pointwise convergence

$$\begin{aligned}\lim_{\sigma\to 0} f_0(x,y) &= 1, \quad y \in (-\infty, y_0(x)),\\ \lim_{\sigma\to 0} f_0(x,y) &= 0, \quad y \in (y_0(x), \infty),\end{aligned}$$

as well as

$$\begin{aligned}\lim_{\delta\to 0} f_0(x,y) &= 1, \quad y \in (-\infty, y_0(x)),\\ \lim_{\delta\to 0} f_0(x,y) &= 0, \quad y \in (y_0(x), \infty).\end{aligned}$$

Roughly speaking, the internal layer (around $y_0(x)$) connecting the constant parts will have vanishing measure.

Remark 3.5.3 *Note that $\chi_1^{(0)} = \tilde{\mu}_x(B_x^{(1)}) + \gamma_x u_1^{(0)}$ satisfies the homogeneous equation (2.53) as well. This could make one think that consequently $\mathcal{L}_x\chi_1^{(0)}(x,\cdot) = 0$ contradicting the assumption $\mathcal{N}(\mathcal{L}_x) = \mathrm{span}\{\mathbf{1}(y)\}$. However, $\chi_1^{(0)}(x,\cdot)$ is almost everywhere differentiable only excluding the points $m^{(1)}(x)$ and $m^{(2)}(x)$, such that $\chi_1^{(0)}(x,\cdot) \notin \mathcal{D}(\mathcal{L}_x)$ with $\mathcal{D}(\mathcal{L}_x)$ consisting of all continuous functions $f = f(y) \in L^2(\tilde{\mu}_x)$, such that f' is locally absolutely continuous and $f'' - w(y)\, f \in L^2(\tilde{\mu}_x)$, where $w(y) = (D_y\tilde{V})^2/\sigma^4 - \Delta_y\tilde{V}/\sigma^2$. The k-th order approximations $\chi_1^{(k)}(x,\cdot)$ actually serve to make $\chi_1(x,\cdot)$ smooth on the whole axis.*

Asymptotics of $\overline{\mathcal{L}}_{\mathrm{B}}$

We are now in position to show $\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$. For this purpose, we have to show $\langle \mathbf{1}, D_x\chi_1\rangle_{\tilde{\mu}_x} \to 0$ as $\delta \to 0$. It is sufficient to asymptotically evaluate $\langle \mathbf{1}, D_x\chi_1^{(0)}\rangle_{\tilde{\mu}_x}$, for $\lambda_1(x)$, $D_x\lambda_1(x) \to 0$ as $\delta \to 0$. To simplify notation we will use the smallness parameter $g = -2/(\sigma^2 \ln \delta)$ and evaluate the expression for vanishing g. According to (3.53)&(3.54), we immediately obtain

$$\begin{aligned}
&\big\langle \mathbf{1}, D_x\chi_1^{(0)}\big\rangle_{\tilde{\mu}_x} \\
&\quad = \quad \frac{-1}{\tilde{Z}(x)} \int_{m^{(1)}(x)}^{m^{(2)}(x)} D_x \left(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}} \right) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y. \quad (3.55)
\end{aligned}$$

The key point for the asymptotic computation is to show that the major contribution to the value of the integral

$$\begin{aligned}
F(x) \quad &:= \quad \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}(\tilde{V}(x,\tilde{y})-\tilde{V}_{\max}(x))}\mathrm{d}\tilde{y}, \qquad (3.56)\\
\tilde{V}_{\max}(x) \quad &= \quad \max\{\tilde{V}(x,y) \,:\, y \in \mathbf{R}\} \,=\, V(x, y_0(x)) \,+\, \frac{1}{g},
\end{aligned}$$

does asymptotically not vanish to fast as $g \to 0$. We expect that the main contribution arises from the interval $[y_0(x) - g^{3/2}, y_0(x) + g^{3/2}]$. This can be presaged by determining those points $y \in [m^{(1)}(x), m^{(2)}(x)]$ such that

$$\frac{2}{\sigma^2}\big(V(x,y) + V_{\mathrm{corr}}(x,y) - \tilde{V}_{\max}(x)\big) \,\leq\, \mathrm{ord}(1).$$

Using

$$\begin{aligned}
V_{\mathrm{corr}}(x,y) \quad &= \quad \frac{1}{g}\exp\left(-\frac{1}{2}\left(\frac{y-y_0(x)}{g}\right)^2\right)\\
&= \quad \frac{1}{g}\sum_{k=0}^{\infty}\frac{1}{(-2)^k\,k!}\left(\frac{y-y_0(x)}{g}\right)^{2k}, \qquad (3.57)
\end{aligned}$$

yields the desired result

$$V_{\mathrm{corr}}(x,y) - \frac{1}{g} \,\leq\, \mathrm{ord}(1) \qquad \Longleftrightarrow \qquad |y - y_0(x)| \,\leq\, \mathrm{ord}(g^{3/2}).$$

Therefore, we restrict to determine the integral

$$\tilde{F}(x) \quad = \quad \int_{y_0(x)-g^{3/2}}^{y_0(x)+g^{3/2}} e^{\frac{2}{\sigma^2}(\tilde{V}(x,\tilde{y})-\tilde{V}_{\max}(x))}\mathrm{d}\tilde{y}, \qquad (3.58)$$

for small values of g. To this end, we use

$$V_{\rm corr}\big(x, y_0(x) + g^{3/2}y\big) \; - \; \frac{1}{g} \;\; = \;\; -\frac{1}{2}y^2 \; + \; \sum_{k\geq 2} \frac{g^{k-1}}{(-2)^k\, k!} y^{2k}, \qquad (3.59)$$

$$V(x, y_0 + g^{3/2}y) - V(x, y_0(x)) \;\; = \;\; -\frac{1}{2}\omega_0(x)\, g^3\, y^2 \; + \; \mathcal{O}((g^{3/2}|y|)^3) \qquad (3.60)$$

For the first equality we used (3.57), for the second Taylor-expansion of $V(x,\cdot)$ around $y_0(x)$. With it (3.58) can be written in the asymptotic limit $g \to 0$ as

$$\tilde{F}(x) \;\; \simeq \;\; g^{3/2} \int_{-1}^{1} e^{-\frac{1}{2}\frac{2}{\sigma^2}y^2} e^{-\frac{1}{2}\frac{2}{\sigma^2}\omega_0(x) g^3 y^2}\, {\rm d}y,$$

where we omitted the remainder terms in (3.59)&(3.60) containing positive powers of g, as $e^{-g^k} \doteq 1$ for small g and $k > 0$. For the same reason we can simplify $\tilde{F}(x)$ further, and, consequently, asymptotically obtain a Gaussian under the integral:

$$\tilde{F}(x) \;\; \simeq \;\; g^{3/2} \int_{-1}^{1} e^{-\frac{1}{2}\frac{2}{\sigma^2}y^2}\, {\rm d}y \; = \; g^{3/2}\sqrt{2\,\pi}\, \Big(\Phi\big(\frac{\sqrt{2}}{\sigma}\big) - \Phi\big(-\frac{\sqrt{2}}{\sigma}\big)\Big),$$

where Φ denotes the primitive of the standard Gaussian. Consequently, in the asymptotic limit $\delta \to 0$ (respectively, $g \to 0$) we obtain

$$\begin{aligned} \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})} {\rm d}\tilde{y} \; &= \; e^{\frac{2}{\sigma^2}(\frac{1}{g} + V(x, y_0(x)))}\, F(x) \\ &\geq \;\; e^{\frac{2}{\sigma^2}\left(\frac{1}{g} + V(x,y_0(x))\right)}\, \tilde{F}(x) \; \simeq \; C(x,\sigma)\, e^{\frac{2}{\sigma^2}\frac{1}{g}}\, g^{3/2}, \end{aligned} \qquad (3.61)$$

where C denotes a function depending on x and the noise intensity σ.

In order to determine (3.55) we inspect the concerned derivatives wrt. x:

$$\begin{aligned} D_x \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, {\rm d}\tilde{y} \; &= \; \int_{m^{(1)}(x)}^{m^{(2)}(x)} D_x\tilde{V}(x,\tilde{y})\; e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, {\rm d}\tilde{y} \\ &\quad + D_x m^{(2)}(x)\; e^{\frac{2}{\sigma^2}\tilde{V}(x, m^{(2)}(x))} \; - \; D_x m^{(1)}(x)\; e^{\frac{2}{\sigma^2}\tilde{V}(x, m^{(1)}(x))}, \\ D_x \int_{m^{(1)}(x)}^{y} & e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, {\rm d}\tilde{y} \\ = \;\; & \int_{m^{(1)}(x)}^{y} D_x\tilde{V}(x,\tilde{y})\; e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, {\rm d}\tilde{y} \; - \quad D_x m^{(1)}(x)\; e^{\frac{2}{\sigma^2}\tilde{V}(x, m^{(1)}(x))}. \end{aligned}$$

To estimate the above expressions we simply use that $\tilde{V}(x,\tilde{y})$ is monotonic increasing for $\tilde{y} \in [m^{(1)}(x), y_0(x)]$, which immediately implies

$$\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, {\rm d}\tilde{y} \;\; \leq \;\; d(x)\, e^{\frac{2}{\sigma^2}\tilde{V}(x,y)}, \quad \text{for } y \in [m^{(1)}(x), y_0(x)], \qquad (3.62)$$

$$d(x) \;\; := \;\; m^{(2)}(x) - m^{(1)}(x). \qquad (3.63)$$

This is a very coarse approximation, but it is sufficient to obtain the desired result. The key point in the above estimate is that the fast growing term (fast growing around the saddle point) $e^{\frac{2}{\sigma^2}\tilde{V}(x,y)}$ (for $g \to 0$) will be killed by the invariant density in (3.55). We furthermore need the following estimates:

$$\begin{aligned} \max\{|D_x\tilde{V}(x,y)| : \ y \in [m^{(1)}(x), m^{(2)}(x)]\} &= C_1(x) + \frac{1}{g^3}C_2(x), \quad (3.64) \\ \max_{i=1,2} |D_x y_i(x)|\, e^{\frac{2}{\sigma^2}\tilde{V}(x,y_i(x))} &= C_3(\sigma, x), \quad (3.65) \end{aligned}$$

for some positive functions C_1, C_2 only depending on x, and $C_3(\sigma, x) = \mathrm{ord}(1)$ in the limit $g \to 0$. We use (3.62), (3.64), and (3.65) and obtain the following estimates:

$$\begin{aligned} &\Big|D_x \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, \mathrm{d}\tilde{y}\Big| \\ &\quad \le \ \big(C_1(x) + \frac{1}{g^3}C_2(x)\big) \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y} + 2C_3, \quad (3.66) \\ &\Big|D_x \int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\, \mathrm{d}\tilde{y}\Big| \\ &\quad \le \ \big(C_1(x) + \frac{1}{g^3}C_2(x)\big) d(x) e^{\frac{2}{\sigma^2}\tilde{V}(x,y)} \ + \ C_3. \quad (3.67) \end{aligned}$$

Let us apply the above estimations to the integral I in (3.55):

$$I(g,x,\sigma) \ = \ \int_{m^{(1)}(x)}^{m^{(2)}(x)} D_x\Bigg(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\Bigg) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y.$$

We break the interval $[m^{(1)}(x), m^{(2)}(x)]$ into two intervals $[m^{(1)}(x), y_0(x)]$ and $[y_0(x), m^{(2)}(x)]$, that is,

$$\begin{aligned} I(g,x,\sigma) &= I_1(g,x,\sigma) + I_2(g,x,\sigma), \\ I_1(g,x,\sigma) &:= \int_{m^{(1)}(x)}^{y_0(x)} D_x\Bigg(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\Bigg) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y, \\ I_2(g,x,\sigma) &:= \int_{y_0(x)}^{m^{(2)}(x)} D_x\Bigg(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\Bigg) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y. \end{aligned}$$

We determine I_1, which is decomposed according to

$$\begin{aligned} I_1 &= I_1^{(1)}(g,x,\sigma) - I_1^{(2)}(g,x,\sigma), \\ I_1^{(1)} &= \int_{m^{(1)}(x)}^{y_0(x)} \frac{D_x \int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}} e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y, \\ I_1^{(2)} &= \int_{m^{(1)}(x)}^{y_0(x)} \frac{\left(D_x \int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}\right) \int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\left(\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}\right)^2} e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y. \end{aligned}$$

To approximate $|I_1^{(1)}|$ we use the estimate (3.67) and obtain

$$\begin{aligned} |I_1^{(1)}| &\leq \int_{m^{(1)}(x)}^{y_0(x)} \frac{(C_1(x) + 1/g^3\, C_2(x))d(x) + C_3(\sigma,x)e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\,\mathrm{d}y \\ &\leq d(x)\frac{d(x)\big(C_1(x) + \frac{1}{g^3}C_2(x)\big) + C_3(\sigma,x)e^{-\frac{2}{\sigma^2}\tilde{V}(x,m^{(2)}(x))}}{e^{\frac{2}{\sigma^2}\tilde{V}_{\max}(x)}F(x)}, \end{aligned}$$

where $F(x)$ is defined in (3.56). We estimate the denominator according to (3.61), which yields for small g the asymptotic estimate

$$I_1^{(1)}(g,x,\sigma) \lesssim g^{-4.5}\, e^{-\frac{2}{\sigma^2}\frac{1}{g}}\, C_4(\sigma,x),$$

for some function C_4 only depending on x and σ.

In a similar way we approximate $I_1^{(2)}$. To this end, we use the estimate (3.66), which results in

$$\begin{aligned} |I_1^{(2)}(g,x,\sigma)| &\leq \int_{m^{(1)}(x)}^{y_0(x)} \frac{(C_1(x) + 1/g^3\, C_2(x) + C_3(\sigma,x))d(x)}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\,\mathrm{d}y \\ &\lesssim g^{-4.5}\, e^{-\frac{2}{\sigma^2}\frac{1}{g}}\, C_5(\sigma,x), \end{aligned}$$

for some function C_5 only depending on x and σ.

The estimate on the remaining integral $|I_2|$ is obtained in an analogous way. To this end, we use

$$\begin{aligned} &\int_{y_0(x)}^{m^{(2)}(x)} D_x\left(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\right) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y \\ &\quad = -\int_{y_0(x)}^{m^{(2)}(x)} D_x\left(\frac{\int_{y}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\right) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y, \end{aligned}$$

together with the fact that

$$\int_y^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y} \;\le\; e^{\frac{2}{\sigma^2}\tilde{V}(x,y)}(y_0(x)-m^{(2)}(x)), \qquad y\in[y_0(x),m^{(2)}(x)].$$

Putting everything together we obtain in the asymptotic limit $g\to 0$

$$\begin{aligned} |I| &\le \int_{m^{(1)}(x)}^{m^{(2)}(x)} \left| D_x\left(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\right)\right| e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y \\ &\lesssim g^{-4.5}\, e^{-\frac{2}{\sigma^2}\frac{1}{g}}\, C_6(\sigma,x), \end{aligned} \tag{3.68}$$

for a function C_6 only depending on x,σ.

