Theory of eigenvalues for periodic non-stationary Markov processes: the Kolmogorov operator and its applications

Theory of eigenvalues for periodic non-stationary Markov processes: the Kolmogorov operator and its applications

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Abstract
We present an eigenvalue theory to study the stochastic dynamics of non-stationary time-periodic Markov processes. The analysis is carried out by solving an integral operator of the Fredholm type, i.e. considering complex-valued functions fulfilling the Kolmogorov compatibility condition. We show that the asymptotic behaviour of the stochastic process is characterized by the smaller time-scale associated with the spectrum of the Kolmogorov operator. The presence of time-periodic elements in the evolution equation for the semigroup leads to a Floquet analysis. The first non-trivial Kolmogorov's eigenvalue is interpreted from a physical point of view. This non-trivial characteristic time-scale strongly depends on the interplay between the stochastic behaviour of the process and the time-periodic structure of the Fokker–Planck equation for continuous processes, or the periodically modulated master equation for discrete Markov processes. We present pedagogical examples in a finite-dimensional vector space to calculate the Kolmogorov characteristic time-scale for discrete Markov processes.

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1. General statements

It is well known that from a given stochastic prescription [1, 2] (Stratonovich, Ito, etc) any stochastic differential equation (SDE) with a delta-correlated Gaussian noise leads to a well-defined Markov process [3]. A continuous Markov process is completely characterized by its Fokker–Planck operator (FPO), which can immediately be written from the corresponding SDE. If some parameter of the SDE is time dependent, the stochastic process will not be stationary. Particularly if such a dependence is time periodic the stochastic process is called a periodic non-stationary Markov process (PNMP) [1, 4, 5]. This classification also applies

for a discrete Markov process, i.e., characterized by a master equation (ME); this case will be presented in the last section.

Now we want to discuss a method for solving a Fokker–Planck dynamics with time-periodic drift or diffusion matrix. Let the Fokker–Planck equation be

$$\partial_t P(q,t) = \left[-\frac{\partial}{\partial q_\nu} K^\nu(q,t) + \frac{\epsilon}{2} \frac{\partial^2}{\partial q_\nu \partial q_\mu} Q^{\nu\mu}(q,t) \right] P(q,t)$$
$$= \mathcal{L}_{\text{FP}}(q, \partial_q, t) P(q,t). \tag{1.1}$$

Here q stands for the set of variables $(q_1, \ldots, q_n)$ and summation over the double appearing indices ν, μ is understood. The drift $K^\nu(q,t)$ and diffusion matrix $Q^{\nu\mu}(q,t)$ are supposed to be time periodic with time-discrete translation invariance $t \to t + T$, i.e.,

$$K^\nu(q, t+T) = K^\nu(q,t) \tag{1.2}$$
$$Q^{\nu\mu}(q, t+T) = Q^{\nu\mu}(q,t). \tag{1.3}$$

ϵ is the parameter which measures the noise strength. The propagator (conditional probability density) of the Fokker–Planck dynamics $P(q,t|q_0,t_0)$ is a solution of (1.1) with the initial condition

$$P(q, t_0|q_0, t_0) = \delta(q - q_0).$$

The propagator is non-negative for any q and q_0 and satisfies normalization to 1 on a given state space $\mathcal{D}$. If K^ν and $Q^{\nu\mu}$ are time independent the Fokker–Planck dynamics can be mapped into an eigenvalue problem, then the propagator could be expanded into a biorthonormal set of eigenfunctions of the FPO, indeed only closely related to the Sturm–Liouville problem [2]. The need of the adjoint eigenfunctions is due to the fact that in general the FPO is neither Hermitian nor normal [3, 4, 6]. In the restricted case of detailed balance, the problem can be mapped into a self-adjoint negative semi-definite eigenvalue problem, which shows the existence of a complete set of eigenfunctions with negative (or zero) eigenvalues for some restricted state space $\mathcal{D}$ (see Elliott's theorem for a rigorous proof [7]), but for general FPOs not even the existence of a complete set of eigenfunctions can be proved.

In the present work, we use the Floquet structure of the FPO or the master equation to build up a characteristic value theory of an integral equation (the Fredholm equation of the second kind with a non-symmetric kernel [8]). This approach based on a biorthogonal eigenvector system, of the time-evolution operator in one period of time, can be used to obtain the characteristic time-scales of the non-stationary stochastic problem. This procedure is more amenable from the numerical point of view than other previous approaches [1, 9, 10] as we discuss in section 6.3.

Our approach can also be extended to the periodic non-stationary quantum problem; in this case the Kolmogorov compatibility condition is just the 'fundamental composition law' for the quantum time displacement operator.

In the following sections, we will give some applications of the eigenvalue theory, i.e., we deduce some connections between eigenvalues, eigenfunctions and quantities which characterize the dynamics and mixing of the system, such as correlation functions, the Lyapunov function, the spectrum and the generalized switching time between attractors [11].

2. The Kolmogorov operator

Every solution $f(q,t)$ of the Fokker–Planck equation (1.1) satisfies the Kolmogorov compatibility condition

$$f(q,t) = \int P(q,t|q',t') f(q',t') \, \mathrm{d}q', \tag{2.1}$$

for all $t' \leqslant t$.

Definition. *The Kolmogorov operator is given by* $(t_2 \geqslant t_1)$

$$\mathcal{U}(t_2, t_1) : f(q) \to \int P(q, t_2 | q', t_1) f(q') \, \mathrm{d}q',$$

i.e. the evolution of every solution of the Fokker–Planck equation is obtained by the application of the Kolmogorov operator

$$f(q, t_2) = \mathcal{U}(t_2, t_1) f(q, t_1).$$

This is once again the Kolmogorov compatibility condition.

Proposition. *The Kolmogorov operator satisfies the semigroup laws*

$$\mathcal{U}(t_1, t_1) = \mathrm{i}d \tag{2.2}$$

$$\mathcal{U}(t_3, t_1) = \mathcal{U}(t_3, t_2)\mathcal{U}(t_2, t_1). \tag{2.3}$$

If the FPO is time periodic (see (1.2)–(1.3)), the Kolmogorov operator has the periodicity

$$\mathcal{U}(t_2 + T, t_1 + T) = \mathcal{U}(t_2, t_1). \tag{2.4}$$

Property (2.2) follows from the initial condition for the propagator, and property (2.3) from the Chapman–Kolmogorov equation, which is valid for every Markov process. From (1.1) to (1.3), it is easy to see that the propagator has the periodicity

$$P(q, t + T | q_0, t_0 + T) = P(q, t | q_0, t_0),$$

from which property (2.4) follows. Due to the fact that the propagator generally is not symmetric under the transformation $q \leftrightarrow q_0$, the Kolmogorov operator in general is not self-adjoint. Its adjoint is given by

$$\mathcal{U}(t_2, t_1)^+ : \phi(q) \to \int \phi(q') P(q', t_2 | q, t_1) \, \mathrm{d}q'.$$

Proposition. *The adjoint Kolmogorov operator satisfies*

$$\mathcal{U}(t_1, t_1)^+ = \mathrm{i}d \qquad \mathcal{U}(t_3, t_1)^+ = \mathcal{U}(t_2, t_1)^+ \mathcal{U}(t_3, t_2)^+, \tag{2.5}$$

and if the FPO is time periodic (1.2)–(1.3)

$$\mathcal{U}(t_2 + T, t_1 + T)^+ = \mathcal{U}(t_2, t_1)^+.$$

These properties follow immediately from the corresponding properties of the Kolmogorov operator.

If $\phi(q, t)$ is a solution of the Fokker–Planck backwards equation

$$\partial_t \phi(q, t) = \left[K^\nu(q, t) \frac{\partial}{\partial q_\nu} + \frac{\epsilon}{2} Q^{\nu\mu}(q, t) \frac{\partial^2}{\partial q_\nu \partial q_\mu} \right] \phi(q, t)$$
$$= \mathcal{L}_{\mathrm{FP}}(q, \partial_q, t)^+ \phi(q, t), \tag{2.6}$$

then its evolution backwards in time is obtained by the application of the adjoint Kolmogorov operator

$$\phi(q, t_1) = \mathcal{U}(t_2, t_1)^+ \phi(q, t_2). \tag{2.7}$$

We will call this equation the *adjoint Kolmogorov compatibility* condition.

