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RATE DESCRIPTION OF MARKOV PROCESSES WITH TIME DEPENDENT PARAMETERS*

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Dedicated to Professor Andrzej Fuliński on the occasion of his 70th birthday

A projection of a Markov process onto the dynamics of its metastable states is performed by means of conveniently defined site localizing functions. The method is illustrated by a simple model with time dependent transition rates. In this particular case an alternative method is available. The results of both methods are compared and found to agree with each other.

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1. Introduction

The description of physical, chemical or biological processes by simple models often becomes possible by a separation of time scales of the underlying microscopic dynamics [1,2]. For example, thermally activated transitions between locally stable states typically occur on a much slower time scale than the fast motion in the vicinity of these locally stable states [3]. On the long time scales on which the transitions occur, the fast dynamics leads to a complete loss of memory. Therefore, the escape from a locally stable state is characterized by a single total rate which in general is the sum of individual rates describing transitions into those states that can be reached

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from the considered state. A quantitative description of the transition dynamics is then provided by a Markovian master equation [4]. Such a kinetic description has often been assumed to hold also when some of the parameters characterizing the microscopic dynamics of the system vary in time [5], in particular also in the context of stochastic resonance [6] and Brownian motors [7]. As a consequence one then has to allow for time dependent rates. For a sufficiently slow change of the parameters usually the instantaneous rates are assumed at least to provide a qualitative description [8]. Recently master equations with instantaneous rates were derived for Fokker–Planck processes with metastable states and slowly varying parameters [9].

Here we want to illustrate the reduction to a master equation by a particularly simple example. The starting point is a Markovian three state process with the states $\{1,2,3\}$. There are transitions between the neighboring states 1 and 2, as well as between 2 and 3 but no direct transitions between 1 and 3. Moreover, we assume the process to reside predominantly in either of the states $\{1,3\}$ and only rarely in 0. In other words, the rates out of the state 2 are much larger than those out of the other two "metastable" states $\{1,3\}$.

In Sect. 2 we shortly review the main assumptions underlying the reduction of a continuous process described by a Fokker–Planck equation to a discrete process governed by a master equation. The states of this discrete process correspond to the metastable states of the original continuous process. In Sect. 3 we apply this approach to a simple model with two slow states and one fast state and compare it with the result of the adiabatic elimination of the fast state. The paper ends with a summary in Sect. 4.

2. Multistable systems at small noise

We consider a Markov process $\boldsymbol{X}(t) = (X_1(t), \dots X_n(t))$ whose probability density $\rho(\boldsymbol{x}, t)$ to find the process at time t at the state space point $\boldsymbol{x}$ is governed by the Fokker–Planck equation

$$\dot{\rho}(\boldsymbol{x}, t) = L(t)\rho(\boldsymbol{x}, t)\,, \tag{1}$$

where $L(t)$ denotes the Fokker–Planck operator

$$L(t) = -\frac{\partial}{\partial x_i} K_i(\boldsymbol{x}, t) + \frac{\partial^2}{\partial x_i \partial x_j} D_{i,j}(\boldsymbol{x}, t)\,. \tag{2}$$

If not explicitly excluded, summation over double indices is always understood. For the process $\boldsymbol{X}(t)$ the following properties are assumed to hold:

(i) The time dependence of the drift vector $K_i(\boldsymbol{x}, t)$ and the diffusion matrix $D_{i,j}(\boldsymbol{x}, t)$ is slow in a way that will be specified below.

(ii) The deterministic motion that results when the diffusion matrix vanishes has m time dependent attracting asymptotic states. The time dependence of the drift is so slow that the asymptotic states can be approximated by the adiabatic stable fixed points

$$K_i(x_\alpha(t), t) = 0\,, \tag{3}$$

where $\alpha = 1 \ldots m$ labels the asymptotic states which are distinct from each other for all times t. These states are locally stable for all times. They do neither merge nor bifurcate at any instant of time. Their domains of attraction are denoted by $\mathcal{D}_\alpha(t)$. They partition the whole state space $\cup_{\alpha=1}^{m} \mathcal{D}_\alpha(t) = \mathbb{R}^n$.

(iii) The presence of noise leading to a finite diffusion matrix destabilizes the deterministically stable states and renders them metastable. The noise is weak enough so that most of the time the process is found close to one of these states; it only very rarely leads to transitions between them.