Asymptotics of $\overline{\mathcal{L}}_{\mathbf{E}}$

Using the estimates in the last subsection it is only a small step to derive $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$. To this end, we have to show for $i,j=1,2$

$$\left\langle \chi_i, \mathcal{L}_y\chi_j\right\rangle_{\tilde{\mu}_x} \;\to\; 0, \qquad \text{as } g\to 0.$$

As χ_i will be bounded in the maximum norm, it is sufficient to show $\left\langle \mathbf{1}, \mathcal{L}_y\chi_j\right\rangle_{\tilde{\mu}_x} \to 0$. As before, we restrict the consideration to the zeroth order approximation $\chi_1^{(0)}$ of χ_1 that is given in (3.53). We split the generator $\mathcal{L}_y$ into its parts $(\sigma^2/2)\Delta_x$ and $D_x\tilde{V}\,D_x$ and average wrt. $\tilde{\mu}_x$. Using $\tilde{Z}(x)=\mathrm{ord}(1)$ necessitates to estimate $\tilde{I}=I(g,x,\sigma)$ and $\widehat{I}=\widehat{I}(g,x,\sigma)$ with

$$\tilde{I} \;=\; \int_{m^{(1)}(x)}^{m^{(2)}(x)} D_xD_x\left(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\right) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y, \tag{3.69}$$

$$\widehat{I} \;=\; \int_{m^{(1)}(x)}^{m^{(2)}(x)} D_x\tilde{V}(x,y)D_x\left(\frac{\int_{m^{(1)}(x)}^{y} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}{\int_{m^{(1)}(x)}^{m^{(2)}(x)} e^{\frac{2}{\sigma^2}\tilde{V}(x,\tilde{y})}\mathrm{d}\tilde{y}}\right) e^{-\frac{2}{\sigma^2}\tilde{V}(x,y)}\mathrm{d}y. \tag{3.70}$$

We resort to the predecing results. With it we easily obtain an approximation of the integral (3.70) by using (3.64) and (3.68). This yields for a function C_7 the asymptotic estimate

$$|\widehat{I}| \;\lesssim\; g^{-7.5}\, e^{-\frac{2}{\sigma^2}\frac{1}{g}}\, C_7(\sigma,x).$$

An estimate for the integral (3.70) is obtained by considering the estimates in the last subsection and thinking about the consequences of the additional derivative. In so doing, we observe that the slowest decaying parts now contain the terms

$$\begin{aligned} \big(\max\{|D_x\tilde{V}(x,y)|:\; y\in[m^{(1)}(x),m^{(2)}(x)]\}\big)^2 &= (C_1(x)+\frac{1}{g^3}C_2(x))^2 \\ &= \mathrm{ord}(1/g^6), \\ \max\{|D_{xx}\tilde{V}(x,y)|:\; y\in[m^{(1)}(x),m^{(2)}(x)]\} &= \mathrm{ord}(1/g^5), \end{aligned}$$

and, consequently, for C_8 only depending on x, σ we obtain

$$|\tilde{I}| \lesssim g^{-7.5}\, e^{-\frac{2}{\sigma^2}\frac{1}{g}}\, C_8(\sigma, x).$$

The strategy enables us to obtain a more general result, namely,

$$\left\langle u_j(x,\cdot), \mathcal{L}_y \chi_j \right\rangle_{\tilde{\mu}_x} \to 0, \qquad \text{as } g \to 0, \tag{3.71}$$

for every eigenfunction $u_j(x,\cdot)$ of $\mathcal{L}_x$. This can be seen by carefully inspecting the computation of the last results together with the most feasible assumption

$$\int_{m^{(1)}(x)}^{m^{(2)}(x)} |u_j(x,y)| \mathrm{d}y = \mathrm{ord}(1),$$

in the asypmotic limit $g \to 0$.

3.5.4 Modeling of Metastable Transitions Induced by x Dynamics

Using the results from Section 3.5.3, there is no loss of generality in the next assumption that will allow to present the metastable transitions that are induced by the x dynamics mathematically rigorous in an appropriate asymptotic limit.

Assumption 3.5.4 *Subsequently, we use the following working assumption on the exchange term $\overline{\mathcal{L}}_{\mathrm{E}}$:*

$$\overline{\mathcal{L}}_{\mathrm{E}} = \tilde{\epsilon}\, \widehat{\mathcal{L}}_{\mathrm{E}}, \qquad 0 < \tilde{\epsilon} \ll 1, \quad \widehat{\mathcal{L}}_{\mathrm{E}} = \mathrm{ord}(1).$$

The parameter $\tilde{\epsilon}$ measures the ratio of the correlation time of the x dynamics constrained to a metastable subset to the x-induced transition process between the metastable sets relaxing the system to its invariant distribution.

The long-time effective behaviour that can emerge from system (3.49) will depend on the ordering of the parameter $\tilde{\epsilon}$ describing the "size" of the operator $\overline{\mathcal{L}}_{\mathrm{E}}$. Note that the boundary term $\overline{\mathcal{L}}_{\mathrm{B}}$ does not have to be considered, for it has no contribution in the nullspace of $\overline{\mathcal{L}}$. Therefore we consider the operator $\Upsilon = \Upsilon(\tilde{\epsilon})$ as a perturbation of the operator $\overline{\mathcal{L}}$, that is, we are concerned with the case where $\Upsilon(\tilde{\epsilon})$ is given formally by

$$\Upsilon(\tilde{\epsilon}) = \overline{\mathcal{L}} + \tilde{\epsilon}\, \widehat{\mathcal{L}}_{\mathrm{E}}.$$

Let us now consider an isolated eigenvalue $\bar{\lambda}$ of $\overline{\mathcal{L}}$ with finite multiplicity m. Since $\Upsilon(\tilde{\epsilon})$ converges to $\overline{\mathcal{L}}$ as $\tilde{\epsilon} \to 0$, there are exactly m eigenvalues of $\Upsilon(\tilde{\epsilon})$ in the neighbourhood of $\bar{\lambda}$ and these eigenvalues tend as $\tilde{\epsilon} \to 0$

to $\bar\lambda$. Our primary interest is limited to the eigenvalue $\bar\lambda = 0$ which has multiplicity $m = 2$ and corresponds to the eigenspace

$$\begin{aligned}\mathcal{R}(\mathbf{P}) &= \operatorname{span}\left\{\begin{pmatrix}\mathbf{1}(x)\\0\end{pmatrix},\begin{pmatrix}0\\\mathbf{1}(x)\end{pmatrix}\right\}\\ &= \operatorname{span}\left\{\begin{pmatrix}\mathbf{1}(x)\\\mathbf{1}(x)\end{pmatrix},\begin{pmatrix}\mathbf{1}(x)/\mu(B^{(1)})\\-\mathbf{1}(x)/\mu(B^{(2)})\end{pmatrix}\right\},\end{aligned}$$

where $\mathbf{P}$ denotes the orthogonal projection. Thus, we will write $\bar\lambda_0 = \bar\lambda_1 = 0$ with $\bar\lambda_0$ corresponding to the eigenspace span$\{(\mathbf{1},\mathbf{1})^T\}$ and $\bar\lambda_1 = 0$ to span$\{(\mathbf{1}/\mu(B^{(1)}), -\mathbf{1}/\mu(B^{(2)}))^T\}$. The corresponding orthogonal projections are denoted $\mathbf{P}_0$ and $\mathbf{P}_1$, respectively. We denote by $\bar\lambda_k$, $k \geq 2$ the negative eigenvalues of $\overline{\mathcal{L}}$ in decreasing order, the corresponding projections are $\mathbf{P}_k$. We characterize as $\bar\lambda_k^{\tilde\epsilon}$, $k \in \mathbf{N}$ the eigenvalues of $\Upsilon(\tilde\epsilon)$ which tend to $\bar\lambda_k$ as $\tilde\epsilon \to 0$ and as $\mathbf{P}_k^{\tilde\epsilon}$ the respective projections. Then, we have

$$|\bar\lambda_k^{\tilde\epsilon} - \bar\lambda_k| = \mathcal{O}(\tilde\epsilon), \qquad \|\mathbf{P}_k^{\tilde\epsilon} - \mathbf{P}_k\|_{\mathbf{H}} = \mathcal{O}(\tilde\epsilon^{1/2}).$$

The result goes back to a theorem of Kato ([21, Theorem 4.9, Chapter VIII,4]) that can be applied to sectorial operators with stable eigenvalues and is stated in terms of sectorial forms. According to (3.43) we have $\bar\lambda_0^{\tilde\epsilon} = 0 = \bar\lambda_0$ and $\mathbf{P}_0^{\tilde\epsilon} = \mathbf{P}_0$. The eigenvalue $\bar\lambda_1^{\tilde\epsilon}$ can be expanded wrt. $\tilde\epsilon$ and the theorem in the book of Kato provides us with the asymptotic expansion

$$\bar\lambda_1^{\tilde\epsilon} = \bar\lambda_1 + \tilde\epsilon\,\bar\lambda_1^{(1)} + o(\epsilon) = \tilde\epsilon\,\bar\lambda_1^{(1)} + o(\epsilon),$$

where $\bar\lambda_1^{(1)}$ is the eigenvalue of $(\mathbf{P}_0 + \mathbf{P}_1)\widehat{\mathcal{L}}_{\mathrm{E}}(\mathbf{P}_0 + \mathbf{P}_1) = \mathbf{P}_1\widehat{\mathcal{L}}_{\mathrm{E}}\mathbf{P}_1$. The result likewise can be obtained by using first order perturbation methods.

Evaluation of $\tilde\epsilon\,\bar\lambda_1^{(1)}$

We evaluate the expression $\mathbf{P}_1\overline{\mathcal{L}}_{\mathrm{E}}\mathbf{P}_1$, where

$$\mathbf{P}_1 = \left\langle \cdot\,, \begin{pmatrix}\alpha_1\mathbf{1}(x)\\\alpha_2\mathbf{1}(x)\end{pmatrix}\right\rangle_{\mathbf{H}} \cdot \begin{pmatrix}\alpha_1\mathbf{1}(x)\\\alpha_2\mathbf{1}(x)\end{pmatrix}, \tag{3.72}$$

$$\alpha_1 = \sqrt{\frac{\mu(B^{(2)})}{\mu(B^{(1)})}}, \qquad \alpha_2 = -\sqrt{\frac{\mu(B^{(1)})}{\mu(B^{(2)})}}. \tag{3.73}$$

First we apply $\overline{\mathcal{L}}_{\mathrm{E}}$ to $(\alpha_1\mathbf{1}(x), \alpha_2\mathbf{1}(x))^T$. This yields

$$\overline{\mathcal{L}}_{\mathrm{E}}\begin{pmatrix}\alpha_1\mathbf{1}(x)\\\alpha_2\mathbf{1}(x)\end{pmatrix} = \begin{pmatrix}\frac{1}{\mu_x(B_x^{(1)})}\big\langle\chi_1, \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2)\big\rangle_{\mu_x}\\ \frac{1}{\mu_x(B_x^{(2)})}\big\langle\chi_2, \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2)\big\rangle_{\mu_x}\end{pmatrix}.$$

The explicit value for $\tilde\epsilon\,\bar\lambda_1^{(1)}$ now is obtained by

$$\begin{aligned}\tilde\epsilon\,\bar\lambda_1^{(1)} &= \left\langle\overline{\mathcal{L}}_{\mathrm{E}}\begin{pmatrix}\alpha_1\mathbf{1}(x)\\\alpha_2\mathbf{1}(x)\end{pmatrix}, \begin{pmatrix}\alpha_1\mathbf{1}(x)\\\alpha_2\mathbf{1}(x)\end{pmatrix}\right\rangle_{\mathbf{H}}\\ &= \big\langle(\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2)\big\rangle_{\mu}.\end{aligned} \tag{3.74}$$

Interpretation of $\tilde{\epsilon}\,\bar{\lambda}_1^{(1)}$

Without loss of generality we may assume $\delta \sim \epsilon^2$. For $\delta \sim \epsilon$ (see Section 3.6), the system relaxes to its invariant density $\bar{\mu}$ at time $t = \mathrm{ord}(1)$ such that $\overline{\mathcal{L}}_{\mathrm{E}}$ is neglected anyway and nothing is to show.

We are interested in the most dominant eigenvalue $\lambda^\epsilon \neq 0$ of the full generator $\mathcal{L}^\epsilon$. Denoting u^ϵ the corresponding (normalized) eigenvector, we make the following perturbation ansatz:

$$\begin{aligned} u^\epsilon &= u^{(0)} + \epsilon\, u^{(1)} + \epsilon^2\, u^{(2)} + ... \\ \lambda^\epsilon &= \lambda^{(0)} + \epsilon\, \lambda^{(1)} + \epsilon^2\, \lambda^{(2)} + ... \end{aligned}$$

The following consideration shows $\lambda^{(0)} \ll 1$: The scaling assumption (3.18) with $\delta \sim \epsilon^2$ implies that the transition rates along the y dynamics from $B_x^{(1)}$ to $B_x^{(2)}$ (and vice versa) scale with $\delta/\epsilon \ll 1$. This is explicitly realized if the potential barrier at the boundary of $B_x^{(1)}$ and $B_x^{(2)}$ for fixed x logarithmically increases. But this will effect the same barrier increase on every fibre of the slow state space (if it is affected from the metastable decomposition). Therefore, the transition rates to jump from $B^{(1)}$ to $B^{(2)}$ in the entire state space will asymptotically go to zero. This means that $\lambda^\epsilon \ll 1$ which results in $\lambda^{(0)} \ll 1$. Now, we insert the above expansion in the eigenvalue equation

$$\mathcal{L}^\epsilon u^\epsilon \;=\; \big(\frac{1}{\epsilon}\mathcal{R}_x + \mathcal{L}_y + \frac{\delta}{\epsilon}\mathcal{L}_x^{\mathrm{act}}\big)u^\epsilon \;=\; \lambda^\epsilon u^\epsilon,$$

and get via comparison of powers of ϵ:

$$\begin{aligned} \epsilon^{-1}: &\quad \mathcal{R}_x u^{(0)} = 0, \\ \epsilon^{0}: &\quad \mathcal{R}_x u^{(1)} + \mathcal{L}_y u^{(0)} \;=\; \lambda^{(0)} u^{(0)}. \end{aligned}$$

This immediately yields $\tilde{\Pi} u^{(0)} = u^{(0)}$ with $\tilde{\Pi}$ given in (3.21), i.e.,

$$u^{(0)}(x,y) \;=\; U_0(x) + U_1(x)\, u_1(x,y) \;=\; \sum_{i=1}^{2} \big(U_0(x) + \alpha_i^x U_1(x)\big)\chi_i(x,y),$$

for some functions U_0, U_1 only depending on x and α_i^x, $i = 1,2$ defined in (3.25). In a next step we obtain

$$\tilde{\Pi}\mathcal{L}_y\tilde{\Pi} u^{(0)} \;=\; \lambda^{(0)} u^{(0)},$$

which equivalently is written

$$(\overline{\mathcal{L}} + \overline{\mathcal{L}}_{\mathrm{B}} + \overline{\mathcal{L}}_{\mathrm{E}}) \begin{pmatrix} U_0(x) + \alpha_1^x U_1(x) \\ U_0(x) + \alpha_2^x U_1(x) \end{pmatrix} \;=\; \lambda^{(0)} \begin{pmatrix} U_0(x) + \alpha_1^x U_1(x) \\ U_0(x) + \alpha_2^x U_1(x) \end{pmatrix}.$$

Comparing the order of the RHS (remember $\lambda^{(0)} \ll 1$) with the order of the LHS ($\overline{\mathcal{L}}_{\mathrm{B}} \ll 1$ and $\overline{\mathcal{L}}_{\mathrm{E}} \ll 1$) reveals

$$\begin{aligned}\overline{\mathcal{L}}^{(1)}(U_0(x) + \alpha_1^x U_1(x)) &\ll 1,\\ \overline{\mathcal{L}}^{(2)}(U_0(x) + \alpha_2^x U_1(x)) &\ll 1.\end{aligned}$$

This can only be realized if $U_0(x) + \alpha_i^x U_1(x)$ asymptotically belongs to the nullspace of $\overline{\mathcal{L}}^{(i)}$ for $i = 1, 2$. But this entails in the asymptotic limit $\epsilon \to 0$

$$U_0(x) + \alpha_i^x U_1(x) \in \mathrm{span}\{\mathbf{1}(x)\},$$

and, consequently, with α_1, α_2 given in (3.73),

$$u^{(0)}(x, y) \simeq \alpha_1 \chi_1(x, y) + \alpha_2 \chi_2(x, y).$$

Summarisingly, in the limit $\epsilon \to 0$ the dominant eigenvector of $\mathcal{L}^\epsilon$ can be approximated by

$$u^\epsilon(x, y) \simeq \alpha_1 \chi_1(x, y) + \alpha_2 \chi_2(x, y). \tag{3.75}$$

We then obtain by using (3.74)

$$\begin{aligned}\lambda^\epsilon &= \langle u^\epsilon, \mathcal{L}^\epsilon u^\epsilon \rangle_\mu\\ &\simeq \big\langle (\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}^\epsilon(\alpha_1\chi_1 + \alpha_2\chi_2)\big\rangle_\mu\\ &= \frac{1}{\epsilon}\big\langle (\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}_x(\alpha_1\chi_1 + \alpha_2\chi_2)\big\rangle_\mu + \tilde{\epsilon}\bar{\lambda}_1^{(1)},\end{aligned}$$

which shows that $\tilde{\epsilon}\bar{\lambda}_1^{(1)}$ is correlated with the metastable transitions between $B^{(1)}$ and $B^{(2)}$ (in full dynamics' description) that are induced by the x dynamics.