3. Evolution in one period of time

Now we consider the space of all complex-valued functions with finite norm satisfying the Kolmogorov compatibility condition. In particular, we are interested in the eigenvalue problem of $\mathcal{U}(t+T, t)$. Since the Kolmogorov operator in general is not self-adjoint, we are looking for a complete biorthonormal set of eigenfunctions of $\mathcal{U}(t+T, t)$ and its adjoint $\mathcal{U}(t+T, t)^+$:

$$\mathcal{U}(t+T, t) f_i(q, t) = k_i f_i(q, t) \tag{3.1}$$

$$\mathcal{U}(t+T, t)^+ \phi_i(q, t+T) = k_i \phi_i(q, t+T) \tag{3.2}$$

$$\{\phi_i, f_j\} = \int \phi_i(q, t+T) f_j(q, t)\, \mathrm{d}q = \delta_{ij}. \tag{3.3}$$

Using the definitions and properties of the previous section, the next lemma follows immediately.

Lemma. *Let $f(q, t)$ satisfy the Kolmogorov compatibility condition (2.1) and $\phi(q, t)$ satisfy the adjoint Kolmogorov compatibility condition (2.7), then we have*

(a) *If $f(q, t_0)$ is an eigenfunction of $\mathcal{U}(t_0 + T, t_0)$ with eigenvalue k then $f(q, t)$ is an eigenfunction of $\mathcal{U}(t+T, t)$ with the same eigenvalue k for all t.*
If $\phi(q, t_0 + T)$ is an eigenfunction of $\mathcal{U}(t_0 + T, t_0)^+$ with eigenvalue k then $\phi(q, t+T)$ is an eigenfunction of $\mathcal{U}(t+T, t)^+$ with the same eigenvalue k for all t.
(b) *The eigenfunctions $f_i(q, t)$ and $\phi_i(q, t)$ have the Floquet structure*

$$f_i(q, t) = \mathrm{e}^{-\lambda_i t} g_i(q, t) \qquad \phi_i(q, t) = \mathrm{e}^{\lambda_i t} \gamma_i(q, t), \tag{3.4}$$

where the functions $g_i(q, t)$ and $\gamma_i(q, t)$ are periodic in t:

$$g_i(q, t+T) = g_i(q, t) \qquad \gamma_i(q, t+T) = \gamma_i(q, t) \tag{3.5}$$

and λ_i must be chosen in such a way that the eigenvalue k_i has the form

$$k_i = \mathrm{e}^{-\lambda_i T}.$$

(c) *The integral $\int \phi(q, t+T) f(q, t)\, \mathrm{d}q$ does not depend on t, i.e., the scalar product $\{\phi, f\}$ in (3.3) is well defined.*

Proof.

(a) Since $\mathcal{U}(t+T, t)$ is periodic in t it is enough to show the proof for $t_0 + T > t > t_0$:

$$\begin{aligned}
\mathcal{U}(t+T, t) f(q, t) &= \mathcal{U}(t+T, t) \mathcal{U}(t, t_0) f(q, t_0) \\
&= \mathcal{U}(t+T, t_0) f(q, t_0) \\
&= \mathcal{U}(t+T, t_0+T) \mathcal{U}(t_0+T, t_0) f(q, t_0) \\
&= \mathcal{U}(t+T, t_0+T) k f(q, t_0) \\
&= k \mathcal{U}(t, t_0) f(q, t_0) \\
&= k f(q, t).
\end{aligned}$$

The proof for $\phi(q, t)$ can be stated analogously.
(b) Let $k_i = \mathrm{e}^{-\lambda_i T}$ then $g_i(q, t)$ is periodic in t:

$$\begin{aligned}
g_i(q, t+T) &= \mathrm{e}^{\lambda_i(t+T)} f_i(q, t+T) \\
&= \mathrm{e}^{\lambda_i(t+T)} \mathcal{U}(t+T, t) f_i(q, t) \\
&= \mathrm{e}^{\lambda_i(t+T)} k_i f_i(q, t) \\
&= \mathrm{e}^{\lambda_i t} f_i(q, t) \\
&= g_i(q, t).
\end{aligned}$$

The proof for $\phi_i(q, t)$ is again completely analogous.

(c) Let $t_2 > t_1$:

$$\int \phi(q, t_1 + T) f(q, t_1) \, dq = \int (\mathcal{U}(t_2 + T, t_1 + T)^+ \phi(q, t_2 + T)) f(q, t_1) \, dq$$

$$= \int (\mathcal{U}(t_2, t_1)^+ \phi(q, t_2 + T)) f(q, t_1) \, dq$$

$$= \int \phi(q, t_2 + T)(\mathcal{U}(t_2, t_1) f(q, t_1)) \, dq$$

$$= \int \phi(q, t_2 + T) f(q, t_2) \, dq.$$

Up to now this lemma was in principle only a conclusion from the time periodicity of our problem (i.e. the Floquet theorem [9]). If we further take into account that our equations describe probability distributions of Markov processes, we can make the following conclusions.

(d) *There always exists an eigenvalue $k_0 = 1$ ($\lambda_0 = 0$) with a constant adjoint eigenfunction $\phi_0(q, t) = \gamma_0(q, t) = 1$.*

(e) *Eigenfunctions for other eigenvalues have zero integral*

$$\int f_i(q, t) \, dq = \int g_i(q, t) \, dq = 0, \qquad \text{for} \quad k_i \neq 1.$$

(f) *If the drift and diffusion matrix are not singular, the eigenvalue $k_0 = 1$ is not degenerate, and its eigenfunction is the asymptotic time-periodic distribution* (ATPD) *$f_0(q, t) = g_0(q, t) = P_{\mathrm{as}}(q, t)$.*

(g) *All other eigenvalues have a modulus smaller than* 1

$$|k_i| < 1, \qquad \text{i.e. real part } \lambda_i > 0, \qquad \text{for} \quad i = 1, 2, \dots. \qquad \Box$$

Proof.

(d) Since the propagator is a normalized probability density we have $\mathcal{U}(t + T, t)1 = \int P(q', t + T | q, t) \, dq' = 1$.

(e) Since the Fokker–Planck dynamics conserves the integral we have $\int f_i(q, t + T) \, dq = \int f_i(q, t) \, dq = e^{-\lambda_i t} \int g_i(q, t) \, dq$ but the periodicity of $g_i(q, t)$ gives $\int f_i(q, t + T) \, dq = e^{-\lambda_i(t+T)} \int g_i(q, t + T) \, dq = e^{-\lambda_i(t+T)} \int g_i(q, t) \, dq$. Both are only possible if either $e^{-\lambda_i T} (= k_i) = 1$ or $\int g_i(q, t) \, dq = 0$ and therefore $\int f_i(q, t) \, dq = 0$.

(f) Under these conditions [5], the system approaches a unique ATPD $P_{\mathrm{as}}(q, t)$ for $t \to \infty$. The eigenfunctions with eigenvalue 1 are precisely the time-periodic functions satisfying (3.1). But $P_{\mathrm{as}}(q, t)$ is the only such function (besides scalar multiples).