(iv) For fixed system parameters, *i.e.* for constant values of the drift and the diffusion, the system approaches a state of thermal equilibrium characterized by an equilibrium probability density $\rho_0(\boldsymbol{x}, t)$ to which we will refer as *frozen equilibrium probability density.* With respect to the frozen equilibrium probability density the process obeys the symmetry of detailed balance

$$L(t)\hat{\rho}_0(t) = \hat{\rho}_0(t)\tilde{L}^+(t)\,, \tag{4}$$

where $L^+(t)$ denotes the backward Fokker–Planck operator

$$L^+(t) = K_i(\boldsymbol{x}, t)\frac{\partial}{\partial x_i} + D_{i,j}(\boldsymbol{x}, t)\frac{\partial^2}{\partial x_i \partial x_j}\,. \tag{5}$$

The tilde denotes the operation of time reversal, *i.e.* $\tilde{x}_i = \epsilon_i x_i$ (no summation over i) with parities $\epsilon_i = \pm 1$ depending on whether x_i is even or odd under time reversal. The hat indicates a multiplication operator, *i.e.* $\hat{\rho}_0(t)\, f(\boldsymbol{x}) = \rho_0(\boldsymbol{x}, t)\, f(\boldsymbol{x})$.

Under these restrictions the transitions between the metastable states are governed by a master equation for the probabilities $p_\alpha(t)$ for finding the process in either of the states α [9]. It reads

$$\dot{p}_\alpha(t) = \sum_{\alpha' \neq \alpha} \left[r_{\alpha,\alpha'}(t) p_{\alpha'}(t) - r_{\alpha',\alpha}(t) p_\alpha(t) \right]. \tag{6}$$

The rate $r_{\alpha,\alpha'}(t)$ denotes the probability of a transition from state α' to state α at time t per unit time. It is given in terms of the frozen equilibrium density and site localizing functions $\chi_\alpha(\boldsymbol{x},t)$ which are one on $\mathcal{D}_a(t)$ and zero elsewhere with the exception of a small regions near the boundary of $\mathcal{D}_\alpha(t)$ where $\chi_\alpha(\boldsymbol{x},t)$ smoothly interpolates between zero and one. It is the solution of the homogeneous backward equation

$$\begin{aligned} L^+(t)\chi_\alpha(\boldsymbol{x},t) &= 0\,, \\ \chi_\alpha(\boldsymbol{x},t) &= 1 \quad \text{for } \boldsymbol{x}\in\partial d_a(t)\,, \\ \chi_\alpha(\boldsymbol{x},t) &= 0 \quad \text{for } \boldsymbol{x}\in\partial d_{a'}(t) \text{ for all } \alpha'\neq\alpha\,. \end{aligned} \tag{7}$$

Here $d_\alpha(t)$ and $d_{\alpha'}(t)$ denote small regions about the respective states α or α', and $\partial d_\alpha(t)$ and $\partial d_{\alpha'}(t)$ the respective boundaries. These regions are just those parts of the state space where the probability density is high and therefore they represent the metastable states. The precise choice of these regions does not matter under the weak noise condition *(iii)*. Note that $\chi_\alpha(\boldsymbol{x},t)$ is a splitting probability of the frozen system; it gives the probability that a trajectory starting at $\boldsymbol{x}$ first reaches the metastable state α before it eventually visits the other states α', provided that the drift and diffusion are kept constant at their values which they have at a fixed time t. Within the excluded regions $d_\alpha(t)$ and $d_{\alpha'}(t)$ the function $\chi_\alpha(\boldsymbol{x},t)$ can be represented by the respective constant value that it assumes at the boundaries of these regions. We here only mention that asymptotic methods which were developed for mean first passage times can also be employed to determine the splitting probabilities [4, 10, 11]. The probability of finding the process in one of the metastable states, say α, $p_\alpha(t)$, follows from the solution $\rho(\boldsymbol{x},t)$ of the Fokker–Planck equation by means of the site localizing function $\chi_\alpha(\boldsymbol{x},t)$ [9]

$$p_\alpha(t) = \int d^n\boldsymbol{x}\;\chi_\alpha(\boldsymbol{x},t)\;\rho(\boldsymbol{x},t)\,. \tag{8}$$