In Appendix E we present an illustrative picture that nicely shows the varying structure of the second eigenvector u^ϵ of the full generator $\mathcal{L}^\epsilon$, if we increase metastability on every fibre of the fast state space. It becomes apparent that the temperature has to be chosen very small such that u^ϵ approximately lies in the span of $\mathbf{1}_{B^{(1)}}$ and $\mathbf{1}_{B^{(2)}}$. For small values of β however, u^ϵ will be an approximate linear combination of $\mathbf{1}_{B_x^{(1)}}$ and $\mathbf{1}_{B_x^{(2)}}$ for every fixed x.

3.5.5 Summary of Main Results and Outlook

We briefly summarize the main results obtained in this section. For the asymptotic procedure performed in Section 3.6 and Section 3.7 we moreover need to reformulate the achievements wrt. the coefficients $A_0(x), A_1(x)$ of the basis $\{\mathbf{1}, u_1(x, \cdot)\}$.

Summary

Under the scaling assumption (3.18) with $\delta = \epsilon^2$ we have $\mathcal{L}^\epsilon = (1/\epsilon)\mathcal{R}_x + \mathcal{L}_y + \epsilon\,\mathcal{L}_x^{\text{act}}$, see (3.19). If we expand the density $\rho^\epsilon = \rho^\epsilon(t,\tau,x,y)$ into a power series wrt. ϵ, that is, $\rho^\epsilon = \rho^0 + \epsilon\rho^1 + \mathcal{O}(\epsilon^2)$, insert it into the Fokker-Planck equation (1.3), and compare the coefficients wrt. ϵ we obtain:

$$\begin{aligned} \epsilon^{-1} \;:\quad & \mathcal{R}_x\rho^0 = 0 && (3.76)\\ \epsilon^{0} \;:\quad & \partial_t\rho^0 = \mathcal{R}_x\rho^1 + \mathcal{L}_y\rho^0 && (3.77)\\ \epsilon^{1} \;:\quad & \partial_t\rho^1 + \partial_\tau\rho^0 = \mathcal{R}_x\rho^2 + \mathcal{L}_y\rho^1 + \mathcal{L}_x^{\text{act}}\rho^0. && (3.78) \end{aligned}$$

Equation (3.76) immediately yields $\rho^0 = A_0(t,\tau,x)\mathbf{1}(x,y) + A_1(t,\tau,x)u_1(x,y)$ with $\mathbf{1}$, $u_1(x,\cdot)$ being the dominant eigenfunctions of $\mathcal{L}_x$. If we use (3.27) and (3.28), ρ^0 equivalently is expressed as

$$\rho^0 = c_1(t,\tau,x)\chi_1(x,y) + c_2(t,\tau,x)\chi_2(x,y).$$

Using the orthogonal projection $\tilde{\Pi}$ according to (3.21) (onto the nullspace of $\mathcal{R}_x$) we obtain from equation (3.77) the following three equivalent evolution systems:

$$\begin{aligned} &(i.) && \partial_t\rho^0 = \tilde{\Pi}\mathcal{L}_y\tilde{\Pi}\rho^0, && \rho^0 = \tilde{\Pi}\rho^0 \in L^2(\mu),\\ &(ii.) && \partial_t\vec{A} = \Gamma\vec{A}, && \vec{A} = (A_0, A_1)^T \in \mathbf{L} = L^2(\bar{\mu}) \times L^2(\bar{\mu}), \quad (3.79)\\ &(iii.) && \partial_t\vec{c} = \Upsilon\vec{c}, && \vec{c} = (c_1, c_2)^T \in \mathbf{H} = L^2(\bar{\mu}^{(1)}) \times L^2(\bar{\mu}^{(2)}). \end{aligned}$$

By exploiting $\chi_i \approx \mathbf{1}_{B_x^{(i)}}$, $i = 1,2$ we demonstrated in a straightforward but tedious calculation that Υ actually allows for an absorbing interpretation: The operator Υ can be decomposed into a diagonal matrix $\overline{\mathcal{L}}$ consisting of effectively computable Fokker-Planck generators and a second term $\overline{\mathcal{L}}_{\text{E}}$ that represents some exchange on a scale that is longer than the order one time scale t. This is formulated by introducing a smallness parameter $\tilde{\epsilon}$ such that

$$\partial_t\vec{c} \;=\; (\overline{\mathcal{L}} + \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\text{E}})\vec{c}, \qquad \tilde{\epsilon} \ll 1,\;\; \widehat{\mathcal{L}}_{\text{E}} = \text{ord}(1).$$

Thus, the solution over time scale t will be given by $\vec{c}(t) = \exp(t\overline{\mathcal{L}})\vec{c}(t=0)$, whereas $\widehat{\mathcal{L}}_{\text{E}}$ has to be taken to the corresponding equation of order $\text{ord}(\tilde{\epsilon})$. To this end, we have to relate $\tilde{\epsilon}$ to the parameter ϵ and distinguish between $\tilde{\epsilon} \ll \epsilon$, $\epsilon \ll \tilde{\epsilon} \ll 1$ and $\tilde{\epsilon} = \text{ord}(\epsilon)$.

The key role for the solution on any time scale $t \gg 1$ (with time variable $\tau \ll 1$) is established by the nullspace of $\overline{\mathcal{L}}$. Again, first order perturbation serves as the effective tool that will allow us to explicitly derive the model:

$$\overline{\mathcal{L}} + \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\text{E}} = \bar{\lambda}_0\mathbf{P}_0 + \sum_{k\geq 1}(\bar{\lambda}_k + \tilde{\epsilon}\bar{\lambda}_k^{(1)} + o(\tilde{\epsilon}))\mathbf{P}_k^{\tilde{\epsilon}}, \quad \|\mathbf{P}_k^{\tilde{\epsilon}} - \mathbf{P}_k\|_{\mathbf{H}} = \mathcal{O}(\sqrt{\tilde{\epsilon}}),$$

with $\bar{\lambda}_0 = \bar{\lambda}_1 = 0$, $\bar{\lambda}_k < 0$ for $k \geq 2$, $\mathbf{P} = \mathbf{P}_0 + \mathbf{P}_1$ denoting the orthogonal projection onto $\mathcal{N}(\overline{\mathcal{L}})$, and $\lambda_1^{(1)} = \mathbf{P}\widehat{\mathcal{L}}_{\mathrm{E}}\mathbf{P}$. Using the spectral decomposition of $\overline{\mathcal{L}}$, the solution $\vec{c}(t,\tau,x)$ is expressed as

$$\vec{c}(t,\tau,x) \;=\; \mathbf{P}\vec{c}(t=0,\tau,x) \;+\; \sum_{k\geq 2} e^{t\bar{\lambda}_k}\mathbf{P}_k\vec{c}(t=0,\tau,x),$$

which is obtained as the asymptotic limit of $\exp(t(\overline{\mathcal{L}} + \tilde{\epsilon}\widehat{\mathcal{L}}_{\mathrm{E}}))\vec{c}(t=0,\tau,x)$. We observe that the evaluation on the next time scale is carried out in the range of $\mathbf{P}$ as $\bar{\lambda}_k < 0$ for $k \geq 2$.

Strategy for Evaluation Longest Time Scale

To give the reader an idea of how to derive the solution over time $\tau \ll 1$, we demonstrate the proceeding for the easiest case $\epsilon \ll \tilde{\epsilon} \ll 1$. In this situation, we have to set $\tau = \tilde{\epsilon}\,t$ establishing an order that has to be arranged between equation (3.77) and equation (3.78). We do have no pre-existing information on the evolution over τ, thus we simply set

$$\begin{aligned} \epsilon^0 \;&:\quad \partial_t\vec{c} \;=\; \overline{\mathcal{L}}\vec{c} \,+\, \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\mathrm{E}}\vec{c}, \\ \tilde{\epsilon}^1 \;&:\quad \partial_\tau\vec{c} \;=\; 0. \end{aligned}$$

Following an intuitive approach, we propose to take $\widehat{\mathcal{L}}_{\mathrm{E}}$ to the correct order, which yields

$$\begin{aligned} \epsilon^0 \;&:\quad \partial_t\vec{c} \;=\; \overline{\mathcal{L}}\vec{c}, \\ \tilde{\epsilon}^1 \;&:\quad \partial_\tau\vec{c} \;=\; \widehat{\mathcal{L}}_{\mathrm{E}}\vec{c}. \end{aligned}$$

(The case of $\tilde{\epsilon} = \mathrm{ord}(\epsilon)$ is somewhat more complicated, for we have to embed the $\mathrm{ord}(\tilde{\epsilon})$ information into equation (3.78).) Projecting the $\mathrm{ord}(\tilde{\epsilon})$ equation onto the nullspace of $\overline{\mathcal{L}}$ and using $\mathbf{P}\vec{c}(t) = \mathbf{P}\vec{c}(t=0)$ provides us with the evolution equation over time τ:

$$\partial_\tau\mathbf{P}\vec{c}(t=0,\tau,x) \;\;=\;\; \mathbf{P}\widehat{\mathcal{L}}_{\mathrm{E}}\mathbf{P}\vec{c}(t=0,\tau,x).$$

Finally, we explicitly show how to obtain the evolution equation in a mathematically rigorous way. To this end, we prefer the representation of $\vec{c}$ by means of the eigenvalue expansion of $\overline{\mathcal{L}} + \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\mathrm{E}}$. The key step is to take the derivative of $\vec{c}$ wrt. τ by incorporating the $\mathrm{ord}(\tilde{\epsilon})$ terms. Thus, we take

$$\begin{aligned} \vec{c}^{\,\tilde{\epsilon}}(t,\tau,x) \;&=\; \mathbf{P}_0\vec{c}(t=0) \,+\, \sum_{k\geq 1} e^{t\bar{\lambda}_k^{\tilde{\epsilon}}}\mathbf{P}_k^{\tilde{\epsilon}}\vec{c}(t=0), \\ \bar{\lambda}_k^{\tilde{\epsilon}} \;&=\; \bar{\lambda}_k \,+\, \tilde{\epsilon}\,\bar{\lambda}_k^{(1)} \,+\, o(\tilde{\epsilon}). \end{aligned}$$

as the basis of our computation. Now, if we notionally replace $\tilde{\epsilon}\,t$ by τ, take the derivative wrt. τ, and let $\tilde{\epsilon} \to 0$, we obtain

$$\partial_\tau\vec{c}^{\,\epsilon} \;\;\longrightarrow\;\; \partial_\tau\vec{c} + \sum_{k\geq 1}\bar{\lambda}_k^{(1)}\mathbf{P}_k\vec{c}(t=0), \qquad \text{as } \tilde{\epsilon} \to 0,$$

such that we finally arrive at

$$\partial_\tau \vec{c} \;=\; (\partial_\tau \vec{c})^{\rm old} + \sum_{k\geq 1} \bar{\lambda}_k^{(1)} \mathbf{P}_k \vec{c}(t=0). \tag{3.80}$$

In case of a pre-existing equation for $\partial_\tau \vec{c}$ (e.g, for $\tilde{\epsilon} = \epsilon$ we consider equation (3.78)), we have to replace $(\partial_\tau \vec{c})^{\rm old}$ by the information obtained from this equation, otherwise we set $(\partial_\tau \vec{c})^{\rm old} = 0$. Therefore, the assumption $\epsilon \ll \tilde{\epsilon} \ll 1$ implies

$$\partial_\tau \vec{c}(t,\tau,x) \;=\; \sum_{k\geq 1} \bar{\lambda}_k^{(1)} \mathbf{P}_k \vec{c}(t=0,\tau,x).$$

Again, we apply the orthogonal projection $\mathbf{P}$ to both sides of the equation and obtain

$$\begin{aligned} \partial_\tau \mathbf{P}\vec{c}(t=0,\tau,x) &= \bar{\lambda}_1^{(1)} \mathbf{P}_1 \vec{c}(t=0,\tau,x), \\ \bar{\lambda}_1^{(1)} &= \mathbf{P}\widehat{\mathcal{L}}_{\rm E}\mathbf{P} \;=\; \mathbf{P}_1 \widehat{\mathcal{L}}_{\rm E} \mathbf{P}_1. \end{aligned}$$

For a pathwise realization of the corresponding Markov chain, we write

$$\mathbf{P}\vec{c}(t=0,\tau,x) \;=\; b_1(\tau) \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix} + b_2(\tau) \begin{pmatrix} 0 \\ \mathbf{1}(x) \end{pmatrix},$$

with uniquely determined coefficients b_1, b_2. Using the inner product of $\mathbf{H}$ given in (3.37) together with (3.72) yields

$$\begin{aligned} \partial_\tau \vec{b} &= |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix} \vec{b}, \qquad (3.81) \\ \vec{b}(\tau) &= \begin{pmatrix} b_1(\tau) \\ b_2(\tau) \end{pmatrix} = \begin{pmatrix} \int c_1(t=0,\tau,x) \bar{\mu}^{(1)}(\mathrm{d}x) \\ \int c_2(t=0,\tau,x) \bar{\mu}^{(2)}(\mathrm{d}x) \end{pmatrix}. \end{aligned}$$

The solution is effectively computable by using

$$\tilde{\epsilon}\, \bar{\lambda}_1^{(1)} \;=\; \big\langle (\alpha_1 1\chi_1 + \alpha_2 \chi_2), \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2) \big\rangle_\mu.$$

This nicely illustrates that eventually only the eigenvalue $\mathbf{P}\overline{\mathcal{L}}_{\rm E}\mathbf{P}$ will be needed to evaluate the motion over time $\tau = \tilde{\epsilon}\, t$ (instead of computing the operator $\overline{\mathcal{L}}_{\rm E}$ as a whole). For the numerical realization note that the vector $\vec{b}$ is considered as density normalized relative to $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$. As outlined in Remark 2.2.3, the matrix in equation (3.81) actually generates a transition process on state space $\{1,2\}$, for it is self-adjoint in the weighted space $l^2(\psi)$.

Reformulation wrt. A_0, A_1

Finally, we need to reformulate the evolution equation $\partial_t \vec{c} = (\overline{\mathcal{L}} + \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\rm E})\vec{c}$ wrt. the coefficients A_0, A_1 of the eigenvector basis $\{\mathbf{1}, u_1(x,\cdot)\}$. In case of executing the asymptotic procedure (including every possible scenario) in terms of the orthogonal basis $\{\chi_1, \chi_2\}$, the notation is getting out of hand. Thus, we prefer to use the projections onto the eigenfunctions $\mathbf{1}$ and $u_1(x,\cdot)$ instead. It should be clear that results obtained in either of the two pictures can be transformed into the other.