(g) Since every solution of the Fokker–Planck dynamics approaches the ATPD $P_{\mathrm{as}}(q, t)$ for $t \to \infty$ all other eigenfunctions must vanish for $t \to \infty$, so $|k_i|$ must be smaller than 1. This proof follows from the existence of the Lyapunov function for PNMP [5], but part (g) of the lemma can also be proved without using the uniqueness of the ATPD. Consider (3.2); thus from the definition of the adjoint Kolmogorov operator it follows that

$$k_i \phi_i(q, t + T) = \int \phi_i(q', t + T) P(q', t + T | q, t) \, dq'. \qquad (3.6)$$

Now we use that the propagator is non-negative for any q and q' and satisfies normalization to 1, and denote q by q_m if q is such that $|\phi_i(q, t + T)| = \max$. Then from (3.6)

$$|k_i| |\phi_i(q_m, t + T)| = \left| \int \phi_i(q', t + T) P(q', t + T | q_m, t) \, dq' \right|$$

$$\leqslant \int |\phi_i(q', t + T)| P(q', t + T | q_m, t) \, dq'$$

$$\leqslant \int |\phi_i(q_m, t+T)| P(q', t+T|q_m, t)\, \mathrm{d}q'$$
$$\leqslant |\phi_i(q_m, t+T)|,$$

so therefore $|k_i| \leqslant 1$. □

For the rest of the paper, we will order the eigenvalues with decreasing modulus $1 = k_0 > |k_1| > |k_2| > \cdots$, i.e., λ_i with increasing real part.

Up to now nothing is said about the completeness of the eigenfunctions system. Actually this cannot be proved in general [2, 7]. But lemmas a and b show that from the existence of a complete set of eigenfunctions for some fixed time t_0 follows the existence for all times t. For further conclusions, we assume that such a complete set of eigenfunctions exists, so that the functions $f_i(q, t)$ and $\phi_i(q, t)$ satisfy

$$\int \phi_i(q, t+T) f_j(q, t)\, \mathrm{d}q = \delta_{ij}$$
$$\sum_{i=0}^{\infty} \phi_i(q', t+T) f_i(q, t) = \delta(q' - q). \tag{3.7}$$

Now we can expand every function $h(q, t)$ which satisfies the Kolmogorov compatibility condition (2.1) in a series of eigenfunctions

$$h(q, t) = \sum_{i=0}^{\infty} A_i f_i(q, t) = \sum_{i=1}^{\infty} A_i\, \mathrm{e}^{-\lambda_i t} g_i(q, t),$$

where the coefficients A_i can be obtained from

$$A_i = \{\phi_i, h\} = \int \phi_i(q, t+T) h(q, t)\, \mathrm{d}q.$$

In particular, the propagator can be written as

$$P(q, t|q_0, t_0) = \sum_{i=0}^{\infty} A_i(q_0, t_0)\, \mathrm{e}^{-\lambda_i(t-t_0)} g_i(q, t), \tag{3.8}$$

where the coefficients $A_i(q_0, t_0)$ are periodic in t_0. This can easily be seen from the periodicity of $P(q, t|q_0, t_0)$ and $g_i(q, t)$.

4. Periodic detailed balance

Proving the existence of a complete set of eigenfunctions of the Kolmogorov operator is still an open question. The problems arise because on one hand the differential representation of the Kolmogorov operator involves a time-ordered exponential [2–4, 6], which is difficult to handle

$$\mathcal{U}(t_2, t_1) = \vec{\mathcal{T}} \exp\left(\int_{t_1}^{t_2} \mathcal{L}_{\mathrm{FP}}(q, \partial_q, \tau)\, \mathrm{d}\tau \right).$$

Here the time-ordering symbol $\vec{\mathcal{T}}$ stipulates that all operators appearing on the right have to be taken in chronological order, i.e., according to decreasing time arguments. On the other hand in its integral representation (2.1), the kernel (i.e. the propagator) is in general not symmetric. For time-independent Markov processes, a symmetrization of the FPO is possible under the condition of detailed balance with even variables under time inversion

$$P(x, t|y, 0) P_{\mathrm{st}}(y) = P(y, t|x, 0) P_{\mathrm{st}}(x).$$

($P_{st}(x)$ is the stationary solution of such a Markov process.) This fact leads to a self-adjoint Fokker–Planck and Kolmogorov operator, which guarantees the completeness of the set of eigenfunctions [2, 3, 6]. Furthermore, under these conditions the symmetrized FPO is negative semi-definite, so that its eigenvalues are negative real numbers, i.e., the eigenvalues of the Kolmogorov operator are real numbers between 0 and 1. In our case, we have no continuous time translation symmetry but a discrete symmetry under the translation $t \rightarrow t + T$. A symmetrization of the Kolmogorov operator is possible under a similar condition as the detailed balance which is compatible with our discrete time translation symmetry and which we will call periodic detailed balance.

Definition. *The periodic detailed balance (PDB) is held if*

$$P(x, t + T | y, t) P_{as}(y, t) = P(y, t + T | x, t) P_{as}(x, t), \qquad \text{for all } x, y, t.$$

Proposition. *If the periodic detailed balance is fulfilled, the Kolmogorov operator $\mathcal{U}(t + T, t)$ is self-adjoint under the scalar product*

$$\{\eta, \xi\} = \int \eta(x)\xi(x)/P_{as}(x, t)\, dx.$$

Proof.

$$\{\eta, \mathcal{U}(t + T, t)\xi\} = \iint \eta(x) P(x, t + T | y, t)\xi(y)/P_{as}(x, t)\, dx\, dy$$

$$= \iint P(y, t + T | x, t)\eta(x)\xi(y)/P_{as}(y, t)\, dx\, dy$$

$$= \{\mathcal{U}(t + T, t)\eta, \xi\}. \qquad \square$$

As we have mentioned before if $\mathcal{U}(t + T, t)$ is an operator in an infinite-dimensional space the completeness of the eigenfunctions (3.7) is a matter for proof in each individual case, but when the Kolmogorov operator is a finite matrix the completeness can in fact be asserted when $\mathcal{U}(t + T, t)$ is symmetric under a specific scalar product, then we have

Corollary. *In a finite-dimensional vector space, if PDB is fulfilled there exists a complete set of eigenfunctions of the Kolmogorov operator $\mathcal{U}(t + T, t)$.*

5. Strong mixing

Strong mixing was originally introduced as one of the several conditions that a stochastic process must satisfy in order that the central limit theorem is applicable. This question does not arise here, since our process is in general non-Gaussian. We are more interested in the strong mixing condition as a form of asymptotic independence.

Definition. *Let $q(t)$ be a realization of a stochastic process. The correlation function is defined by*

$$\langle\langle q(t)q(t')\rangle\rangle = \langle q(t)q(t')\rangle - \langle q(t)\rangle\langle q(t')\rangle,$$

where the simple bracket represents the ensemble average.

Particularly the correlation function is calculated for the long-time limit, i.e., by using for the one-time probability distribution the ATPD $P_{as}(q, t)$. Then the asymptotic two-time second moment is given by

$$\langle q(t)q(t')\rangle_{as} = \iint qq' P(q', t' | q, t) P_{as}(q, t)\, dq\, dq',$$

where we have $t' \geqslant t$ without a loss of generality. We can consider the correlation function as a function of the variables t and $\tau = t' - t$. By using the representation of the propagator in the set of eigenfunctions of the Kolmogorov operator we get

$$\langle\langle q(t + \tau)q(t)\rangle\rangle_{\text{as}} = \sum_{i=1}^{\infty} \mathrm{e}^{-\lambda_i \tau} B_i(t, \tau), \qquad (5.1)$$

where the functions

$$B_i(t, \tau) = \iint qq' A_i(q, t) g_i(q', t + \tau) g_0(q, t) \, \mathrm{d}q \, \mathrm{d}q', \qquad i = 1, 2, 3 \ldots,$$

are periodic functions in t and τ. Therefore, the asymptotic correlation function is an oscillatory decreasing function of τ for every fixed time t, which goes to zero for $\tau \to \infty$. Therefore, under the assumption of the completeness of the eigenfunctions (3.7), we get the following:

Corollary. *Every periodic non-stationary Markov process characterized by a non-singular drift and diffusion matrix is strong mixing.*

5.1. A correlation function for large τ

If we arrange the eigenvalues of the Kolmogorov operator in the order $1 = k_0 > |k_1| > |k_2| > \cdots$ and retain only the slowest decreasing summand in expansion (5.1) of the asymptotic correlation function, we get

$$\langle\langle q(t + \tau)q(t)\rangle\rangle_{\text{as}} \approx \mathrm{e}^{-\lambda_1 \tau} B_1(t, \tau).$$

Then after each period of time in τ the asymptotic correlation function falls by a factor $k_1 = \mathrm{e}^{-\lambda_1 T}$, i.e., the first eigenvalue of the Kolmogorov operator smaller than 1 characterizes the slope of the decay of $\langle\langle q(t + \tau)q(t)\rangle\rangle_{\text{as}}$ as a function of τ.