Its time rate of change is determined by the master equation (6) with rates $r_{\alpha,\alpha'}(t)$ reading [9]

$$\begin{aligned} r_{\alpha,\alpha'}(t) \;=\; & \frac{\displaystyle\int d^n\boldsymbol{x}\;\chi_\alpha(\boldsymbol{x},t)\;L(t)\tilde{\chi}_{\alpha'}(\boldsymbol{x},t)\;\rho_0(\boldsymbol{x},t)}{\displaystyle\int d^n\boldsymbol{x}\;\tilde{\chi}_{\alpha'}(\boldsymbol{x},t)\;\rho_0(\boldsymbol{x},t)} \\ & + \frac{\displaystyle\int d^n\boldsymbol{x}\;\partial\chi_\alpha(\boldsymbol{x},t)/\partial t\;\tilde{\chi}_{\alpha'}(\boldsymbol{x},t)\rho_0(\boldsymbol{x},t)}{\displaystyle\int d^n\boldsymbol{x}\;\tilde{\chi}_{\alpha'}(\boldsymbol{x},t)\;\rho_0(\boldsymbol{x},t)}\,, \end{aligned} \tag{9}$$

where the tilde indicates the time reversed function, $\tilde{\chi}_{\alpha'}(\boldsymbol{x},t) = \chi_{\alpha'}(\tilde{\boldsymbol{x}},t)$. The first term on the right-hand side is the frozen rate that results when the drift and diffusion are kept fixed at their values at a particular time t. The second term is referred to as the geometric correction of the rate. Provided that the condition

$$\left| \int d^n\boldsymbol{x}\, \chi_{\alpha'}(\boldsymbol{x},t)\, \rho_0(\boldsymbol{x},t)\, \frac{\partial}{\partial t}\chi_\alpha(\boldsymbol{x},t) \right| \ll \int d^n\boldsymbol{x}\, \chi_\alpha(\boldsymbol{x},t)\, L(t)\tilde{\chi}_{\alpha'}(\boldsymbol{x},t)\, \rho_0(\boldsymbol{x},t) \tag{10}$$

is fulfilled, the geometric correction can be neglected and the time dependent rates coincide with the frozen ones. The resulting kinetic description holds whenever the time rates of change of drift and diffusion are sufficiently small.

3. A three state process

One of the simplest possible Markovian process that still allows some reduction has three states $\{1,2,3\}$ where the states 1 and 3 are considered as metastable and 2 is a rarely visited intermediate state. There is only one outgoing rate $k_1(t)$ from 1 to 2 and the corresponding one $k_3(t)$ from 3 to 2. In order that the state 2 is only rarely visited, these rates are assumed to be much smaller than the rates $q_1(t)$ and $q_3(t)$ which lead from the intermediate state 2 to 1 and 3, respectively. Then, the master equation for the considered process has the form:

$$\begin{pmatrix} \dot{p}_1(t) \\ \dot{p}_2(t) \\ \dot{p}_3(t) \end{pmatrix} = \begin{pmatrix} -k_1(t) & q_1(t) & 0 \\ k_1(t) & -(q_1(t)+q_3(t)) & k_3(t) \\ 0 & q_3(t) & -k_3(t) \end{pmatrix} \begin{pmatrix} p_1(t) \\ p_2(t) \\ p_3(t) \end{pmatrix}, \tag{11}$$

where

$$k_1(t), k_2(t) \ll q_1(t), q_2(t)\,. \tag{12}$$

Moreover, we assume that also the rates of change of all rates are slow compared to the fast rates $q_1(t)$ and $q_3(t)$:

$$\frac{\dot{k}_\alpha(t)}{k_\alpha(t)}, \frac{\dot{q}_\alpha(t)}{q_\alpha(t)} \ll q_1(t), q_3(t), \quad \alpha = 1,3\,. \tag{13}$$

The forward operator $L(t)$ is hence given by

$$L(t) = \begin{pmatrix} -k_1(t) & q_1(t) & 0 \\ k_1(t) & -(q_1(t)+q_3(t)) & k_3(t) \\ 0 & q_3(t) & -k_3(t) \end{pmatrix}, \tag{14}$$

and the corresponding backward operator becomes

$$L^{+}(t) = \begin{pmatrix} -k_1(t) & k_1(t) & 0 \\ q_1(t) & -(q_1(t)+q_3(t)) & q_3(t) \\ 0 & k_3(t) & -k_3(t) \end{pmatrix}. \tag{15}$$