The description wrt. to the coefficients A_0, A_1 is now obtained by decomposing the generator Γ in equation (3.79) according to $\Gamma = \overline{\Gamma} + \overline{\Gamma}_{\rm B} + \overline{\Gamma}_{\rm E}$ where $\overline{\Gamma}$, $\overline{\Gamma}_{\rm B}$ and $\overline{\Gamma}_{\rm E}$ are the respective equivalents to $\overline{\mathcal{L}}$, $\overline{\mathcal{L}}_{\rm B}$ and $\overline{\mathcal{L}}_{\rm E}$, i.e.,

$$\overline{\Gamma} = \mathcal{S}^{-1}\overline{\mathcal{L}}\mathcal{S}, \quad \overline{\Gamma}_{\rm B} = \mathcal{S}^{-1}\overline{\mathcal{L}}_{\rm B}\mathcal{S}, \quad \overline{\Gamma}_{\rm E}\overline{\Gamma}_{\rm E} = \mathcal{S}^{-1}\overline{\mathcal{L}}_{\rm E}\mathcal{S}.$$

The operators $\mathcal{S}$ and $\mathcal{S}^{-1} = \tilde{\mathcal{S}}$ are given in (3.33)&(3.34). Following (3.49) we get

$$\overline{\Gamma}_{\rm B} \ll 1, \qquad \overline{\Gamma}_{\rm E} \ll 1,$$

and, consequently, by using

$$\vec{U} \in \mathcal{N}(\overline{\Gamma}) \Rightarrow \mathcal{S}\vec{U} \in \mathcal{N}(\overline{\mathcal{L}}) \Rightarrow \overline{\Gamma}_{\rm B}\vec{U} = 0,$$

we can neglect $\overline{\Gamma}_{\rm B}$ on longer time scales. We establish Assumption 3.5.4 for $\overline{\Gamma}_{\rm E}$ and obtain

$$\overline{\Gamma}_{\rm E} = \tilde{\epsilon}\,\widehat{\Gamma}_{\rm E}, \qquad \tilde{\epsilon} \ll 1, \quad \widehat{\Gamma}_{\rm E} = \mathrm{ord}(1),$$

which implies that Γ is given formally by

$$\Gamma = \overline{\Gamma} + \tilde{\epsilon}\,\widehat{\Gamma}_{\rm E}.$$

With it we obtain two equivalent formulations for the evolution of $\rho^0 = A_0\mathbf{1} + A_1 u_1 = c_1\chi_1 + c_2\chi_2$:

$$(i.) \qquad \partial_t \vec{A} = \overline{\Gamma}\vec{A} + \tilde{\epsilon}\,\widehat{\Gamma}_{\rm E}\vec{A}, \qquad \vec{A} = (A_0, A_1)^T \in \mathbf{L}, \tag{3.82}$$

$$(ii.) \qquad \partial_t\, \vec{c} \,=\, \overline{\mathcal{L}}\,\vec{c} + \tilde{\epsilon}\,\widehat{\mathcal{L}}_{\rm E}\,\vec{c}, \qquad \vec{c} = (c_1, c_2)^T \in \mathbf{H}. \tag{3.83}$$

The properties of the operators appearing in (3.83) can be carried over to the respective operators in (3.82) (and vice versa) by using the orthogonal transformation $\mathcal{S}$. For example we easily get for $\vec{A} = (A_0, A_1)^T \in \mathbf{L}$

$$\langle \Gamma\vec{A}, \vec{A}\rangle_{\mathbf{L}} = \langle \Upsilon\mathcal{S}\vec{A}, \mathcal{S}\vec{A}\rangle_{\mathbf{H}}, \qquad \langle \overline{\Gamma}\vec{A}, \vec{A}\rangle_{\mathbf{L}} = \langle \overline{\mathcal{L}}\mathcal{S}\vec{A}, \mathcal{S}\vec{A}\rangle_{\mathbf{H}},$$

such that dissipativity and self-adjointness of Γ and $\overline{\Gamma}$ follow from the respective properties of Υ and $\overline{\mathcal{L}}$. Moreover, we do have equal eigenvalues

for Υ and Γ, as well as for $\overline{\mathcal{L}}$ and $\overline{\Gamma}$. The corresponding eigenfunctions differ solely in the transformation $\mathcal{S}^{-1}$. Therefore, following the perturbation expansion in Section 3.5.4, we obtain the spectral decomposition

$$\begin{aligned} \overline{\Gamma} + \tilde{\epsilon}\,\widehat{\Gamma}_{\mathrm{E}} &= \bar{\lambda}_0 \overline{\mathbf{P}}_0 + \sum_{k\geq 1} (\bar{\lambda}_k + \tilde{\epsilon}\bar{\lambda}_k^{(1)} + o(\tilde{\epsilon}))\overline{\mathbf{P}}_k^{\tilde{\epsilon}}, \qquad (3.84) \\ \mathcal{R}(\overline{\mathbf{P}}_k^{\tilde{\epsilon}}) &= \mathcal{R}(\mathcal{S}^{-1}\mathbf{P}_k^{\tilde{\epsilon}}), \qquad \mathcal{R}(\overline{\mathbf{P}}_k) = \mathcal{R}(\mathcal{S}^{-1}\mathbf{P}_k). \end{aligned}$$

where $\|\overline{\mathbf{P}}_k^{\tilde{\epsilon}} - \overline{\mathbf{P}}_k\|_{\mathbf{L}} = \mathcal{O}(\sqrt{\tilde{\epsilon}})$. A simple calculation yields

$$\begin{aligned} \mathcal{N}(\Gamma) &= \mathcal{R}(\overline{\mathbf{P}}_0) = \mathrm{span}\left\{ \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix} \right\}, \\ \mathcal{N}(\overline{\Gamma}) &= \mathcal{R}(\overline{\mathbf{P}}_0 + \overline{\mathbf{P}}_1) = \mathrm{span}\left\{ \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix}, \frac{1}{\gamma} \begin{pmatrix} \mu_x(B_x^{(1)}) - \mu(B^{(1)}) \\ \gamma_x \end{pmatrix} \right\}, \end{aligned}$$

with $\gamma = \sqrt{\mu(B^{(1)})\mu(B^{(2)})}$, where we have chosen an orthonormal basis in $\mathcal{N}(\overline{\Gamma})$.

3.6 Multiscale Asymptotics with $\delta \sim \epsilon$

In this section we now consider the situation where the spectral gap δ of $\mathcal{L}_x$ is comparable to ϵ, i.e., $\delta \sim \epsilon$, and use the corresponding Fokker-Planck equation for a systematic expansion in ϵ.

The postulation $\delta \sim \epsilon$ implicates $(1/\epsilon)\mathcal{L}_x = \mathcal{L}_x^{\mathrm{act}} + (1/\epsilon)\mathcal{R}_x$, such that the conformational changes on the fast fibre do not alter with vanishing ϵ. Therefore, the metastable transitions induced by the fast dynamics happen on the same time scale as the slow motion in x and the system relaxes to its final invariant distribution $\bar{\mu}$ at time $t \sim 1$. There is no need to go to higher order terms.

We proceed in two steps. First we use systematic perturbation methods to explicitly derive the averaged evolution equation for the slow variable alone. To this end, we use the orthogonal projections onto the dominant eigenfunctions $u_0 = \mathbf{1}$, $u_1(x,\cdot)$ of the fast generator $\mathcal{L}_x$. This entails the derivation of an evolution system formulated in terms of the coefficients A_0, A_1. In a second step we reformulate the averaged system wrt. the coefficients c_1, c_2 of the approximate stepfunctions χ_1, χ_2. This finally provides a clear insight into the Markov nature of the process and allows for a pathwise realization within the SDE formulation.

In this situation, the generator of the Fokker-Planck equation (1.3) is given by

$$\mathcal{L}^{\epsilon} = \frac{1}{\epsilon}\mathcal{R}_x + \mathcal{L}_y + \mathcal{L}_x^{\mathrm{act}}, \qquad (3.85)$$

where we use the decomposition (3.19) with $\delta = \epsilon$. The second order perturbation methods in Section 3.7 require a more careful analysis including the timescale of the fastest motion additionally to time $t \sim 1$. Although it is not coercively mandatory here, for reasons of consistency we introduce by now a second time scale $s = t/\epsilon$ on which the fast motion in y happens. This involves that the initial probability density not necessarily has to lie in the nullspace of $\mathcal{R}_x$. Thus, we seek for a formal asymptotic solution of (1.3) with to distinguished time scales

$$\rho^\epsilon(s,t,x,y) \;=\; \rho^0(s,t,x,y) \;+\; \epsilon\,\rho^1(s,t,x,y) \;+\; \epsilon^2\,\rho^2(s,t,x,y) \;+ ..., \quad s \;=\; \frac{t}{\epsilon}.$$

We treat these two time scales as if they were independent being consistent to the separation between s and t. Thus, we set

$$\frac{\partial}{\partial t} \;\mapsto\; \frac{1}{\epsilon}\frac{\partial}{\partial s} \;+\; \frac{\partial}{\partial t}.$$

We insert the perturbation expansion of ρ^ϵ in (1.3) with $\mathcal{L}^\epsilon$ specified in (3.85). Equating equal powers in ϵ gives the following sequence of equations:

$$\epsilon^{-1} \;:\quad \partial_s\rho^0 \;=\; \mathcal{R}_x\rho^0 \tag{3.86}$$

$$\epsilon^{0} \;:\quad \partial_s\rho^1 \;+\; \partial_t\rho^0 \;=\; \mathcal{R}_x\rho^1 \;+\; \mathcal{L}_y\rho^0 \;+\; \mathcal{L}_x^{\mathrm{act}}\rho^0 \tag{3.87}$$

1. step: (3.86) immediately yields that ρ^0 is given by

$$\begin{aligned} \rho^0(s,t,x,y) &= \exp(s\mathcal{R}_x)A(t,x,y), \\ A(t=0,x,y) &= \rho^0(s=0,t=0,x,y) \\ &= \rho^\epsilon(s=0,t=0,x,y). \end{aligned}$$

By using (3.3) we get

$$A(t,x,y) \;=\; \sum_k A_k(t,x)\cdot u_k(x,y),$$

such that ρ^0 is rewritten according to

$$\rho^0(s,t,x,y) = A_0(t,x) + A_1(t,x)u_1(x,y) + \sum_{k\geq 2} e^{s\lambda_k(x)}A_k(t,x)u_k(x,y) \tag{3.88}$$

where $\lambda_k(x)$, $k \geq 2$ denote the non-zero eigenvalues of $\mathcal{R}_x$ associated to the eigenfunctions $u_k(x,\cdot)$ and arranged in decreasing order. For the dominant eigenfunctions of $\mathcal{L}_x$ we have $u_0 = \mathbf{1}(x,\cdot), u_1(x,\cdot) \in \mathcal{N}(\mathcal{R}_x)$.

2. step: In the same way we expand ρ^1 wrt. the eigenfunctions of $\mathcal{L}_x$ which yields

$$\rho^1(s,t,x,y) \;=\; \sum_{k\geq 0} C_k(s,t,x)\cdot u_k(x,y).$$

By applying the projections $\langle\cdot, u_i(x,\cdot)\rangle_{\mu_x}$, $i=0,1$ on equation (3.87), we get:

$$\begin{aligned}
\partial_s C_0 &= h_0, \qquad h_0(s,t,x) := \langle \mathbf{1}, (-\partial_t + \mathcal{L}_y)\rho^0\rangle_{\mu_x},\\
\partial_s C_1 &= h_1 + \tilde{\lambda}_1(x)A_1, \qquad h_1(s,t,x) := \langle u_1, (-\partial_t + \mathcal{L}_y)\rho^0\rangle_{\mu_x}.
\end{aligned}$$

By using (3.88) we can expand h_i, $i=0,1$ according to

$$\begin{aligned}
h_i(s,t,x) &= H_{i0}(t,x) + H_{i1}(t,x) + \sum_{k\geq 2} e^{s\lambda_k(x)} H_{ik}(t,x),\\
H_{ik} &= \langle u_i, (-\partial_t + \mathcal{L}_y)(A_k u_k)\rangle_{\mu_x}.
\end{aligned}$$

It follows that

$$\begin{aligned}
C_0(s,t,x) &= C_0(s=0,t,x) + (H_{00}+H_{01})(t,x)\cdot s\\
&\quad + \sum_{k\geq 2} \frac{H_{0k}}{\lambda_k(x)}(e^{s\lambda_k(x)}-1),\\
C_1(s,t,x) &= C_1(s=0,t,x) + (H_{10}+H_{11})(t,x)\cdot s + \tilde{\lambda}_1(x)A_1(t,x)\cdot s\\
&\quad + \sum_{k\geq 2} \frac{H_{1k}}{\lambda_k(x)}(e^{s\lambda_k(x)}-1).
\end{aligned}$$

Equations (3.86)&(3.87) require as a solvability condition that

$$H_{00}+H_{01} = 0, \tag{3.89}$$
$$H_{10}+H_{11} = -\tilde{\lambda}_1 A_1. \tag{3.90}$$

If the above equations were not satisfied, the unresolved variable y would induce order $\mathcal{O}(1/\epsilon)$ effects on the slow variable x contradicting the very criterion for the distinction between these variables. Thus, the solvability condition (3.89)&(3.90) provides us with closed equations for the slow variable x over time scale $t = \mathrm{ord}(1)$:

$$\partial_t A_0 = \langle \mathbf{1}, \mathcal{L}_y(A_0 + A_1 u_1)\rangle_{\mu_x}, \tag{3.91}$$
$$\partial_t A_1 = \langle u_1, \mathcal{L}_y(A_0 + A_1 u_1)\rangle_{\mu_x} + \tilde{\lambda}_1(x)A_1. \tag{3.92}$$

Reformulation wrt. Coefficients c_1, c_2

To obtain an explicit interpretation of the above equations we set $\vec{A} = (A_0, A_1)^T$ and express the evolution equations as

$$\begin{aligned}
\partial_t \vec{A} &= \Gamma\vec{A} + \tilde{\Lambda}_1\vec{A},\\
\tilde{\Lambda}_1 &= \begin{pmatrix} 0 & 0\\ 0 & \tilde{\lambda}_1(x)\end{pmatrix},
\end{aligned} \tag{3.93}$$

where Γ is defined in (3.23) (for $M = 2$). Using the operators $\mathcal{S}$, $\mathcal{S}^{-1}$ given in (3.33)&(3.34), the evolution wrt. the coefficients c_1, c_2 (recall: $A_0 u_0 + A_1 u_1 = c_1\chi_1 + c_2\chi_2$) is governed by the system

$$\partial_t \vec{c} = \Upsilon \vec{c} + \mathcal{S}\tilde{\Lambda}_1 \mathcal{S}^{-1}\vec{c}, \qquad \vec{c} = (c_1, c_2)^T \in \mathbf{H} = L^2(\bar{\mu}^{(1)}) \times L^2(\bar{\mu}^{(2)}),$$

where Υ is defined in (3.41) and

$$\mathcal{S}\tilde{\Lambda}_1\mathcal{S}^{-1} \;=\; |\tilde{\lambda}_1| \begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix}.$$

Subsequently, we use the notation

$$\mathcal{Q} = \mathcal{Q}_x \;:=\; |\tilde{\lambda}_1(x)| \begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix}. \tag{3.94}$$

As outlined in Section 3.5.2, Υ is decomposed according to

$$\Upsilon \;=\; \overline{\mathcal{L}} + \overline{\mathcal{L}}_{\mathrm{B}} + \overline{\mathcal{L}}_{\mathrm{E}}, \qquad \overline{\mathcal{L}}_{\mathrm{B}} \ll 1,\ \overline{\mathcal{L}}_{\mathrm{E}} \ll 1.$$

The operators are defined in (3.46), (3.47), and (3.48). As $\overline{\mathcal{L}}_{\mathrm{B}}$ and $\overline{\mathcal{L}}_{\mathrm{E}}$ are vanishing in the asymptotic limit $\epsilon \to 0$, they do not have to be considered on time scale $t \sim 1$.

Final System

Conclusively, the evolution system for the vector $\vec{c} = \vec{c}(t, x)$ reads

$$\partial_t \vec{c} \;=\; \begin{pmatrix} \overline{\mathcal{L}}^{(1)} & 0 \\ 0 & \overline{\mathcal{L}}^{(2)} \end{pmatrix} \vec{c} + |\tilde{\lambda}_1| \begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix} \vec{c}. \tag{3.95}$$

where $\overline{\mathcal{L}}^{(i)}$, $i = 1, 2$ is the Fokker-Planck generator of the averaged potential $\overline{V}^{(i)}$ according to (3.44). The system (3.95) exactly corresponds to the conditionally averaged system obtained in [43]. Note that $\tilde{\lambda}_1(x)$ is replaced by $\lambda_1(x)/\epsilon$.