5.2. The Lyapunov function

Another interesting object, which also gives dynamical information of a stochastic process, is the Lyapunov function. Traditionally, this function was introduced in order to analyse the decay of the initial preparation of the system.

Definition. *Let the system be prepared in one point q_0 at some certain time t_0. The Lyapunov function is defined by*

$$\mathcal{H}(t) = \int P(q, t|q_0, t_0) \ln \frac{P(q, t|q_0, t_0)}{P_{\text{as}}(q, t)} \, \mathrm{d}q.$$

Note that for every q_0, $\mathcal{H}(t)$ is a non-negative decreasing function and that the approach of the system from the preparation point q_0 towards the ATPD is characterized by the decreasing of $\mathcal{H}(t)$ [5]. If we again assume (3.7) and make use of the expansion of the propagator in eigenfunctions of the Kolmogorov operator and take only the slowest decreasing part we get the following:

Corollary. *In the long-time regime the Lyapunov function $\mathcal{H}(t)$ is an oscillatory decreasing function, which falls by a factor k_1^2 in each period of time.*

Note that in the asymptotic regime the decay of the correlation function (as a function of τ) is slower than the decay of the Lyapunov function. In the next section, we present an example showing this fact.

It is possible to interpret the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ that appears in the eigenvalue k_1 as a generalization of the Kramers escape time for periodic non-stationary Markov processes. An important question for stationary processes, conveniently answered in terms of the FPO framework, is what is the time required for the passage of a prepared initial state to the final stationary state? Historically this problem was first studied by Kramers [12], and many mathematicians [13] and physicists [14] have developed different perturbation approaches to tackle this fundamental problem for bistable situations with clearly separated time-scales. In the present section, we were concerned with a similar question but for a non-stationary periodically modulated Markov process. But because the system periodically reaches a situation where the stabilities and instabilities may not be well pronounced, the analysis is even more complex than in the Kramers problem due to the disparate time-scales that the system may have [11]. Therefore, the hope to find an analytical expression characterizing the passage times is even more unlikely, so in the next section we introduce discrete Markov processes in order to find some analytical answers to the characterization of λ_1^{-1}.

6. Applications to finite-dimensional vector spaces

A continuous nonlinear stochastic Markovian process can rarely be solved analytically, and solving the integral equation related to the Kolmogorov eigenvalue problem is even more complex. If we can arrange the eigenvalues of the Kolmogorov operator $\mathcal{U}(t + T, t)$ in the form $1 = k_0 > |k_1| > |k_2| > \cdots$, we have shown that the asymptotic behaviour of the periodic non-stationary process is controlled by k_1. The important point to remark here is that by finding the first non-trivial eigenvalue of Kolmogorov's operator, we get the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ which controls the asymptotic stochastic relaxation of the system, see section 5. In fact, in previous works [11] we have studied numerically a noise-induced order–disorder transition by employing the mentioned integral operator $\mathcal{U}(t + T, t)$. Here we will extend our presentation concerning the Floquet analysis of *non-stationary periodically modulated* processes to the case when the Markov process is discrete. In this situation, the evolution equation of the process is controlled by a master equation rather than by a Fokker–Planck one, so in order to solve $\mathcal{U}(t + T, t)$, we only have to deal with a matrix eigenvalue problem.

The ME of an arbitrary discrete Markov process is characterized by a master Hamiltonian matrix $\mathbf{H}$ of finite dimension $N \times N$ (we exclude here the analysis of a system whose range is denumerably infinite). This matrix $\mathbf{H}$ is real and in general non-symmetric, and it must fulfil the fundamental conditions

$$\mathbf{H}_{jl} \geqslant 0, \qquad j \neq l, \qquad \mathbf{H}_{jj} = -\sum_{l(\neq j)} \mathbf{H}_{lj}.$$

Therefore, for a *non-stationary* Markov process, any result will have to be based on the *two* properties: (1) $\mathbf{H}_{jl}(t) \geqslant 0$, $j \neq l$ and (2) for each l we have $\sum_j \mathbf{H}_{jl}(t) = 0$. This means that in general the instantaneous matrix $\mathbf{H}(t)$ cannot be diagonalized. Consider now the situation when the process is non-stationary but *periodically modulated*. In this case, we have the additional temporal symmetry $\mathbf{H}_{jl}(t) = \mathbf{H}_{jl}(t + T)$; thus we can apply our Floquet analysis of section 3. In this case, the Kolmogorov integral problem reduces to an eigenvector analysis. This fact can be seen by noting that the Kolmogorov operator is

$$\mathcal{U}(t_2, t_1) = \vec{\mathcal{T}} \exp \left(\int_{t_1}^{t_2} \mathbf{H}(\tau) \, d\tau \right) \equiv \mathbf{P}(t_2 \mid t_1), \tag{6.1}$$

where $\mathbf{P}(t_2 \mid t_1)$ is the matrix Green's function of the ME $\dot{\mathbf{P}} = \mathbf{H}(t) \cdot \mathbf{P}$. Note the similitude with the propagator introduced in section 2 when we deal with a continuous Markov process.

From this comment it is trivial to see that the Kolmogorov eigenvalue problem, see (3.1)–(3.3), reduces to a simple eigenvector problem of dimension N. We remark that in order to fully characterize the temporal behaviour of an arbitrary discrete N-level PNMP, the Kolmogorov operator technique turns out to be a suitable and fundamental approach to tackle that sort of non-stationary problems.

6.1. Master equation toy model

A toy discrete stochastic process which, in the present context, can analytically be solved is the so-called *dichotomic process* [2–4, 15] originally introduced by Kubo and Anderson. As we pointed out before, in opposition to continuous Markov processes, the dichotomic process has two discrete levels and the evolution equation that governs its propagator is the ME. Then the Kolmogorov operator approach can immediately be applied.

Here we will work out a non-stationary dichotomic process for the case when the ME has a discrete symmetry under the time translation $t \rightarrow t + T$. In the present case, the Kolmogorov operator is a 2×2 matrix (6.1), and the eigenvalues problem (3.1)–(3.3) reads

$$\begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \cdot \begin{pmatrix} f_i(1, t) \\ f_i(2, t) \end{pmatrix} = k_i \begin{pmatrix} f_i(1, t) \\ f_i(2, t) \end{pmatrix} \tag{6.2}$$

$$(\phi_i(1, t + T) \quad \phi_i(2, t + T)) \cdot \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} = k_i(\phi_i(1, t + T) \quad \phi_i(2, t + T)) \tag{6.3}$$

$$\{\vec{\phi}_i, \vec{f}_j\} \equiv (\phi_i(1, t + T) \quad \phi_i(2, t + T)) \cdot \begin{pmatrix} f_j(1, t) \\ f_j(2, t) \end{pmatrix} = \delta_{ij}, \qquad \forall i, j = 0, 1. \tag{6.4}$$

As we commented in the lemma, the elements of the propagator are evaluated in one period of time

$$P_{\alpha\beta} \equiv P_{\alpha\beta}(t + T \mid t), \qquad \forall \alpha, \beta = 1, 2,$$

and they are periodic functions of t fulfilling the normalization conditions

$$P_{11} + P_{21} = 1, \qquad P_{12} + P_{22} = 1.$$

As expected, the one-time asymptotic time-periodic (ATP) probability (vector) of the discrete system $P_{as}(\alpha, t), \forall \alpha, \beta = 1, 2$, is related to the propagator (matrix) in the long-time limit.