In a first, direct approach we perform an adiabatic elimination of the fast, intermediate state 2 by setting $\dot{p}_2(t) = 0$ in Eq. (11). This yields for the remaining two states the reduced master equation:

$$\begin{pmatrix} \dot{p}_1(t) \\ \dot{p}_3(t) \end{pmatrix} = \begin{pmatrix} -\frac{q_3(t)}{q_1(t)+q_3(t)}k_1(t) & \frac{q_1(t)}{q_1(t)+q_3(t)}k_3(t) \\ \frac{q_3(t)}{q_1(t)+q_3(t)}k_1(t) & -\frac{q_1(t)}{q_1(t)+q_3(t)}k_3(t) \end{pmatrix} \begin{pmatrix} p_1(t) \\ p_3(t) \end{pmatrix}. \tag{16}$$

The reduction method that we reviewed in the previous section presents an alternative approach. Although this method refers to a Fokker–Planck dynamics, it is not difficult to transfer it to the present discrete process. For this purpose we first determine the frozen equilibrium solution $p^0(t)$ as the solution of the three state master equation with the left-hand side put equal to zero. It is given by:

$$p^0(t) = \frac{1}{k_1(t)k_3(t) + q_1(t)k_3(t) + q_3(t)k_1(t)} \begin{pmatrix} q_1(t)k_3(t) \\ k_1(t)k_3(t) \\ q_3(t)k_1(t) \end{pmatrix}. \tag{17}$$

Next, we determine the site localizing "functions" $\chi_1(t)$ and $\chi_3(t)$, each of which is a time dependent vector with three components. As in the case of a system with continuous state space, these functions coincide with the frozen splitting probabilities. Hence, we fix the value of the 1-component of, say $\chi_1(t)$, to 1 and its 3-component to 0, $\chi_{1,1}(t) = 1$, $\chi_{1,3}(t) = 0$. The remaining second component is determined such that the homogeneous backward equation $L^{+}(t)\chi_1(t) = 0$ is solved with absorbing states 1 and 3, *i.e.* with rates $k_1(t)$ and $k_3(t)$ put to zero. This gives:

$$\chi_1(t) = \begin{pmatrix} 1 \\ \frac{q_1(t)}{q_1(t)+q_3(t)} \\ 0 \end{pmatrix}. \tag{18}$$

Correspondingly, one obtains for the other site localizing function

$$\chi_3(t) = \begin{pmatrix} 0 \\ \frac{q_3(t)}{q_1(t)+q_3(t)} \\ 1 \end{pmatrix}. \tag{19}$$

Note, that the site localizing functions correctly add up to the unit vector:

$$\chi_1(t) + \chi_3(t) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{20}$$

The frozen equilibrium populations of the two considered states are given by

$$\begin{aligned} n_1(t) = \big(\chi_1(t), p^0(t)\big) &\approx \frac{q_1(t)k_3(t)}{q_1(t)k_3(t) + q_3(t)k_1(t)}\,, \\ n_3(t) = \big(\chi_3(t), p^0(t)\big) &\approx \frac{q_3(t)k_1(t)}{q_1(t)k_3(t) + q_3(t)k_1(t)}\,, \end{aligned} \tag{21}$$

where (u, v) denotes the scalar product of the vectors u and v, and where terms of the order $k_1(t)\,k_3(t)$ were neglected on the right-hand side on the basis of the inequalities (12). Using now the definition of the instantaneous rates, see Eq. (9), we find

$$\begin{aligned} r_{1,1}(t) &= \frac{\big(\chi_1(t), L(t)\chi_1(t)p^0(t)\big)}{(\chi_1(t), p^0(t))} \approx -\frac{q_3(t)k_1(t)}{q_1(t) + q_3(t)}\,, \\ r_{1,3}(t) &= \frac{\big(\chi_1(t), L(t)\chi_3(t)p^0(t)\big)}{(\chi_3(t), p^0(t))} \approx \frac{q_1(t)k_3(t)}{q_1(t) + q_3(t)}\,, \end{aligned} \tag{22}$$

where again, terms of the order $k_1(t)k_2(t)$ were neglected. Comparing with the result of the adiabatic elimination of the fast state 2, see Eq. (16), we obtain the identical rates. The remaining rates follow from the conservation of probability, say, $r_{3,1}(t) = -r_{1,1}(t)$. Here, the components of a vector uv are given by the product of the components of the vectors u and v, *i.e.* $(uv)_i = u_i v_i$.