The operator $\overline{\mathcal{L}} + \mathcal{Q}$ is acting as a generator in the weighted space $\mathbf{H}$ and its nullspace is given by

$$\mathcal{N}(\overline{\mathcal{L}} + \mathcal{Q}) \;=\; \mathrm{span}\{(\mathbf{1}(x), \mathbf{1}(x))^T\} \;=\; \mathcal{R}(\mathbf{P}_0).$$

The Markov process that is generated by (3.95) admits the unique invariant probability density $\bar{\mu}(x)$. This is easily seen by considering the inner product (3.37) in $\mathbf{H}$, which suggests to weight the invariant densities $\bar{\mu}^{(1)}$ and $\bar{\mu}^{(2)}$ by $\mu(B^{(1)})$ and $\mu(B^{(2)})$, respectively. Therefore, we obtain

$$\mu(B^{(1)})\bar{\mu}^{(1)}(x) + \mu(B^{(2)})\bar{\mu}^{(2)}(x) \;=\; \mu_x(B_x^{(1)})\bar{\mu}(x) + \mu_x(B_x^{(2)})\bar{\mu}(x) \;=\; \bar{\mu}(x),$$

compare Remark 3.5.1.

Interpretation and Discretization

The evolution system (3.95) allows for pathwise simulation within the SDE formulation by interpreting the matrix $\mathcal{Q} = \mathcal{Q}_x$ for fixed x as a rate matrix generating a transition process between the levels $i = 1$ and $i = 2$. To this end, recall the comments on the generation of two-state Markov chains that are given in Remark 2.2.3. Tailored to system (3.95) we deduce that $\mathcal{Q}_x$ generates a transition process on the state space $\mathbf{S} = \{1, 2\}$ if and only if one of the following equivalent conditions is satisfied:

(i.) $\mathcal{Q}$ is self-adjoint in $\mathbf{H}$;

(ii.) $\mathcal{Q}_x$ is self-adjoint in $l^2(\psi_x)$ where $\psi_x = (\mu_x(B_x^{(1)}), \mu_x(B_x^{(2)}))^T$;

(iii.) $\mathcal{Q}_x^T \psi_x = 0$.

We easily verify $\mathcal{Q}_x^T \psi_x = 0$, which allows to interpret $\mathcal{Q}_x$ as the generator of a Markov chain on $\mathbf{S} = \{1, 2\}$ for *fixed* x.

We follow the line of [43] and shortly discuss a discretization scheme that allows for the pathwise simulation of the Markov process corresponding to system (3.95). Equation (3.95) is discretized in time by means of some simple *splitting scheme*, e.g., by the Trotter scheme which yields (in a somewhat sloppy notation):

$$\begin{aligned} \vec{c}(\mathrm{d}t, \cdot) &= \exp(\mathrm{d}t(\overline{\mathcal{L}} + \mathcal{Q}_x))\, \vec{c}(t = 0, \cdot) \\ &= \exp(\mathrm{d}t\, \overline{\mathcal{L}})\, \exp(\mathrm{d}t\, \mathcal{Q}_x)\, \vec{c}(t = 0, \cdot) + \mathcal{O}(\mathrm{d}t^2), \end{aligned}$$

where $\mathrm{d}t$ (unfortunately) has to be of order $o(\epsilon)$. This restriction follows from $\tilde{\lambda}_1 = \lambda_1/\epsilon$. The advantage of this discretization is that $\exp(\mathrm{d}t\, \overline{\mathcal{L}})$ has a direct pathwise realization since it denotes the time-$\mathrm{d}t$ transport of the Fokker-Planck equations associated with the two SDEs

$$\dot{x} = -D_x \overline{V}^{(i)}(x) + \sigma \dot{W}_1, \qquad i = 1, 2.$$

The second term, $\exp(\mathrm{d}t\, \mathcal{Q}_x)$, allows to calculate the hopping probabilities between the two levels $i = 1$ and $i = 2$:

$$\exp(\mathrm{d}t\, \mathcal{Q}_x) = \begin{pmatrix} 1 + \mu_x(B_x^{(2)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1) & -\mu_x(B_x^{(2)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1) \\ -\mu_x(B_x^{(1)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1) & 1 + \mu_x(B_x^{(1)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1) \end{pmatrix}.$$

Therefore, for every x the matrix is a stochastic matrix for all $\mathrm{d}t \geq 0$.

Now, a single realization of the corresponding Markov process requires two steps at each instance $t_k = t_0 + k\, \mathrm{d}t$.

Step 1: Transport. The first step consists of determining an updated position $x(t + \mathrm{d}t)$ by solving

$$\dot{x} = -D_x \overline{V}^{(i)}(x) + \sigma \dot{W}_1,$$

over $[0, \mathrm{d}t]$ with initial point $x(t)$.

Step 2: Exchange. The second step models the exchange between the states $i = 1$ and $i = 2$. Thus, if $i = 1$, we set $i = 2$ with hopping probability $p_{1\to 2} = -\mu_x(B_x^{(2)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1)$ and remain at $i = 1$ with probability $1 - p_{1\to 2}$. Vice versa, if $i = 2$, we set $i = 1$ with hopping probability $p_{2\to 1} = -\mu_x(B_x^{(1)})(e^{\mathrm{d}t\lambda_1/\epsilon} - 1)$ and remain at $i = 2$ with probability $1 - p_{2\to 1}$. Return to step 1 by setting $x(t) = x(t + \mathrm{d}t)$.

Remark 3.6.1 *The discretization of the ensemble dynamics is realized by executing the above two steps for an ensemble of initial states that represents the initial probability density $\vec{p}(t = 0)$. However, the transport step has to be considered as equivalent to the ensemble description by means of the Fokker-Planck equation in the unweighted space, that is, the ensemble actually has to represent a* probability *density $\vec{p}(t = 0, x) = (p_1(t = 0, x), p_2(t = 0, x))^T$, and* not *a density $\vec{c}(t = 0, x) = (c_1(t = 0, x), c_2(t = 0, x))^T$ normalized relative to $(\bar{\mu}^{(1)}, \bar{\mu}^{(2)})^T$. Therefore, we choose an ensemble according to*

$$\begin{pmatrix} p_1(t=0,x) \\ p_2(t=0,x) \end{pmatrix} = \begin{pmatrix} c_1(t=0,x)\mu(B^{(1)})\bar{\mu}^{(1)} \\ c_2(t=0,x)\mu(B^{(2)})\bar{\mu}^{(2)} \end{pmatrix},$$

such that

$$\begin{aligned} \vec{p}(t,x) &= \exp(t(\overline{\mathcal{A}} + \mathcal{Q}_x^T))\vec{p}(t=0,x) \\ &= \big(\exp(t(\overline{\pounds} + \mathcal{Q}_x))\vec{c}(t=0,x)\big) \begin{pmatrix} \mu(B^{(1)})\bar{\mu}^{(1)} \\ \mu(B^{(2)})\bar{\mu}^{(2)} \end{pmatrix}, \end{aligned}$$

where $\overline{\mathcal{A}}$ denotes the Fokker-Planck generator in the unweighted space $L^2(\mathbf{R})\times L^2(\mathbf{R})$. A detailed view to the second step now reveals that it is exactly associated to the evolution

$$\exp(\mathrm{d}t\, \mathcal{Q}_x^T)\, \vec{p}(t,\cdot) = \big(\exp(\mathrm{d}t\, \mathcal{Q}_x)\big)^T\, \vec{p}(t,\cdot).$$

3.7 Multiscale Asymptotics with $\delta \sim \epsilon^2$

We turn again to the Fokker-Planck equation (1.3) and consider the situation where the spectral gap δ is comparable to ϵ^2, i.e., $\delta \sim \epsilon^2$.

This time, the supposition $\delta \sim \epsilon^2$ implicates $(1/\epsilon)\mathcal{L}_x = \epsilon\mathcal{L}_x^{\mathrm{act}} + (1/\epsilon)\mathcal{R}_x$, such that the metastable transitions along the y dynamics are assumed to happen on a time scale $\mathrm{ord}(\epsilon)$. This is only a special case of the general postulation $\delta \sim \epsilon^r$ with $r > 1$, where the metastable relaxation happens on a time scale that is longer than the ord(1) time scale of the slow dynamics in x.

We proceed in three steps. Analogous to the procedure in Section 3.6 we obtain the evolution system over the order one time scale $t \sim 1$. This time however, the x dynamics only induce a relaxation to the invariant probability

density conditioned upon remaining within one metastable set. The averaged evolution system for the coefficients A_0, A_1 is given in (3.109). According to (3.110), the generator additionally contains the expression $\tilde{\epsilon}\,\overline{\Gamma}$, $\tilde{\epsilon} \ll 1$ that contributes to higher order terms and models the metastable transitions induced by the x dynamics.

Recalling that the metastable transitions along the y direction are governed by the ord(ϵ) term $\epsilon\mathcal{L}_x^{\text{act}}$ (as a part of $\mathcal{L}_x/\epsilon$), in the next step we derive the equation over the longer time scale $t \gg 1$ relaxing the system to its invariant probability density $\bar{\mu}$. To this end, we carefully have to distinguish whether the metastable transitions are dominated by the x or the y dynamics being expressed in an ordering of the parameters $\epsilon, \tilde{\epsilon}$: For $\tilde{\epsilon} \ll \epsilon$, the metastable relaxation occurs on time scale $t \sim \epsilon^{-1}$ and the effective dynamics over the slow time variable $\tau = \epsilon\, t$ is presented in (3.121) in Subsection 3.7.1; in the case of $\tilde{\epsilon} \sim \epsilon$, the metastable relaxation on time scale $t \sim \epsilon^{-1} \sim \tilde{\epsilon}^{-1}$ is induced by both x and y transitions, the corresponding system is given in (3.133) in Subsection 3.7.2; finally, for $\epsilon \ll \tilde{\epsilon}$, the relaxation to $\bar{\mu}$ is governed by system (3.140) in Subsection 3.7.3 that evolves over the slow time variable $\tau = \tilde{\epsilon}\, t$.

The formal derivation of the equations (3.121), (3.133), and (3.140) was performed in the space $\mathbf{L} = L^2(\bar{\mu}) \times L^2(\bar{\mu})$. As the result does not allow for a final interpretation, in the last step we transform the equations into the equivalent formulation wrt. the coefficients c_1, c_2, which is achieved by simply using the matrices $\mathcal{S}$, $\mathcal{S}^{-1}$ from Section 3.5.1. The evolution over time $t \sim 1$ is given in (3.127). The reformulations that finally arise on the longest times scale, are given in (3.125) for $\tau = \epsilon t$, in (3.135) for $\tau = \epsilon\, t = \tilde{\epsilon}\, t$, and (3.142) for $\tau = \tilde{\epsilon} t$. We observe that each system is associated to a Markov process that admits of a direct pathwise realization within the corresponding stochastic model equations.

We turn to Assumption 3.3.1 and suppose its performance with $\delta \sim \epsilon^2$. This implies that the generator $\mathcal{L}^\epsilon$ has the following form:

$$\mathcal{L}^\epsilon \;=\; \frac{1}{\epsilon}\mathcal{R}_x \,+\, \mathcal{L}_y \,+\, \epsilon\mathcal{L}_x^{\text{act}}, \tag{3.96}$$

where we used the decomposition (3.19) with $\delta = \epsilon^2$. In addition to the distinguished time scales $t \sim 1$ and $s \sim 1/\epsilon$, we now have to introduce a third time $\tau = \epsilon\, t \sim \epsilon$, which represents the separated slow scale on which the metastable relaxation occurs[4]. Therefore, we expand $\rho^\epsilon = \rho^\epsilon(s, t, \tau, x, y)$ wrt. ϵ:

$$\begin{aligned} \rho^\epsilon(s,t,\tau,x,y) \;&=\; \rho^0(s,t,\tau,x,y) + \epsilon\rho^1(s,t,\tau,x,y) + \epsilon^2\rho^2(s,t,\tau,x,y) + ..., \\ s \,=\, \frac{t}{\epsilon}, &\qquad\qquad \tau \,=\, \epsilon \cdot t. \end{aligned}$$

[4]More precise, τ will be given by $\tau = max(\epsilon, \tilde{\epsilon})\, t$, where $\tilde{\epsilon}$ is the order of the metastable transitions that happen along the x axis.

Consistent with the separation of scales between s, t, and τ, we treat these three timescales as if they were independent. Thus we set

$$\frac{\partial}{\partial t} \mapsto \frac{1}{\epsilon}\frac{\partial}{\partial s} + \frac{\partial}{\partial t} + \epsilon\frac{\partial}{\partial \tau}. \tag{3.97}$$

We insert the perturbation ansatz for ρ^ϵ in equation (1.3) (with $\mathcal{L}^\epsilon$ due to (3.96)) and use (3.97). By comparison of coefficients of different powers of ϵ we get the following sequence of equation:

$$\begin{aligned}
\epsilon^{-1} &: \quad \partial_s\rho^0 = \mathcal{R}_x\rho^0 && (3.98)\\
\epsilon^{0} &: \quad \partial_s\rho^1 + \partial_t\rho^0 = \mathcal{R}_x\rho^1 + \mathcal{L}_y\rho^0 && (3.99)\\
\epsilon^{1} &: \quad \partial_s\rho^2 + \partial_t\rho^1 + \partial_\tau\rho^0 = \mathcal{R}_x\rho^2 + \mathcal{L}_y\rho^1 + \mathcal{L}_x^{\mathrm{act}}\rho^0. && (3.100)
\end{aligned}$$

By comparing the equations with (3.86)&(3.87) it is anticipated that the formally derived evolution equation for x over timescale t is given by (3.91)&(3.92) with the exception that we have to remove the term $\tilde{\lambda}_1(x)A_1$, which has to be taken to the next order ord(ϵ) equation. We will carry out the procedure up to time t yet, as some interim steps are needed for later use (when we go to order ord(ϵ)).

1. step: (3.98) immediately yields that ρ^0 is given by

$$\begin{aligned}
\rho^0(s,t,\tau,x,y) &= A_0(t,\tau,x) + A_1(t,\tau,x)u_1(x,y)\\
&\quad + \sum_{k\geq 2} e^{s\lambda_k(x)}A_k(t,\tau,x)u_k(x,y), \qquad (3.101)
\end{aligned}$$

where $\lambda_k(x)$, $k \geq 2$ denote the non-zero eigenvalues of $\mathcal{R}_x$ that are associated to the eigenvectors $u_k(x,\cdot)$.