The eigenvalue problem (6.2)–(6.4) can immediately be solved, so we get for the eigenvalue $k_0 = 1$ the right and left eigenvectors

$$\vec{f}_0 \equiv f_0(1, t) \begin{pmatrix} 1 \\ \frac{1 - P_{11}}{1 - P_{22}} \end{pmatrix}, \qquad \vec{\phi}_0 \equiv C \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The function $f_0(1, t)$ and the constant C can be determined from normalization of the ATP probability and the scalar-product condition $\{\vec{\phi}_0, \vec{f}_0\} = 1$.

From the eigenvalue k_1, we get

$$\vec{f}_1 \equiv f_1(1, t) \begin{pmatrix} 1 \\ \frac{P_{11} - 1}{P_{22} - k_1} \end{pmatrix}, \qquad \vec{\phi}_1 \equiv \phi_1(1, t + T) \begin{pmatrix} 1 \\ \frac{P_{11} - k_1}{P_{11} - 1} \end{pmatrix},$$

and from orthogonality, $\{\vec{\phi}_0, \vec{f}_1\} = \{\vec{\phi}_1, \vec{f}_0\} = 0$, we obtain

$$P_{11} + P_{22} = 1 + k_1, \tag{6.5}$$

which is nothing more than the trace of the Kolmogorov operator, see (6.1). From the scalar-product $\{\vec{\phi}_1, \vec{f}_1\} = 1$, we get the condition

$$f_1(1, t)\phi_1(1, t + T) = \left(1 + \frac{P_{11} - k_1}{P_{22} - k_1}\right)^{-1}.$$

Using the Floquet structure (see lemma, part (b)) we know that $f_1(1, t) = e^{-\lambda_1 t} \Theta(t)$ and $\phi_1(1, t+T) = e^{+\lambda_1(t+T)} \Xi(t)$, where $\Theta(t)$ and $\Xi(t)$ are periodic functions of time. It is simple to see that they fulfil

$$\Theta(t) \Xi(t) = k_1 \left(\frac{P_{22} - k_1}{1 - k_1} \right) = k_1 \left(\frac{P_{11} - 1}{k_1 - 1} \right). \tag{6.6}$$

So we arrive at the set of vectors

$$\vec{f}_0 = \frac{1}{1 - k_1} \begin{pmatrix} 1 - P_{22} \\ 1 - P_{11} \end{pmatrix}; \qquad \vec{\phi}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\vec{f}_1 = e^{-\lambda_1 t} \begin{pmatrix} \Theta(t) \\ -\Theta(t) \end{pmatrix}; \qquad \vec{\phi}_1 = e^{+\lambda_1(t+T)} \begin{pmatrix} \Xi(t) \\ \frac{P_{11} - k_1}{P_{11} - 1} \Xi(t) \end{pmatrix}. \tag{6.7}$$

The calculation of the functions $\Theta(t)$ and $\Xi(t)$ can be done by imposing the condition that the following equality holds for any pair of times $\{t, t_0\}$ provided $t \geqslant t_0$:

$$\mathbf{P}(t \mid t_0) = \sum_j \vec{f}_j(t) \cdot \vec{\phi}_j(t_0 + T)^{\mathsf{T}}$$

$$= \frac{1}{1 - k_1} \begin{pmatrix} 1 - P_{22}(t + T \mid t) & 1 - P_{22}(t + T \mid t) \\ 1 - P_{11}(t + T \mid t) & 1 - P_{11}(t + T \mid t) \end{pmatrix}$$

$$+ \frac{e^{\lambda_1(t_0 - t + T)} \Theta(t) \Xi(t_0)}{P_{11}(t_0 + T \mid t_0) - 1} \begin{pmatrix} P_{11}(t_0 + T \mid t_0) - 1 & P_{11}(t_0 + T \mid t_0) - k_1 \\ -P_{11}(t_0 + T \mid t_0) + 1 & -P_{11}(t_0 + T \mid t_0) + k_1 \end{pmatrix}. \tag{6.8}$$

Note that (6.6) follows from (6.8) considering that $\mathbf{P}(t_0 \mid t_0) = \mathbf{I}$, i.e., the identity matrix. Defining $\Gamma(t, t_0) \equiv \text{Tr}[\mathbf{P}(t \mid t_0)] - 1$ we can write the equations

$$\Gamma(t, t_0) e^{-\lambda_1(t_0 - t)} = \frac{\Theta(t)}{\Theta(t_0)} \qquad \frac{P_{11}(t + T \mid t) - 1}{k_1 - 1} \frac{k_1}{\Theta(t)} = \Xi(t), \tag{6.9}$$

from where both functions $\Theta(t)$ and $\Xi(t)$ can be calculated (besides scalar multiples); see (6.15) and (6.17) for two particular cases of $\Gamma(t, t_0)$.

In the present 2×2 model, there are only two important time-scales, T and λ_1^{-1}; interestingly the only function that remains to be calculated is the trace of the propagator, which in fact depends on the temporal structure of $\mathbf{H}(t)$. On the other hand, the decay of the slowest decreasing (antisymmetric) eigenvector $\vec{f}_1$ is dominated by the time-scale λ_1^{-1}.

Note that in the continuous case, the eigenfunction $f_1(q, t)$ has to be antisymmetric with only one zero because such a function can only decay when there is a current across the origin [11]. This situation is analogous to the Kramers metastable problem for stationary Markov processes, mathematically the FPO is parabolic and its propagator can be written as an eigenfunction expansion, with the eigenvalues appearing in exponential decay factors associated with each eigenfunction. Thus, it turns out that the lowest non-trivial eigenvalue of the FPO is just the inverse of the mean first passage time, in the large barrier limit [3]. But this simple interpretation for the Kramers problem, in general, does not appear in periodic non-stationary Markov processes.

The two-point correlation function, (5.1), in the discrete case reads

$$\langle\langle q(t + \tau) q(t) \rangle\rangle_{\text{as}} = \sum_{i=1}^{\infty} e^{-\lambda_i \tau} B_i(t, \tau), \tag{6.10}$$

where

$$B_i(t, \tau) = \frac{1}{k_i} \sum_{\alpha\beta} q_\alpha q_\beta g_i(q_\alpha, t + \tau) \gamma_i(q_\beta, t) g_0(q_\beta, t).$$

Here $A_i(q_0, t_0)$ appearing in (3.8) has been replaced by $\gamma_i(q_\beta, t)/k_i$ and q_α is the arbitrary value that the discrete process can take. The time-periodic vectors $g_i(q_\alpha, t)$ and $\gamma_i(q_\beta, t)$ can be read from the Floquet structure of the eigenvectors associated with the eigenvalue problem (3.1)–(3.3). In the present dichotomic case, these eigenvectors are given in (6.7); then we get

$$\langle\langle q(t + \tau)q(t)\rangle\rangle_{as} = e^{-\lambda_1 \tau} B_1(t, \tau), \tag{6.11}$$

with

$$B_1(t, \tau) = \frac{\Theta(t + \tau)\,\Xi(t)}{k_1}\left(\frac{1 - P_{22}}{1 - k_1}\right)(q_1 - q_2)^2, \tag{6.12}$$

where we have used (6.5).

In order to have an explicit expression for the non-trivial eigenvalue k_1, we need to specify the time-structure of the one period of time propagator $\mathbf{P}(t + T \mid t)$. In general, this matrix is obtained from the solution of the ME

$$\frac{d\mathbf{P}}{dt} = \mathbf{H} \cdot \mathbf{P}, \tag{6.13}$$

where $\mathbf{H}$ is given in terms of the transition probability rate $W_{\alpha\beta}$

$$\mathbf{H} = \begin{pmatrix} -W_{21} & W_{12} \\ W_{21} & -W_{12} \end{pmatrix}. \tag{6.14}$$

As a particular asymmetric model, we assume here that the transition probability rate W_{12} is periodic in time with the structure $W_{12} = \mathcal{A} + \mathcal{B}\cos\omega t$, with $\mathcal{A} - \mathcal{B} \geqslant 0$; and that the reverse transition rate is constant $W_{21} = \mathcal{C} \geqslant 0$. Solving system (6.13) it is possible to write

$$\mathbf{P}(t \mid t_0) \equiv \begin{pmatrix} P_{11}(t \mid t_0) & P_{12}(t \mid t_0) \\ P_{21}(t \mid t_0) & P_{22}(t \mid t_0) \end{pmatrix},$$

with

$$P_{11}(t|t_0) = \Gamma(t, t_0) + \int_{t_0}^{t} (\mathcal{A} + \mathcal{B}\cos\omega t')\Gamma(t, t')\,dt'$$

$$P_{22}(t|t_0) = \Gamma(t, t_0) + \int_{t_0}^{t} \mathcal{C}\,\Gamma(t, t')\,dt'$$

$$P_{21}(t|t_0) = 1 - P_{11}(t|t_0)$$

$$P_{12}(t|t_0) = 1 - P_{22}(t|t_0),$$

where $\Gamma(t, t')$ is

$$\Gamma(t, t') = \exp\left[-(\mathcal{A} + \mathcal{C})(t - t') + \frac{\mathcal{B}}{\omega}(\sin\omega t - \sin\omega t')\right]. \tag{6.15}$$

This expression *completely* solves the Kolmogorov problem we have posed before. As a matter of fact, it can be seen that the following expression holds:

$$1 + \Gamma(t, t') = P_{11}(t|t') + P_{22}(t|t').$$

Therefore, by taking in the former expression $t' = t - T$, and comparing with equation (6.5), the eigenvalue k_1 can be written in the form

$$k_1 = P_{11}(t + T|t) + P_{22}(t + T|t) - 1 = \exp[-(\mathcal{A} + \mathcal{C})T]. \tag{6.16}$$

Note that for the present model, due to the symmetry of the periodic modulation in W_{12}, the Kolmogorov time-scale is independent of $\mathcal{B}$ and it is just characterized by the value $\lambda_1^{-1} = (\mathcal{A} + \mathcal{C})^{-1}$. Nevertheless, as we have already mentioned, in general the time-scale λ_1^{-1} strongly depends on the temporal structure of the matrix $\mathbf{H}(t)$. For example, if the time-dependent W_{12} transition rate were of the Arrhenius type, the eigenvalue k_1 would not be independent of the amplitude of the periodic modulation.

6.1.1. Periodically modulated Arrhenius-like model. Consider an asymmetric Arrhenius-type model, so we now assume that the transition probability rate W_{12} is periodic in time with the temporal structure $W_{12} = \mathcal{A} \exp(b \cos \omega t)$, and as before $W_{21} = \mathcal{C}$ is constant in time. Solving systems (6.13) and (6.14) for this model it is possible to write

$$\Gamma(t, t') = \exp\left[-\mathcal{C}(t - t') - \mathcal{A} \int_{t'}^{t} \exp(b \cos \omega s) \, \mathrm{d}s \right]. \tag{6.17}$$

Therefore, Kolmogorov's time-scale $\lambda_1^{-1} = -T / \log k_1$ reads

$$\lambda_1^{-1} = [\mathcal{C} + \mathcal{A} I_0(b)]^{-1}, \tag{6.18}$$

where $I_0(b)$ is the Hyperbolic or modified Bessel function [16]; in the case $b = 0$, there is no periodic modulation and we reobtain the static or Kramers-like time-scale. In analogy with the splitting problem [3], note that in the static case the rate λ_1 is just given in terms of the Kramers scape rates $\mathcal{C}$ and $\mathcal{A}$.

The non-adiabatic formula (6.18) is therefore a useful starting point to study the relaxation of our stochastic model in the presence of an external periodic modulation. It is interesting to introduce here a perturbation in the amplitude of modulation b, in order to compare Kolmogorov's time-scale λ_1^{-1} with the static time-scale $\tau_s = [\mathcal{C} + \mathcal{A}]^{-1}$. Using the expansion of the Bessel function, from (6.18) we get

$$\lambda_1^{-1} = \tau_s \left(1 - \mathcal{A} \tau_s \left(\frac{b^2}{4} + \cdots \right) \right), \tag{6.19}$$

it is worth pointing here that (6.18) is independent of T, showing therefore that (6.19) is not a perturbative expression in the inverse of the period of the modulation. Thus, the comparison of λ_1^{-1} against T will give information concerning the loss of correlation during the time-scale of the external periodic modulation.

We see from the propagator expansion (3.8), i.e., using (6.8) for a dichotomic process, that by increasing the amplitude of modulation b the antisymmetric Floquet eigenvector $\vec{g}_1(t) = (\Theta(t), -\Theta(t))$ dies out faster to reach the ATP probability (positive vector $\vec{g}_0(t)$). In a similar context, Kolmogorov's eigenvalue k_1 gets smaller for increasing b thus predicting a faster strong mixing of the two-point correlation function (6.11).

We have proved in section 5 that in general the relaxation of the *correlation* and the *Lyapunov* functions is, in the asymptotic limit, controlled by the Kolmogorov time-scale $\sim \mathrm{Re}[\lambda_1]^{-1}$. Therefore, in order to study the asymptotic relaxation of any PNMP, the important task is to determine the first non-trivial eigenvalue k_1. More complex objects can similarly be studied in terms of the biorthogonal set of eigenvectors of $\mathcal{U}(t + T, t)$; for example, this is the case of the stochastic resonance phenomenon.

6.1.2. Stochastic resonance in a 2×2 model. The stochastic resonance is a name *coined* in order to characterize the situation when the addition of noise into a periodically modulated nonlinear system leads to an amplification of the signal-to-noise spectrum, i.e., this is a cooperative result showing the interplay between deterministic and random dynamics in a time-modulated system [10]. The signature of this phenomena can easily be seen from the dynamics of a ME, as it is in the present 2×2 model. Consider the exact expression for the correlation function (6.11). The power spectral density $S(\omega, t)$ is the Fourier transform of the correlation function with respect to the variable τ. Here the time t corresponds to the time at which one begins to take data, and since the phase of the signal with respect to this time is usually not known (in decoherent systems), one assumes that t itself is a random variable

distributed uniformly over one period of the signal. Then the spectral density of interest is the average over the random phase variable

$$S(\omega) = \frac{1}{T} \int_0^T \left[\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega\tau} \langle\langle q(t+\tau)q(t)\rangle\rangle_{as} \, d\tau \right] dt$$

$$= \frac{1}{T} \int_0^T \left[\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega\tau} e^{-\lambda_1\tau} B_1(t,\tau) \, d\tau \right] dt.$$

As we mentioned before, from (6.12), it is simple to see that $B_1(t,\tau)$ is a periodic function of τ, in fact given in terms of $\Theta(t+\tau)$. This τ-dependence implies the destruction of the Lorentzian shape for the spectra, a fact that ultimately leads to the stochastic resonance phenomenon shown in the signal-to-noise spectrum.

For a general time-modulated Markov problem, in order to study the amplification of the signal-to-noise spectrum the important task—in the *asymptotic* analysis—is to consider just the associated key function $B_1(t,\tau)$ in the corresponding expansion (5.1), or (6.10) for discrete Markov processes.

6.2. Diagonalizable models

If the N-level master Hamiltonian can be diagonalized at any *instant* t, we could calculate the spectrum of $\mathcal{U}(t+T,t)$ by the following device. Consider the auxiliary time-parametric eigenvalue problem

$$\mathbf{H}(t') \mid n(t') \rangle = E_n(t') \mid n(t') \rangle,$$

where $E_n(t), n = 0, 1, 2\ldots$, are auxiliary quasienergies. Assuming the existence a complete *braket* set $\mid n(t') \rangle$, i.e., defining a suitable scalar product such that $\sum_n |n(t)\rangle\langle n(t)| = \mathbf{I}$ (the identity matrix) it is possible to show that

$$\mathrm{Tr}[\mathbf{P}(t|t')] = \sum_n \exp \int_{t'}^t E_n(s) \, ds. \tag{6.20}$$

From this expression we can calculate recursively any Kolmogorov's eigenvalue. Using the notation $\Gamma(t+T,t) = \mathrm{Tr}[\mathbf{P}(t+T \mid t)] - 1$, in principle any eigenvalue $k_n = e^{-\lambda_n T}$ can be calculated by noting that

$$\lim_{T\to\infty} \frac{\frac{d}{dT}\Gamma(t+T,t)}{\Gamma(t+T,t)} \to -\lambda_1,$$

and for λ_2 we have

$$\lim_{T\to\infty} \frac{\frac{d}{dT}[\Gamma(t+T,t) - k_1]}{\Gamma(t+T,t) - k_1} \to -\lambda_2,$$

and so forth. We see that the important task is to determine the trace of matrix Green's function $\mathbf{P}(t+T|t)$.