2. step: If we express ρ^1 by

$$\rho^1(s,t,\tau,x,y) = \sum_{k\geq 0} C_k(s,t,\tau,x)\cdot u_k(x,y),$$

and apply the projections $\langle\cdot, u_i(x,\cdot)\rangle_{\mu_x}$, $i \in \mathbf{N}$ on equation (3.99), we get:

$$\begin{aligned}
\partial_s C_i &= h_i, \qquad \text{for } i = 0,1, && (3.102)\\
\partial_s C_i &= h_i + \lambda_i(x)C_i, \qquad \text{for } i \geq 2, && (3.103)
\end{aligned}$$

where $h_i = h_i(s,t,\tau,x)$ is defined by

$$\begin{aligned}
h_i &= \langle u_i, (-\partial_t + \mathcal{L}_y)\rho^0\rangle_{\mu_x}\\
&= H_{i0}(t,\tau,x) + H_{i1}(t,\tau,x) + \sum_{k\geq 2} e^{s\lambda_k(x)}H_{ik}(t,\tau,x),
\end{aligned}$$

with

$$H_{ik} \;=\; \langle u_i, (-\partial_t + \mathcal{L}_y)(A_k u_k)\rangle_{\mu_x}. \tag{3.104}$$

Therefore, the solution of equation (3.102) is

$$\begin{aligned} C_i(s,t,\tau,x) \;&=\; C_i(s=0,t,\tau,x) \;+\; (H_{i0}+H_{i1})(t,\tau,x)\cdot s \\ &\quad + \sum_{k\geq 2} \frac{H_{0k}(t,\tau,x)}{\lambda_k(x)}(e^{s\lambda_k(x)}-1), \quad i=0,1 \end{aligned} \tag{3.105}$$

For $i \geq 2$ we get from equation (3.103)

$$C_i(s,t,\tau,x) \;=\; e^{s\lambda_i(x)}C_i(s=0,t,\tau,x) \;+\; \int_0^s e^{(s-\tilde{s})\lambda_i} h_i(\tilde{s},t,\tau,x)\mathrm{d}\tilde{s} \tag{3.106}$$

$$\begin{aligned} &= e^{s\lambda_i(x)}C_i(s=0,t,\tau,x) \;-\; (H_{i0}+H_{i1})(t,\tau,x)\frac{e^{s\lambda_i(x)}-1}{\lambda_i(x)} \\ &+ \; H_{ii}(t,\tau,x)e^{s\lambda_i(x)}\cdot s + \sum_{k\geq 2, k\neq i} H_{ik}(t,\tau,x)\frac{e^{s\lambda_k(x)}-e^{s\lambda_i(x)}}{\lambda_k(x)-\lambda_i(x)}. \end{aligned}$$

The solvability condition for $i=0$ and $i=1$ (compare (3.89)&(3.90)),

$$H_{i0} \;+\; H_{i1} \;=\; 0,$$

supplies the evolution equation for A_0, A_1 on time scale t:

$$\partial_t A_0 \;=\; \langle \mathbf{1}, \mathcal{L}_y(A_0 + A_1 u_1)\rangle_{\mu_x}, \tag{3.107}$$

$$\partial_t A_1 \;=\; \langle u_1, \mathcal{L}_y(A_0 + A_1 u_1)\rangle_{\mu_x}. \tag{3.108}$$

Using $\vec{A} = (A_0, A_1)^T$, the equations are expressed as

$$\partial_t \vec{A} \;=\; \Gamma \vec{A}, \tag{3.109}$$

where Γ is defined in (3.22) with $M=2$. Exploiting the examinations of the above evolution equation in Section 3.5 admits of decomposing Γ according to (see (3.82))

$$\Gamma \;=\; \overline{\Gamma} \;+\; \tilde{\epsilon}\widehat{\Gamma}_{\mathrm{E}}, \qquad \tilde{\epsilon} \ll 1, \tag{3.110}$$

and, consequently, the equation over time $t = \mathrm{ord}(1)$ asymptotically takes the form

$$\partial_t \vec{A} = \overline{\Gamma}\vec{A} \qquad \Longleftrightarrow \qquad \partial_t \vec{c} = \overline{\mathcal{L}}\vec{c},$$

with $\overline{\mathcal{L}}$ denoting the Fokker-Planck generator wrt. the coefficients $(c_1, c_2) \in \mathbf{H} = L^2(\bar{\mu}^{(1)}) \times L^2(\bar{\mu}^{(1)})$ that is given in (3.46). The solution is $\vec{c}(t,\tau,x) = \exp(t\overline{\mathcal{L}})\vec{c}(t=0,\tau,x)$ and, consequently,

$$\vec{c}(t,\tau,x) \;\longrightarrow\; \mathbf{P}\vec{c}(t=0,\tau,x), \qquad \text{as } t \;\to\; \infty,$$

where $\mathbf{P}$ denotes the projection onto the nullspace of $\overline{\mathcal{L}}$. Therefore, the system relaxes to a probability density that can be described with b_1, $b_2 \in \mathbf{R}^+$ by

$$b_1(\tau)\mu(B^{(1)})\bar{\mu}^{(1)}(x) + b_2(\tau)\mu(B^{(2)})\bar{\mu}^{(2)}(x), \quad \vec{b}(\tau) = \mathbf{P}\vec{c}(t=0,\tau,x), \tag{3.111}$$

where the coefficients $\vec{b} = (b_1, b_2)$ will be parametrized by the longer time scale τ.

We now turn to the evaluation on the slow time scale τ and distinguish between three different situations concerning the order of the smallness parameter $\tilde{\epsilon}$ in (3.110):

(i.) $\tilde{\epsilon} \ll \epsilon$: In this case the operator $\tilde{\epsilon}\,\widehat{\Gamma}_{\mathrm{E}}$ in (3.110) contributes to an order that is longer than the order $\mathrm{ord}(\epsilon^{-1})$ time scale of the metastable y transitions. Therefore, we simply forget about $\tilde{\epsilon}\,\widehat{\Gamma}_{\mathrm{E}}$, define the time variable $\tau = \epsilon\, t$, and resort to equation (3.100);

(ii.) $\tilde{\epsilon} \sim \epsilon$: The situation with $\tilde{\epsilon}$ comparable to ϵ requires to utilize the $\mathrm{ord}(\tilde{\epsilon})$ information that is contained in (3.109) due to (3.110) and explicitly imbed it into the $\mathrm{ord}(\epsilon)$ information given in equation (3.100) (the slow time variable is $\tau = \epsilon\, t = \tilde{\epsilon}\, t$);

(iii.) $\tilde{\epsilon} \gg \epsilon$: Now, the $\mathrm{ord}(\tilde{\epsilon})$ information dominates the information given in equation (3.100). Therefore, we define $\tau = \tilde{\epsilon}\, t$ and take $\widehat{\Gamma}_{\mathrm{E}}$ to the next order equation. This results in the evolution equation $\partial_\tau \vec{A} = \widehat{\Gamma}_{\mathrm{E}}\vec{A}$ which then enables us to obtain the effective configuration.

3.7.1 Final Metastable Relaxation Through Transitions Along Fast Variable Direction: $\tilde{\epsilon} \ll \epsilon$

The solution $\vec{A}$ over time $t = \mathrm{ord}(1)$ is derived by using the spectral decomposition of $\overline{\Gamma}$. According to (3.84), this yields

$$\vec{A}(t,\tau,x) \;=\; \overline{\mathbf{P}}\vec{A}(t=0,\tau,x) \;+\; \sum_{k\geq 2} e^{t\bar{\lambda}_k}\overline{\mathbf{P}}_k\vec{A}(t=0,\tau,x), \tag{3.112}$$

with $\bar{\lambda}_k$, $k \geq 2$ denoting the non-zero eigenvalues of $\overline{\Gamma}$ and $\overline{\mathbf{P}}_k$ the projections onto the corresponding eigenspaces. The orthogonal projection $\overline{\mathbf{P}}$ is the total projection onto the nullspace of $\overline{\Gamma}$. As the last term is decaying in t, we only have to consider the first term for the evaluation over the longest time variable $\tau = \epsilon\, t$. This arises as well out of the subsequent asymptotic procedure.

Now, we consider equation (3.100), resolve it wrt. $\partial_s\rho^2$, and apply the projections $\langle \cdot, u_i(x,\cdot)\rangle_{\mu_x}$ for $i = 0, 1$. If we express ρ^2 in the form

$$\rho^2(s,t,\tau,x,y) \;=\; \sum_{k\geq 0} E_k(s,t,\tau,x)u_k(x,y),$$

the procedure yields equations for the evolution of E_0, E_1 wrt. the fastest time scale $s = t/\epsilon$:

$$\partial_s E_0 \;=\; -\partial_t C_0 \,+\, \sum_{k\geq 0} \langle \mathbf{1}, \mathcal{L}_y(C_k u_k)\rangle_{\mu_x} \,-\, \partial_\tau A_0 \tag{3.113}$$

$$\partial_s E_1 \;=\; -\partial_t C_1 \,+\, \sum_{k\geq 0} \langle u_1, \mathcal{L}_y(C_k u_k)\rangle_{\mu_x} \,-\, \partial_\tau A_1 \,+\, \tilde{\lambda}_1 A_1. \tag{3.114}$$

In order to obtain the solvability condition, let us consider how the RHS depends on the fast time s. To this end, we go back to the **2. step** where we calculated the coefficients C_j, $j \in \mathbf{N}$. For $i = 0, 1$ they are given in (3.105), for $i \geq 2$ in (3.106). We observe the following: For every $i \in \mathbf{N}$ the coefficients C_i can be decomposed into a term that is independent of s and another term that, on its part, is split into terms containing $e^{s\lambda_k}$ for some $k \geq 2$ or $s\, e^{s\lambda_k}$, $k \geq 2$. Note that the solvability condition for C_0, C_1 revealed $H_{i0} + H_{i1} = 0$ for $i = 0, 1$. The terms containing $e^{s\lambda_k}$, $k \geq 2$ or $s\, e^{s\lambda_k}$, $k \geq 2$ do not bother us because they do not violate the solvability condition. Thus, we only have to consider that part of C_i which is independent of s. We denote it by $\bar{C}_i$ and get

$$\bar{C}_i \;=\; C_i(s = 0, t, \tau, x) \,-\, \sum_{k\geq 2} \frac{H_{ik}(t, \tau, x)}{\lambda_k(x)}, \qquad i = 0, 1, \tag{3.115}$$

$$\bar{C}_i \;=\; \frac{(H_{i0} + H_{i1})(t, \tau, x)}{\lambda_k(x)}, \qquad i \geq 2, \tag{3.116}$$

where H_{ik} is defined in (3.104). As A_0, A_1 do not depend on s either, the solvability condition for equations (3.113)&(3.114) leads to an evolution system over time $t = \mathrm{ord}(1)$:

$$\begin{pmatrix} \partial_t \bar{C}_0 \\ \partial_t \bar{C}_1 \end{pmatrix} = \Gamma \begin{pmatrix} \bar{C}_0 \\ \bar{C}_1 \end{pmatrix} + \vec{\Omega} - \begin{pmatrix} \partial_\tau A_0 \\ \partial_\tau A_1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \tilde{\lambda}_1(x) \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \end{pmatrix}, \tag{3.117}$$

where $\vec{\Omega} = (\Omega_0, \Omega_1)^T \in \mathbf{L} = L^2(\bar{\mu}) \times L^2(\bar{\mu})$ is given by

$$\Omega_i(t, \tau, x) \;=\; \sum_{j\geq 2} \left\langle \mathcal{L}_y(\bar{C}_j u_j), u_i(x, \cdot) \right\rangle_{\mu_x}, \qquad i = 0, 1.$$

Now, recall that

$$\Gamma \;=\; \overline{\Gamma} + \overline{\Gamma}_{\mathcal{B}} + \overline{\Gamma}_{\mathrm{E}}, \qquad \overline{\Gamma}_{\mathcal{B}} \ll 1,\ \overline{\Gamma}_{\mathrm{E}} \ll 1.$$

Thus, for the evaluation over $t \sim 1$ we can skip the higher order terms, and asymptotically write $\Gamma = \overline{\Gamma}$. The same consideration applies to $\vec{\Omega}$. In Appendix F we show that there exist functions $\vec{J}_k(\tau, x)$, $\vec{K}(\tau, x) \ll 1$ with

$$\vec{\Omega}(t, \tau, x) \;=\; \sum_{k\geq 2} e^{t\bar{\lambda}_k} \vec{J}_k(\tau, x) \,+\, \vec{K}(\tau, x), \qquad \vec{K} \ll 1 \tag{3.118}$$

with $\bar{\lambda}_k$, $k \geq 2$ denoting the nonzero eigenvalues of $\overline{\Gamma}$. Consequently, we obtain from (3.117) in the asymptotic limit $\epsilon \to 0$

$$\begin{pmatrix} \partial_t \bar{C}_0 \\ \partial_t \bar{C}_1 \end{pmatrix} = \bar{\Gamma} \begin{pmatrix} \bar{C}_0 \\ \bar{C}_1 \end{pmatrix} + \sum_{k\geq 2} e^{t\bar{\lambda}_k} \vec{J}_k(\tau, x) - \begin{pmatrix} \partial_\tau A_0 \\ \partial_\tau A_1 \end{pmatrix} + \tilde{\Lambda}_1 \begin{pmatrix} A_0 \\ A_1 \end{pmatrix}, \quad (3.119)$$

where $\tilde{\Lambda}_1$ is defined in (3.93). We apply the orthogonal projection $\overline{\mathbf{P}} = \overline{\mathbf{P}}_0 + \overline{\mathbf{P}}_1$ onto the nullspace of $\overline{\Gamma}$ and obtain for $\vec{\bar{C}} = (\bar{C}_0, \bar{C}_1)^T$

$$\partial_t \overline{\mathbf{P}} \vec{\bar{C}} \;=\; \sum_{k\geq 2} e^{t\bar{\lambda}_k} \overline{\mathbf{P}} \vec{J}_k(\tau, x) \;+\; \overline{\mathbf{P}}(\tilde{\Lambda}_1 - \partial_\tau)\vec{A},$$

with $\vec{A} = (A_0, A_1)$. Therefore, the solution $\overline{\mathbf{P}}\vec{\bar{C}}$ asymptotically is

$$\begin{aligned} \overline{\mathbf{P}}\vec{\bar{C}}(t,\tau,x) \;&=\; \overline{\mathbf{P}}\vec{\bar{C}}(t=0) \;+\; \sum_{k\geq 2} \int_0^t e^{\tilde{t}\bar{\lambda}_k} \overline{\mathbf{P}} \vec{J}_k \mathrm{d}\tilde{t} \\ &+\; \int_0^t \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 \vec{A}(\tilde{t},\tau,x) - \partial_\tau \vec{A}(\tilde{t},\tau,x)\big)\mathrm{d}\tilde{t} \\ &=\; \overline{\mathbf{P}}\vec{\bar{C}}(t=0) \;+\; \sum_{k\geq 2} \frac{e^{t\bar{\lambda}_k} - 1}{\bar{\lambda}_k} \overline{\mathbf{P}} \vec{J}_k \\ &+\; \int_0^t \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 \vec{A}(\tilde{t},\tau,x) - \partial_\tau \vec{A}(\tilde{t},\tau,x)\big)\mathrm{d}\tilde{t}. \end{aligned} \quad (3.120)$$

To obtain the value of the integral in (3.120), we use (3.112) and substitute it into the equation. This yields

$$\begin{aligned} \int_0^t \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 - \partial_\tau\big)\vec{A}(\tilde{t},\tau,x)\,\mathrm{d}\tilde{t} \;&=\; \sum_{k\geq 0} \int_0^t e^{\tilde{t}\bar{\lambda}_k} \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 - \partial_\tau\big)\overline{\mathbf{P}}_k \vec{A}(t=0)\,\mathrm{d}\tilde{t} \\ =\; \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 - \partial_\tau\big)\overline{\mathbf{P}}\vec{A}(t=0)\,t \;+\; \sum_{k\geq 2} \frac{e^{t\bar{\lambda}_k} - 1}{\bar{\lambda}_k} \overline{\mathbf{P}}\big(\tilde{\Lambda}_1 - \partial_\tau\big)\overline{\mathbf{P}}_k \vec{A}(t=0). \end{aligned}$$

Putting everything together, we observe that the dynamic equation for $\partial_\tau \overline{\mathbf{P}}\vec{A}(t=0,\tau,x)$ is determined from the solvability condition for the solution $\overline{\mathbf{P}}\vec{\bar{C}}$ in (3.120), i.e.,

$$\begin{aligned} &\overline{\mathbf{P}}\big(\tilde{\Lambda}_1 - \partial_\tau\big)\overline{\mathbf{P}}\vec{A}(t=0) \;=\; 0 \\ \iff\; &\partial_\tau \overline{\mathbf{P}}\vec{A}(t=0,\tau,x) \;=\; \overline{\mathbf{P}}\tilde{\Lambda}_1\overline{\mathbf{P}}\vec{A}(t=0,\tau,x). \end{aligned} \quad (3.121)$$

Reformulation wrt. Coefficients c_1, c_2

In the next step we establish the equivalent formulation wrt. the coefficients c_1, c_2. To this end, we use the transformation operator $\mathcal{S}$ defined in (3.33)

and its inverse (3.34) that apply to the matrix $\tilde{\Lambda}_1$ and the projection $\overline{\mathbf{P}}$. Thus we set

$$\tilde{\Lambda}_1 \longrightarrow \mathcal{Q} := \mathcal{S}\tilde{\Lambda}_1\mathcal{S}^{-1} = |\tilde{\lambda}_1(x)| \begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix},$$

whereas the corresponding projection operator $\mathbf{P}$ is now defined by the range of $\mathcal{S}\overline{\mathbf{P}}$ which equals the nullspace of $\overline{\mathcal{L}}$. Therefore, $\mathbf{P}$ is the orthogonal projection onto $\mathrm{span}\{(\mathbf{1}(x),0)^T,(0,\mathbf{1}(x))^T\} \subset \mathbf{H}$, and normalizing the basis leads to

$$\mathbf{P} = \sum_{i=1}^{2} \langle \cdot, \vec{\xi}_i \rangle_{\mathbf{H}} \, \vec{\xi}_i, \tag{3.122}$$

with

$$\vec{\xi}_1 = \frac{1}{\sqrt{\mu(B^{(1)})}} \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix}, \quad \vec{\xi}_2 = \frac{1}{\sqrt{\mu(B^{(2)})}} \begin{pmatrix} 0 \\ \mathbf{1}(x) \end{pmatrix}.$$

The inner product $\langle \cdot, \cdot \rangle_{\mathbf{H}}$ is defined in (3.37). For the vector $\vec{c} = (c_1, c_2)$ we arrive at the evolution equation

$$\partial_\tau \mathbf{P}\vec{c}(t=0) = \mathbf{P}\mathcal{Q}\mathbf{P}\vec{c}(t=0).$$

If we express $\mathbf{P}\vec{c}(t=0)$ by means of the orthogonal basis $\{(\mathbf{1},0)^T,(0,\mathbf{1})^T\}$, the equation results in a system of equations for the coefficients $b_1(\tau), b_2(\tau)$ that has the following form:

$$\partial_\tau b_1 = \int \tilde{\lambda}_1(x)\mu_x(B_x^{(2)})\,\bar{\mu}^{(1)}(x)\,\mathrm{d}x\,(b_1 - b_2), \tag{3.123}$$

$$\partial_\tau b_2 = \int \tilde{\lambda}_1(x)\mu_x(B_x^{(1)})\,\bar{\mu}^{(2)}(x)\,\mathrm{d}x\,(b_2 - b_1). \tag{3.124}$$

Exploiting the relation (3.45) and using the inner product $\langle \cdot, \cdot \rangle_{\bar{\mu}}$ of $L^2(\bar{\mu})$, the system is equivalently expressed with $\vec{b} = \mathbf{P}\vec{c}(t=0)$ as

$$\begin{pmatrix} \partial_\tau b_1 \\ \partial_\tau b_2 \end{pmatrix} = \left\langle |\tilde{\lambda}_1|, (\gamma_x)^2 \right\rangle_{\bar{\mu}} \cdot \begin{pmatrix} -1/\mu(B^{(1)}) & 1/\mu(B^{(1)}) \\ 1/\mu(B^{(2)}) & -1/\mu(B^{(2)}) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, \tag{3.125}$$

with γ_x defined in (3.26). Subsequently we use the abbreviation

$$\overline{\mathcal{Q}} := \left\langle |\tilde{\lambda}_1|, (\gamma_x)^2 \right\rangle_{\bar{\mu}} \cdot \begin{pmatrix} -1/\mu(B^{(1)}) & 1/\mu(B^{(1)}) \\ 1/\mu(B^{(2)}) & -1/\mu(B^{(2)}) \end{pmatrix}. \tag{3.126}$$

Final System

The effective dynamics on time scale $t \sim 1$ are described by the Fokker-Planck equation

$$\partial_t \vec{c} \;=\; \begin{pmatrix} \overline{\mathcal{L}}^{(1)} & 0 \\ 0 & \overline{\mathcal{L}}^{(2)} \end{pmatrix} \vec{c}, \qquad \vec{c}(t,\tau,x) \;=\; \begin{pmatrix} c_1(t,\tau,x) \\ c_2(t,\tau,x) \end{pmatrix} \in \mathbf{H}, \quad (3.127)$$

with $\overline{\mathcal{L}}^{(i)}$, $i = 1, 2$ defined in (3.46). The equation describes the evolution of densities $\vec{c}(t)$ normalized relative to $(\mu(B^{(1)})\bar{\mu}^{(1)}, \mu(B^{(2)})\bar{\mu}^{(2)})^T$, see Remark 3.5.1. Therefore, the probability density at time t is given by

$$\vec{p}(t,\tau,x) \;=\; \begin{pmatrix} c_1(t,\tau,x)\mu(B^{(1)})\bar{\mu}^{(1)}(x) \\ c_2(t,\tau,x)\mu(B^{(2)})\bar{\mu}^{(2)}(x) \end{pmatrix}.$$

Since for $i = 1, 2$

$$c_i(t,\tau,x) \;\longrightarrow\; \int c_i(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \qquad \text{as } t \to \infty,$$

we define

$$b_1(\tau) \;=\; \int c_1(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \quad (3.128)$$

$$b_2(\tau) \;=\; \int c_1(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \quad (3.129)$$

and obtain

$$\int \vec{p}(t=0,\tau,x)\,\mathrm{d}x \;=\; \begin{pmatrix} b_1(\tau)\mu(B^{(1)}) \\ b_2(\tau)\mu(B^{(2)}) \end{pmatrix}, \quad (3.130)$$

describing the probability of the system to be in one of the metastable configurations $i = 1$ or $i = 2$. This illustrates that $\vec{b}(\tau) = (b_1(\tau), b_2(\tau))^T$ is the density normalized relative to $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$, and the corresponding Fokker-Planck equation has to be considered in the ψ-weighted space $\overline{\mathbf{H}} := l^2(\psi)$ endowed with the inner product $\langle \vec{f}, \vec{g} \rangle_\psi = \sum_{i=1}^2 f_i\, g_i\, \mu(B^{(i)})$ for $\vec{f} = (f_1, f_2)^T$, $\vec{g} = (g_1, g_2)^T$. According to (3.125), the evolution of the density $\vec{b} = (b_1, b_2)$ over time τ is expressed as

$$\partial_\tau \vec{b} \;=\; \overline{\mathcal{Q}}\,\vec{b}, \qquad \vec{b} = (b_1, b_2)^T \in \overline{\mathbf{H}}$$

with $\overline{\mathcal{Q}}$ defined in (3.126).

Interpretation and Discretization

According to Remark 2.2.3, the matrix $\overline{\mathcal{Q}} : \overline{\mathbf{H}} \to \overline{\mathbf{H}}$ generates a Markov chain on state space $\mathbf{S} = \{1, 2\}$, which is verified by $\overline{\mathcal{Q}}^T \psi = 0$ with $\psi =$

$(\mu(B^{(1)}), \mu(B^{(2)}))^T$. Therefore, the probabilities at time $\tau = \epsilon\, t$ to jump from one state to the other are contained in the transition matrix $\exp(\tau \overline{\mathcal{Q}})$.

The discretization scheme for a single realization of the Markov process is obtained analogously to the numerical simulation of (3.95) with the exception to include the different time variables $t \sim 1$ and $\tau \sim \epsilon$ into the considerations. Therefore, let us fix ϵ and choose a time step $\mathrm{d}t$ for the discretization over time $t \sim 1$. Then we obtain the time cluster $[t_0 = 0, t_1 = \mathrm{d}t, t_2 = 2\,\mathrm{d}t, ..., t_N = N\,\mathrm{d}t, ...]$. According to $\tau = \epsilon\, t$, the discretized time interval over τ takes the form $[t_0, \epsilon\, t_1, \epsilon\, t_2, ..., \epsilon\, t_N, ...]$, and the internal time step for the discretization over time τ is chosen $\epsilon\,\mathrm{d}t$.

Following the description in Section 3.6, the equation (3.127) has a direct pathwise realization within the SDE formulation

$$\dot{x} \;=\; -D_x \overline{V}^{(i)}(x) \;+\; \sigma \dot{W}, \quad i = 1, 2.$$

The second term, $\exp(\epsilon\,\mathrm{d}t\,\overline{\mathcal{Q}})$, denotes an *exchange* between the two *levels* $i = 1$ and $i = 2$:

$$\begin{aligned}
\exp(\epsilon\,\mathrm{d}t\,\overline{\mathcal{Q}}) &= \begin{pmatrix} 1 - p_{1\to 2}(\mathrm{d}t) & p_{1\to 2}(\mathrm{d}t) \\ p_{2\to 1}(\mathrm{d}t) & 1 - p_{2\to 1}(\mathrm{d}t) \end{pmatrix}, \\
p_{1\to 2}(\mathrm{d}t) &= \mu(B^{(2)})\big(1 - \exp(\mathrm{d}t \frac{\langle \lambda_1, \gamma_x \rangle_{\bar{\mu}}}{\epsilon\, \gamma^2})\big), \\
p_{2\to 1}(\mathrm{d}t) &= \mu(B^{(1)})\big(1 - \exp(\mathrm{d}t \frac{\langle \lambda_1, \gamma_x \rangle_{\bar{\mu}}}{\epsilon\, \gamma^2})\big),
\end{aligned}$$

with $\gamma = \sqrt{\mu(B^{(1)})\mu(B^{(2)})}$. We have used $\tilde{\lambda}_1(x) = \lambda_1(x)/\epsilon^2$, where $\lambda_1(x)$ is the dominant eigenvalue of $\mathcal{L}_x$.

Now, a single realization of the corresponding Markov process requires two steps at each instance $t_k = t_0 + k\,\mathrm{d}t$.

Step 1: Transport. The first step consists of determining an updated position $x(t + \mathrm{d}t)$ by solving

$$\dot{x} \;=\; -D_x \overline{V}^{(i)}(x) \;+\; \sigma \dot{W}_1,$$

over $[0, \mathrm{d}t]$ with initial point $x(t)$.

Step 2: Exchange. The second step models the exchange between the states $i = 1$ and $i = 2$. Thus, if $i = 1$, we set $i = 2$ with hopping probability

$$p_{1\to 2} = \mu(B^{(2)})\big(1 - \exp(\mathrm{d}t \frac{\langle \lambda_1, \gamma_x \rangle_{\bar{\mu}}}{\epsilon\, \gamma^2})\big)$$

and remain at $i = 1$ with probability $1 - p_{1\to 2}$. Vice versa, if $i = 2$, we set $i = 1$ with hopping probability

$$p_{2\to 1} = \mu(B^{(1)})\big(1 - \exp(\mathrm{d}t \frac{\langle \lambda_1, \gamma_x \rangle_{\bar{\mu}}}{\epsilon\, \gamma^2})\big)$$

and remain at $i = 2$ with probability $1 - p_{2\to 1}$. Return to step 1 by setting $x(t) = x(t + \mathrm{d}t)$.

For the propagation of ensemble dynamics we refer to Remark 3.6.1.

3.7.2 Final Metastable Relaxation Through Transitions along Both Fast and Slow Variable Directions: $\tilde{\epsilon} \sim \epsilon$

As in the last subsection, the solution $\vec{A}$ over time $t \sim 1$ is given by (3.112). To derive the evolution system on the longer time scale $t \sim 1/\epsilon$, we introduce the slow time variable $\tau = \epsilon\, t = \tilde{\epsilon}\, t$. The asymptotic strategy presented in Subsection 3.7.1 can almost be adopted with one exception. Due to $\tilde{\epsilon} = \epsilon$, the extra term appearing in (3.110) is $\mathrm{ord}(\epsilon)$, which implies that we have to imbed it into equation (3.100). We refer to Section 3.5.5 where we have shown for the coefficients c_1, c_2 how to join both informations together. However, results obtained in either of the two pictures can be transformed into the other. Using (3.80), the key step is to introduce a time derivative $\partial_\tau \vec{A}$ that is equal to the sum of the 'old' information obtained from equation (3.100) and denoted $(\partial_\tau \vec{A})^{\mathrm{old}}$ and the additional information obtained from equation (3.82), that is,

$$\partial_\tau \vec{A} \;=\; (\partial_\tau \vec{A})^{\mathrm{old}} + \sum_{k\geq 1} \bar{\lambda}_k^{(1)} \overline{\mathbf{P}}_k \vec{A}(t=0). \tag{3.131}$$

Now, we basically have to possibilities to derive the final evolution equation. One way is to repeat the procedure of Subsection 3.7.1 up to the point where we find an explicit expression for $\partial_\tau \vec{A}$. This is fulfilled in equations (3.113)&(3.114). Resolving the equations wrt. $\partial_\tau A_0$, $\partial_\tau A_1$ gives an explicit equation for $(\partial_\tau \vec{A})^{\mathrm{old}}$. Now, we use (3.131) and proceed analogously to Subsection 3.7.1. Corresponding to equation (3.119), we arrive with $\vec{\bar{C}} = (\bar{C}_0, \bar{C}_1)$ at

$$\partial_t \vec{\bar{C}} \;=\; \overline{\Gamma} \vec{\bar{C}} + \sum_{k\geq 2} e^{t\bar{\lambda}_k} \vec{J}_k - \partial_\tau \vec{A} + \sum_{k\geq 1} \bar{\lambda}_k^{(1)} \overline{\mathbf{P}}_k \vec{A}(t=0) + \tilde{\Lambda}_1 \vec{A}.$$

If we continue the computation analogously to Subsection 3.7.1 by applying the orthogonal projection $\overline{\mathbf{P}}$ to both sides and exploit

$$\overline{\mathbf{P}}\big(\sum_{k\geq 1} \bar{\lambda}_k^{(1)} \overline{\mathbf{P}}_k\big) \;=\; \bar{\lambda}_1^{(1)} \overline{\mathbf{P}}_1,$$

we finally end up with the solvability condition

$$\overline{\mathbf{P}}(-\partial_\tau + \bar{\lambda}_1^{(1)} \overline{\mathbf{P}}_1 + \tilde{\Lambda}_1) \overline{\mathbf{P}} \vec{A}(t=0) \;=\; 0. \tag{3.132}$$

Condition (3.132) then provides us with the evolution equation on the longest time scale τ:

$$\partial_\tau \overline{\mathbf{P}} \vec{A}(t=0) \;=\; \overline{\mathbf{P}} \tilde{\Lambda}_1 \overline{\mathbf{P}} \vec{A}(t=0,\tau,x) \;+\; \bar{\lambda}_1^{(1)} \overline{\mathbf{P}}_1 \vec{A}(t=0). \tag{3.133}$$

The above evolution equation can also be obtained directly by applying the orthogonal projection $\overline{\mathbf{P}}$ onto the nullspace of $\overline{\Gamma}$ already to equation (3.131). Then we obtain with $\overline{\mathbf{P}}\vec{A}(t,\tau,x) = \overline{\mathbf{P}}\vec{A}(t=0,\tau,x)$

$$\partial_\tau \overline{\mathbf{P}}\vec{A}(t=0) \;=\; (\partial_\tau \overline{\mathbf{P}}\vec{A}(t=0))^{\mathrm{old}} \,+\, \bar{\lambda}_1^{(1)}\overline{\mathbf{P}}_1\vec{A}(t=0). \qquad (3.134)$$

Again, we repeat the procedure from Subsection 3.7.1 until we arrive at (3.121), which is the solution for $(\partial_\tau \overline{\mathbf{P}}\vec{A}(t=0))^{\mathrm{old}}$. Now, we use (3.134) and immediately retain (3.133).