We note that in general a time-parametric master Hamiltonian matrix $\mathbf{H}(t)$ cannot be diagonalized; on the other hand only if the condition of PDB is fulfilled the diagonalization of $\mathcal{U}(t+T,t)$ could be assured, see section 4.

In order to get more insight into the structure of the Kolmogorov spectrum let us now consider a particular non-symmetric 3×3 model. Assume that the master Hamiltonian has the particular structure

$$\mathbf{H} = \begin{pmatrix} -(\beta+\gamma) & \alpha & \alpha \\ \beta & -(\alpha+\gamma) & \beta \\ \gamma & \gamma & -(\alpha+\beta) \end{pmatrix}, \tag{6.21}$$
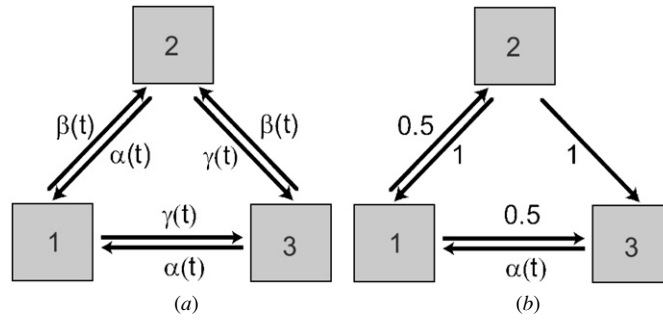
Figure 1. (*a*) Schematic drawing representing the transition rates in the 3-level stochastic process characterized by the master Hamiltonian (6.21). Note that in principle the transition rates can be time-periodically modulated. (*b*) Schematic drawing representing the transition rates characterized by the master Hamiltonian (6.24).

where α, β, γ are positive possible time-periodic functions. The physical interpretation of this $\mathbf{H}(t)$ can easily be done by using a level diagrammatic representation, see figure 1(*a*). Solving system (6.13) for this model it is possible to write a closed equation for the trace of the propagator, then we get

$$\begin{aligned}
\Gamma(t, t') &= \mathrm{Tr}[\mathbf{P}(t \mid t')] - 1 \\
&= 2 \exp\left[-\int_{t'}^{t} (\alpha(s) + \beta(s) + \gamma(s))\, \mathrm{d}s \right].
\end{aligned} \tag{6.22}$$

We see that even when there is a degenerated quasienergy for (6.21), i.e., $E_0(t) = 0$, $E_{1,2}(t) = -\alpha - \beta - \gamma$, due to the fact that this $\mathbf{H}(t)$ can be diagonalized at any *instant t*, expression (6.22) is in accordance with (6.20). From (6.22) it is possible to see that Kolmogorov's time-scale λ_1^{-1} is given, for this particular case, in terms of one period of time area of the transition rates.

6.3. About the Suzuki–Trotter approach

If $\mathbf{H}(t)$ cannot be diagonalized at any instant t, nothing more can be told concerning the possibility of finding analytically the non-trivial eigenvalue k_1 of the Kolmogorov operator. Therefore, in order to end the analysis of the spectrum of $\mathcal{U}(t + T, t)$, we give here a numerical approach that can easily be implemented in a finite-dimensional vector space.

Consider the formal expression (6.1) to represent the Kolmogorov operator. Following the theory of time-ordered exponential, any ordered exponential operator can be expressed by an ordinary exponential operator in terms of the super-operator $\mathbf{T}$ as [17]

$$\vec{\mathcal{T}} \exp\left(\int_{t}^{t+T} \mathbf{H}(\tau)\, \mathrm{d}\tau \right) = \exp[T(\mathbf{H}(t) + \mathbf{T})],$$
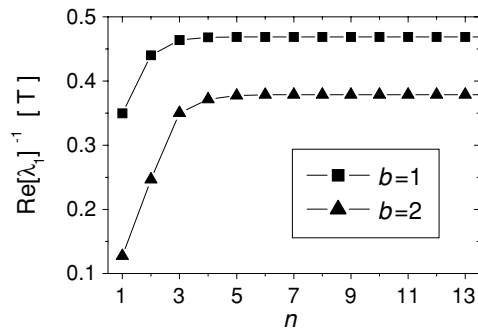
where the super-operator $\mathbf{T}$ is defined by its action over any operator (differentiable or not) $\mathbf{A}(t)$ and $\mathbf{B}(t)$:

$$\mathbf{A}(t)\, \mathrm{e}^{T\mathbf{T}} \mathbf{B}(t) = \mathbf{A}(t + T) \mathbf{B}(t).$$

Thus, using Trotter's formula it is possible to prove that

$$\mathcal{U}(t + T, t) = \lim_{n \to \infty} \mathrm{e}^{\frac{T}{n}\mathbf{H}(t+T)} \cdots \mathrm{e}^{\frac{T}{n}\mathbf{H}(t+\frac{2T}{n})}\, \mathrm{e}^{\frac{T}{n}\mathbf{H}(t+\frac{T}{n})}. \tag{6.23}$$

Figure 2. Plot of the Kolmogorov time-scale $\mathrm{Re}[\lambda_1]^{-1} = T/\ln|k_1|^{-1}$ using (6.23) for $\mathcal{A} = 1$, $T = 1$ and $b = 1, 2$, as a function of the iteration number n. Suzuki–Trotter's discretization time is T/n.

From this expression for $\mathcal{U}(t + T, t)$, the characteristic polynomial can be calculated as a perturbation in the small parameter T/n.

In order to study how fast is the convergence of this approach, let us tackle an interesting 3×3 model. This situation may physically correspond to the case when a periodically modulated external pumping is acting on some discrete *level 3* to produce a current to the *level 1*, while the rest of transition rates W_{ij} are time independent. We can, for example, consider

$$\mathbf{H}(t) = \begin{pmatrix} -1 & 1 & \alpha(t) \\ 0.5 & -2 & 0 \\ 0.5 & 1 & -\alpha(t) \end{pmatrix}. \tag{6.24}$$

Clearly this is an out of equilibrium model with a diode between states *2* and *3*, see figure 1(*b*). Now we assume an Arrhenius-like form for the time-periodic transition rate $\alpha(t) = \mathcal{A}\,\mathrm{e}^{b\cos\omega t}$. It is simple to see that if at time t', $\alpha(t') = 3$ or 1, the matrix $\mathbf{H}(t')$ cannot be diagonalized. Thus, in order to calculate the eigenvalue k_1, we apply the Suzuki–Trotter approach to estimate the characteristic polynomial of $\mathcal{U}(t + T, t)$

$$\mathcal{P}(k) = \det|\mathbf{P}(t + T \mid t) - k\mathbf{1}|.$$

By studying the eigenvalues $k_{1,2}$ we found that the convergence of (6.23) is well defined, and good results are obtained just for $n \sim 10$. In addition, the trivial root $k_0 = 1$ is always present for any n as was expected by normalization of the propagator. In figure 2, we show the calculation of the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ for $\mathcal{A} = 1$ and $b = 1, 2$ as a function of n (in the present case, $k_{1,2}$ are two conjugated eigenvalues and the saturation values of $\mathrm{Re}[\lambda_1]^{-1} = T/\ln|k_1|^{-1}$ are 0.4688 and 0.3788 for $b = 1, 2$, respectively). We have checked that (6.23) provides a straightforward method to calculate the first non-trivial time-scale $\mathrm{Re}[\lambda_1]^{-1}$ of periodically modulated discrete Markov processes. As expected, comparing the present 3×3 case with the similar 2-level system of section 6.1.1, by increasing the amplitude of the periodic modulation b, the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ decreases predicting a faster relaxation of the associated antisymmetric eigenvector $\vec{g}_1(t)$.

Finally, as a practical application of the corollary of section 5.2, we calculated the Lyapunov function associated with the stochastic process characterized by the 3×3 master Hamiltonian (6.24), for two cases $b = 1$ and $b = 2$. The two cases are plotted in figure 3 in semi-log scale. The lines are functions of the form $f(t) = C\exp(-2\,\mathrm{Re}[\lambda_1(b)]t)$, where the
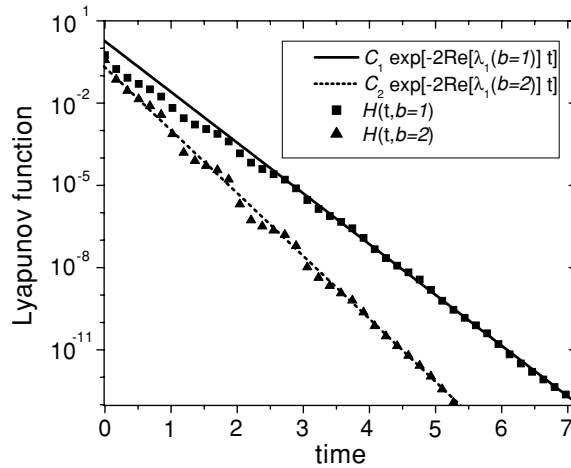
Figure 3. Plot of the calculation of the Lyapunov function $\mathcal{H}(t)$ for the 3-level problem of figure 1(b) for $\mathcal{A} = 1$ and $b = 1, 2$ versus the theoretical prediction of the corollary of section 5.2. The time is shown in units of T.

two numerical values of $\mathrm{Re}[\lambda_1(b)]$ shown in figure 2 have been used. A fitting constant C has been adjusted to match the calculations of the Lyapunov function

$$\mathcal{H}(t) = \sum_{q_\alpha} \mathbf{P}(q_\alpha, t \mid q_\beta, 0) \ln \frac{\mathbf{P}(q_\alpha, t \mid q_\beta, 0)}{P_{\mathrm{as}}(q_\alpha, t)},$$

where we have taken $q_\beta = \delta_{\beta,1}$ as the initial condition. The matrix elements $\mathbf{P}(q_\alpha, t \mid q_\beta, 0)$ were taken from (6.1) with the use of the Suzuki–Trotter approach to represent $\mathcal{U}(t, 0)$. Using previous experience [5] the probability $P_{\mathrm{as}}(q_\alpha, t)$ was calculated from

$$P_{\mathrm{as}}(q_\alpha, \tau) = \lim_{m \to \infty} \sum_{q_1} \cdots \sum_{q_m} \mathbf{P}(q_\alpha, \tau \mid q_m, 0) \prod_{j=1}^{m} \mathbf{P}(q_j, T \mid q_{j-1}, 0).$$

This equation gives the asymptotic time-periodic probability as the product of m one period propagator multiplied by the propagator from 0 to $\tau (\tau \leqslant T)$, which corresponds to a simple multiplication of matrices. We have used m between 10 and 20 to reach the asymptotic regime. The prediction of the corollary of section 5.2 was excellent to reproduce the relaxation of $\mathcal{H}(t)$ in its long-time regime.

6.4. Final discussions

In the present paper, we have introduced the Kolmogorov eigenvalue approach to study the stochastic dynamics of the continuous or discrete periodic non-stationary Markov process, by exploring its Floquet structure. This theory is encoded in the lemma of section 3, reducing the analysis to an eigenvalue problem of a Fredholm equation with a non-symmetrical kernel. In general, we have proved that the asymptotic relaxation of a periodically modulated Markov process is governed by the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ which is characterized by the real part of the first non-trivial eigenvalue k_1 of the Kolmogorov operator.

In section 6.1, we have discussed pedagogical examples showing the interplay of the combined effect of fluctuations and external time-periodic modulations. Taking for example an Arrhenius-like model for the time-modulation of the transition rates, we have shown that

if the amplitude of periodic modulation is small, there is a range of values of the physical parameters where the time-scale $\mathrm{Re}[\lambda_1]^{-1}$ is of the order of the Kramers time. But in general the mechanism leading to diffusion is non-trivial and the calculation of λ_1 is of great value to understand the relaxation and mixing of periodically modulated Markov processes. We have shown that Kolmogorov's spectrum analysis is also of interest in the study of the stochastic resonance [18], and in non-equilibrium (order–disorder) phase transitions by considering the relaxation of the asymptotic two-time correlation function [11].

For a finite-dimensional vector space, if the Kolmogorov operator cannot be diagonalized we could only expect a Jordan form for $\mathcal{U}(t + T, t)$. Nevertheless finding the first non-trivial eigenvalue k_1 gives a very important piece of information concerning the asymptotic relaxation of any discrete periodic non-stationary Markov process. As a matter of fact we have also presented the Suzuki–Trotter approach to calculate the characteristic polynomial in order to get the spectrum of the Kolmogorov operator. To end the section concerning finite-dimensional vector spaces, we worked out an example showing that a Suzuki–Trotter numerical approach is a very suitable algorithm to tackle the calculation of the Kolmogorov time-scale for discrete periodic non-stationary Markov processes.

Acknowledgments

References

[1] Stratonovich R L 1963 *Topics in the Theory of Random Noise* (London: Gordon and Breach)
[2] Horsthemke W and Lefever R 1984 *Noise-Induced Transitions* (Berlin: Springer) , and reference therein
[3] van Kampen N G 1992 *Stochastic Processes in Physics and Chemistry* 2nd edn (Amsterdam: North-Holland)
[4] Cáceres M O 2003 (in spanish) *Estadística de no equilibrio y medios desordenados* (Reverté S.A., Barcelona)
[5] Caceres M O, Becker A and Kramer L 1991 *Phys. Rev.* A **43** 6581
[6] Risken H 1984 *The Fokker–Planck Equation* (Berlin: Springer) , and reference therein
[7] Elliott J 1955 *Trans. Am. Math. Soc.* **78** 406
[8] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill)
    Montroll E W 1985 *The Wonderful World of Stochastic, a Tribute to E.W. Montroll* ed M F Shlesinger and G H Wiess (Amsterdam: North-Holland) p 217
[9] See for example, Moulton F R 1958 *Differential Equations* (New York: Macmillan) chapter XVII
    Also the quasienergy approach presented by Shirley J H 1965 *Phys. Rev.* B **138** 979
[10] Gammaitoni L, Hänggi P, Jung P and Marchesoni F 1998 *Rev. Mod. Phys.* **70** 223 , and references therein
[11] Becker A, Caceres M O and Kramer L 1992 *Phys. Rev.* A **46** R4463
[12] Kramers H A 1940 *Phys. (Utrecht)* **7** 284
[13] Schuss Z and Matkowsky B J 1979 *SIAM J. Appl. Math.* **35** 604
    Matkowsky B J, Schuss Z and Matkowsky B J 1977 *SIAM J. Appl. Math.* **33** 365
[14] Langer J S 1969 *Ann. Phys., NY* **54** 258
    Landauer R and Swanson J A 1961 *Phys. Rev.* **121** 1668
    Graham R and Schenzle A 1981 *Phys. Rev.* A **23** 1302
[15] Caceres M O and Budini A A 1997 *J. Phys. A: Math. Gen.* **30** 8427
[16] Spanier J and Oldham K B 1987 *An Atlas of Functions* (Berlin: Springer)
[17] Suzuki M 1993 *Proc. Japan Acad.* B **69** 161
[18] Chattah A K, Briozzo C B, Osenda O and Caceres M O 1996 *Mod. Phys. Lett.* B **10** 1085