Reformulation wrt. Coefficients c_1, c_2

As in the last subsection we opt for a presentation of the evolution equation (3.133) wrt. the coefficients c_1, c_2. To this end, we go ahead as in Section 3.7.1, and use the transformation operator $\mathcal{S}$ defined in (3.33) and its inverse (3.34) that apply to the matrix $\tilde{\Lambda}_1$, the total projection $\overline{\mathbf{P}}$ and the projection $\overline{\mathbf{P}}_1$. Thus we set

$$\tilde{\Lambda}_1 \;\longrightarrow\; \mathcal{Q} := \mathcal{S}\tilde{\Lambda}_1\mathcal{S}^{-1} \,=\, |\tilde{\lambda}_1(x)| \begin{pmatrix} -\mu_x(B_x^{(2)}) & \mu_x(B_x^{(2)}) \\ \mu_x(B_x^{(1)}) & -\mu_x(B_x^{(1)}) \end{pmatrix},$$

whereas the corresponding projection operators $\mathbf{P}$ and $\overline{\mathbf{P}}_1$ are now defined by the range of $\mathcal{S}\overline{\mathbf{P}}$ and $\mathcal{S}\overline{\mathbf{P}}_1$, respectively. The projection $\mathbf{P}_1$ is defined in (3.72), and $\mathbf{P}$ is given in (3.122). For the vector $\vec{c} = (c_1, c_2)$ we arrive at the evolution equation

$$\partial_\tau \mathbf{P}\vec{c}(t=0) \,=\, \mathbf{P}\mathcal{S}\tilde{\Lambda}_1\mathcal{S}^{-1}\mathbf{P}\vec{c}(t=0) \,+\, \bar{\lambda}_1^{(1)}\mathbf{P}_1\vec{c}(t=0).$$

If we express $\mathbf{P}\vec{c}(t=0)$ by means of the orthogonal basis $\{(\mathbf{1},0)^T, (0,\mathbf{1})^T\}$, the equation results in a system of equations for the coefficients $b_1(\tau), b_2(\tau)$ that has the following form:

$$\begin{aligned} \partial_\tau b_1 \;&=\; \Big(\int \tilde{\lambda}_1(x)\mu_x(B_x^{(2)})\,\bar{\mu}^{(1)}(x)\,\mathrm{d}x \,+\, \bar{\lambda}_1^{(1)}\mu(B^{(2)})\Big)(b_1 - b_2), \\ \partial_\tau b_2 \;&=\; \Big(\int \tilde{\lambda}_1(x)\mu_x(B_x^{(1)})\,\bar{\mu}^{(2)}(x)\,\mathrm{d}x \,+\, \bar{\lambda}_1^{(1)}\mu(B^{(1)})\Big)(b_2 - b_1). \end{aligned}$$

Exploiting relation (3.45) and using the inner product $\langle\cdot,\cdot\rangle_{\bar{\mu}}$ of $L^2(\bar{\mu})$, we can express the system as

$$\begin{pmatrix} \partial_\tau b_1 \\ \partial_\tau b_2 \end{pmatrix} \;=\; \overline{\mathcal{Q}}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} + |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, \qquad (3.135)$$

where $\overline{\mathcal{Q}}$ is given in (3.126). Subsequently, we abbreviate

$$\overline{\mathcal{E}} \;=\; |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix}. \qquad (3.136)$$

Final System

The effective dynamics on time scale $t \sim 1$ are described by the Fokker-Planck equation

$$\partial_t \vec{c} \;=\; \begin{pmatrix} \overline{\mathcal{L}}^{(1)} & 0 \\ 0 & \overline{\mathcal{L}}^{(2)} \end{pmatrix} \vec{c}, \qquad \vec{c}(t,\tau,x) \;=\; \begin{pmatrix} c_1(t,\tau,x) \\ c_2(t,\tau,x) \end{pmatrix} \in \mathbf{H},$$

with $\overline{\mathcal{L}}^{(i)}$, $i = 1, 2$ defined in (3.46). The equation describes the evolution of densities $\vec{c}(t)$ normalized relative to $(\mu(B^{(1)})\bar{\mu}^{(1)}, \mu(B^{(2)})\bar{\mu}^{(2)})^T$, see Remark 3.5.1. Therefore, the probability density at time t is given by

$$\vec{p}(t,\tau,x) \;=\; \begin{pmatrix} c_1(t,\tau,x)\mu(B^{(1)})\bar{\mu}^{(1)}(x) \\ c_2(t,\tau,x)\mu(B^{(2)})\bar{\mu}^{(2)}(x) \end{pmatrix}.$$

Since for $i = 1, 2$

$$c_i(t,\tau,x) \;\longrightarrow\; \int c_i(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \qquad \text{as } t \to \infty,$$

we define

$$\begin{aligned} b_1(\tau) &= \int c_1(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \\ b_2(\tau) &= \int c_1(t=0,\tau,x)\,\bar{\mu}^{(i)}(x)\,\mathrm{d}x, \end{aligned}$$

and obtain

$$\int \vec{p}(t=0,\tau,x)\,\mathrm{d}x \;=\; \begin{pmatrix} b_1(\tau)\mu(B^{(1)}) \\ b_2(\tau)\mu(B^{(2)}) \end{pmatrix},$$

describing the probability of the system to be in one of the metastable configurations $i = 1$ or $i = 2$. This illustrates that $\vec{b}(\tau) = (b_1(\tau), b_2(\tau))^T$ is the density normalized relative to $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$, and the corresponding Fokker-Planck equation has to be considered in the ψ-weighted space $\overline{\mathbf{H}} := l^2(\psi)$ endowed with the inner product $\langle \vec{f}, \vec{g} \rangle_\psi = \sum_{i=1}^2 f_i\, g_i\, \mu(B^{(i)})$ for $\vec{f} = (f_1, f_2)^T$, $\vec{g} = (g_1, g_2)^T$. According to (3.135), the evolution of the density $\vec{b} = (b_1, b_2)$ over time τ is expressed as

$$\partial_\tau \vec{b} \;=\; (\overline{\mathcal{Q}} + \overline{\mathcal{E}})\vec{b}, \qquad \vec{b} = (b_1, b_2)^T \in \overline{\mathbf{H}},$$

with $\overline{\mathcal{Q}}$ defined in (3.126), and $\overline{\mathcal{E}}$ given in (3.136).

Interpretation and Discretization

As outlined in Remark 2.2.3, the matrices $\overline{\mathcal{Q}} : \overline{\mathbf{H}} \to \overline{\mathbf{H}}$ as well as $\overline{\mathcal{E}} : \overline{\mathbf{H}} \to \overline{\mathbf{H}}$ generate Markov chains on state space $\mathbf{S} = \{1, 2\}$. This is easily verified by

$\overline{\mathcal{Q}}^T\psi = 0 = \overline{\mathcal{E}}^T\psi$ with $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$. Therefore, we set $\overline{\mathcal{R}} = \overline{\mathcal{Q}}+\overline{\mathcal{E}}$, and the probabilities at time $\tau = \epsilon\, t = \tilde{\epsilon}\, t$ to jump from one state to the other are contained in the transition matrix $\exp(\tau\overline{\mathcal{R}})$.

The discretization scheme for a single realization of the Markov process is the same as in Subsection 3.7.1 with the exception that we have to replace $\overline{\mathcal{Q}}$ by $\overline{\mathcal{R}}$ and set $\epsilon = \tilde{\epsilon}$. The second term, $\exp(\epsilon\, \mathrm{d}t\, \overline{\mathcal{R}})$, gives the exchange between the two *levels* $i = 1$ and $i = 2$:

$$\exp(\epsilon\, \mathrm{d}t\, \overline{\mathcal{R}}) = \begin{pmatrix} 1 - p_{1\to 2}(\mathrm{d}t) & p_{1\to 2}(\mathrm{d}t) \\ p_{2\to 1}(\mathrm{d}t) & 1 - p_{2\to 1}(\mathrm{d}t) \end{pmatrix}, \tag{3.137}$$

$$p_{1\to 2}(\mathrm{d}t) = \mu(B^{(2)})\Big(1 - \exp\big(\mathrm{d}t\,\big(\lambda_1^{(1)}\epsilon + \frac{\langle\lambda_1, \gamma_x\rangle_{\bar{\mu}}}{\epsilon\,\gamma^2}\big)\big)\Big), \tag{3.138}$$

$$p_{2\to 1}(\mathrm{d}t) = \mu(B^{(1)})\Big(1 - \exp\big(\mathrm{d}t\,\big(\lambda_1^{(1)}\epsilon + \frac{\langle\lambda_1, \gamma_x\rangle_{\bar{\mu}}}{\epsilon\,\gamma^2}\big)\big)\Big), \tag{3.139}$$

with $\gamma = \sqrt{\mu(B^{(1)})\mu(B^{(2)})}$. Note that $\epsilon\bar{\lambda}_1^{(1)}$ is explicitly given by

$$\epsilon\,\bar{\lambda}_1^{(1)} = \Big\langle(\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2)\Big\rangle_\mu.$$

Now, a single realization of the corresponding Markov process requires two steps at each instance $t_k = t_0 + k\,\mathrm{d}t$.

Step 1: Transport. The first step consists of determining an updated position $x(t + \mathrm{d}t)$ by solving

$$\dot{x} = -D_x\overline{V}^{(i)}(x) + \sigma\dot{W}_1,$$

over $[0, \mathrm{d}t]$ with initial point $x(t)$.

Step 2: Exchange. The second step models the exchange between the states $i = 1$ and $i = 2$. Thus, if $i = 1$, we set $i = 2$ with hopping probability

$$p_{1\to 2} = \mu(B^{(2)})\Big(1 - \exp\big(\mathrm{d}t\,\big(\lambda_1^{(1)}\epsilon + \frac{\langle\lambda_1, \gamma_x\rangle_{\bar{\mu}}}{\epsilon\,\gamma^2}\big)\big)\Big)$$

and remain at $i = 1$ with probability $1 - p_{1\to 2}$. Vice versa, if $i = 2$, we set $i = 1$ with hopping probability

$$p_{2\to 1} = \mu(B^{(1)})\Big(1 - \exp\big(\mathrm{d}t\,\big(\lambda_1^{(1)}\epsilon + \frac{\langle\lambda_1, \gamma_x\rangle_{\bar{\mu}}}{\epsilon\,\gamma^2}\big)\big)\Big)$$

and remain at $i = 2$ with probability $1 - p_{2\to 1}$. Return to step 1 by setting $x(t) = x(t + \mathrm{d}t)$.

For the propagation of ensemble dynamics we refer to Remark 3.6.1.

3.7.3 Final Metastable Relaxation Through Transitions along Slow Variable Directions: $\tilde{\epsilon} \gg \epsilon$

The situation with $\epsilon \ll \tilde{\epsilon} \ll 1$ requires to introduce the time variable $\tau = \tilde{\epsilon}\, t$ and use the ord$(\tilde{\epsilon})$ term in (3.110) to receive the dynamics over τ. Therefore, we set

$$\partial_\tau \vec{A} \;=\; \sum_{k\geq 1} \bar{\lambda}_k^{(1)} \overline{\mathbf{P}}_k \vec{A}(t=0),$$

which immediately leads to the equation

$$\partial_\tau \overline{\mathbf{P}} \vec{A}(t=0,\tau,x) \;=\; \bar{\lambda}_1^{(1)} \overline{\mathbf{P}}_1 \vec{A}(t=0,\tau,x). \tag{3.140}$$

Reformulation wrt. Coefficients c_1, c_2

Using the results from above, the equivalent formulation wrt. $\vec{c} = (c_1, c_2)^T$ is given by the evolution equation

$$\partial_\tau \mathbf{P} \vec{c}(t=0,\tau,x) \;=\; \bar{\lambda}_1^{(1)} \mathbf{P}_1 \vec{c}(t=0,\tau,x).$$

We write

$$\mathbf{P}\vec{c}(t=0,\tau,x) \;=\; b_1(\tau) \begin{pmatrix} \mathbf{1}(x) \\ 0 \end{pmatrix} + b_2(\tau) \begin{pmatrix} 0 \\ \mathbf{1}(x) \end{pmatrix},$$

with uniquely determined coefficients b_1, b_2. Using the inner product of $\mathbf{H}$ given in (3.37) together with (3.72) yields

$$\begin{aligned} \partial_\tau \vec{b} \;&=\; |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix} \vec{b}, \\ \vec{b}(\tau) \;&=\; \begin{pmatrix} b_1(\tau) \\ b_2(\tau) \end{pmatrix} = \begin{pmatrix} \int c_1(t=0,\tau,x) \bar{\mu}^{(1)}(\mathrm{d}x) \\ \int c_2(t=0,\tau,x) \bar{\mu}^{(2)}(\mathrm{d}x) \end{pmatrix}. \end{aligned}$$

Final System

The effective dynamics on time scale $t \sim 1$ are described by the Fokker-Planck equation

$$\partial_t \vec{c} \;=\; \begin{pmatrix} \overline{\mathcal{L}}^{(1)} & 0 \\ 0 & \overline{\mathcal{L}}^{(2)} \end{pmatrix} \vec{c}, \qquad \vec{c}(t,\tau,x) \;=\; \begin{pmatrix} c_1(t,\tau,x) \\ c_2(t,\tau,x) \end{pmatrix} \in \mathbf{H}, \tag{3.141}$$

with $\overline{\mathcal{L}}^{(i)}$, $i = 1, 2$ defined in (3.46). As before, we define

$$\begin{aligned} b_1(\tau) \;&=\; \int c_1(t=0,\tau,x)\, \bar{\mu}^{(i)}(x)\, \mathrm{d}x, \\ b_2(\tau) \;&=\; \int c_1(t=0,\tau,x)\, \bar{\mu}^{(i)}(x)\, \mathrm{d}x, \end{aligned}$$

and obtain the evolution system for the density $\vec{b} = (b_1, b_2)$ over time τ according to

$$\begin{aligned} \partial_\tau \vec{b} &= \overline{\mathcal{E}}\,\vec{b}, \qquad \vec{b} = (b_1, b_2)^T \in \overline{\mathbf{H}}, \\ \overline{\mathcal{E}} &= |\bar{\lambda}_1^{(1)}| \begin{pmatrix} -\mu(B^{(2)}) & \mu(B^{(2)}) \\ \mu(B^{(1)}) & -\mu(B^{(1)}) \end{pmatrix}, \end{aligned} \tag{3.142}$$

with $\overline{\mathbf{H}} = l^2(\psi)$ where $\psi = (\mu(B^{(1)}), \mu(B^{(2)}))^T$.

Interpretation and Discretization

The discretization scheme for a single realization of the Markov process is the same as in Subsection 3.7.2 with the exception that we have to replace $\overline{\mathcal{R}}$ by $\overline{\mathcal{E}}$.

The second term, $\exp(\epsilon\,\mathrm{d}t\,\overline{\mathcal{E}})$, gives the exchange between the two *levels* $i = 1$ and $i = 2$:

$$\exp(\tilde{\epsilon}\,\mathrm{d}t\,\overline{\mathcal{R}}) = \begin{pmatrix} 1 + \mu(B^{(2)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big) & -\mu(B^{(2)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big) \\ -\mu(B^{(1)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big) & 1 + \mu(B^{(1)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big) \end{pmatrix}.$$

Note that $\tilde{\epsilon}\bar{\lambda}_1^{(1)}$ is explicitly given by

$$\tilde{\epsilon}\,\bar{\lambda}_1^{(1)} = \Big\langle (\alpha_1\chi_1 + \alpha_2\chi_2), \mathcal{L}_y(\alpha_1\chi_1 + \alpha_2\chi_2) \Big\rangle_\mu.$$

Now, a single realization of the corresponding Markov process requires two steps at each instance $t_k = t_0 + k\,\mathrm{d}t$.

Step 1: Transport. The first step consists of determining an updated position $x(t + \mathrm{d}t)$ by solving

$$\dot{x} = -D_x \overline{V}^{(i)}(x) + \sigma \dot{W}_1,$$

over $[0, \mathrm{d}t]$ with initial point $x(t)$.

Step 2: Exchange. The second step models the exchange between the states $i = 1$ and $i = 2$. Thus, if $i = 1$, we set $i = 2$ with hopping probability $p_{1\to 2} = -\mu(B^{(2)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big)$ and remain at $i = 1$ with probability $1 - p_{1\to 2}$. Vice versa, if $i = 2$, we set $i = 1$ with hopping probability $p_{2\to 1} = -\mu(B^{(1)})\big(e^{\mathrm{d}t\,\tilde{\epsilon}\bar{\lambda}_1^{(1)}} - 1\big)$ and remain at $i = 2$ with probability $1 - p_{2\to 1}$. Return to step 1 by setting $x(t) = x(t + \mathrm{d}t)$.

For the propagation of ensemble dynamics we refer to Remark 3.6.1.