Finally, we investigate the "geometric" contributions to the rates and in particular the conditions under which they can be neglected. The corresponding ratios of $\big(d\chi_\alpha(t)/dt, \chi_{\alpha'}(t)p^0(t)\big)$ and $\big(\chi_\alpha(t), L(t)\chi_{\alpha'}(t)p^0(t)\big)$ are readily calculated to yield:

$$\begin{aligned} \left| \frac{\big(d\chi_1(t)/dt, \chi_1(t)p^0\big)}{(\chi_1(t), L(t)\chi_1(t)p^0(t))} \right| &= \frac{|\dot{q}_1(t)q_3(t) - q_1(t)\dot{q}_3(t)|}{q_3(t)\,(q_1(t) + q_3(t))^2}\,, \\ \left| \frac{\big(d\chi_1(t)/dt, \chi_3(t)p^0\big)}{(\chi_1(t), L(t)\chi_3(t)p^0(t))} \right| &= \frac{|\dot{q}_1(t)q_3(t) - q_1(t)\dot{q}_3(t)|}{q_1(t)\,(q_1(t) + q_3(t))^2}\,. \end{aligned} \tag{23}$$

Using the above required conditions on the time scales, see Eq. (13), we find that the right-hand sides are much smaller than one. Hence, the geometric corrections are much smaller than the frozen rates and therefore can safely be neglected.

4. Summary

In the present paper we reviewed the conditions under which a kinetic description of the transition dynamics between metastable states is valid for a time dependent system and illustrated the reduction procedure by a simple example. Here, the generalization from a Fokker–Planck to a master equation dynamics is straightforward. Moreover, a direct elimination of the single fast state of this model leads to appropriate results for the rates. In the present case there are no extra conditions to be satisfied in order that the geometric contributions to the rates can be neglected. We must though emphasize that this is not always the case. For example for a periodically driven bistable Brownian oscillator the geometric corrections become important if the noise becomes extremely weak and the driving frequency is kept fixed [9]. The crossover between the regimes of slow driving and weak noise [12] is not yet understood even in this, otherwise thoroughly investigated, archetypical model of stochastic resonance.

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REFERENCES

[1] H. Haken, *Synergetics, An Introduction*, Springer Verlag, Berlin 1983.

[2] A. Fuliński, W.J. Kramarczyk, *Physica A* **39**, 575 (1968).

[3] P. Hänggi, P. Talkner, M. Borkovec, *Rev. Mod. Phys.* **62**, 251 (1990); E. Pollak, P. Talkner, *Chaos*, in press.

[4] D. Ryter, H. Meyer, *Physica A* **142**, 122 (1987); G. Moro, *J. Chem. Phys.* **103**, 7514 (1995).

[5] B. McNamara, K. Wiesenfeld, *Phys. Rev.* **A39**, 4854 (1989); R.D. Astumian, B. Robertson, *J. Chem. Phys.* **91**, 4891 (1989); U. Zürcher, C.R. Doering, *Phys. Rev.* **E47**, 3862 (1993); I.A. Goychuk, E.G. Petrov, V. May, *J. Chem. Phys.* **103**, 4937 (1995); P. Talkner, *Ann. Phys.* (Leipzig) **9**, 741 (2000); R. Rozenfeld, J.A. Freund, A. Neimann, L. Schimansky-Geier, *Phys. Rev.* **E64**, 051107 (2001); R.D. Astumian, *Appl. Phys. A: Mater. Sci. Process.* **75**, 193 (2002); P. Talkner, *Physica A* **325**, 124 (2003); P. Talkner, Ł. Machura, M. Schindler, P. Hänggi, J. Łuczka, *New J. Phys.* **7**, 14 (2005); online: `http:www.njp.org`

[6] L. Gammaitoni, P. Hänggi, P. Jung, F. Marchesoni, *Rev. Mod. Phys.* **70**, 223 (1998).

[7] P. Reimann, *Phys. Rep.* **361**, 57 (2002); R.D. Astumian, P. Hänggi, *Phys. Today* **55**(11), 33 (2002).

[8] M. Bier, R.D. Astumian, *Phys. Lett.* **A247**, 385 (1990); I. Derenyi, R.D. Astumian, *Phys. Rev. Lett.* **82**, 2623 (1999); M. Bier, I. Derenyi, M. Kostur, R.D. Astumian, *Phys. Rev.* **E59**, 6422 (1999).

[9] P. Talkner, J. Łuczka, *Phys. Rev.* **E69**, 046109 (2004).

[10] B.J. Matkowsky, Z. Schuss, *SIAM J. Appl. Math.* **42**, 822 (1982).

[11] P. Talkner, *Z. Phys.* **B68**, 201 (1987); P. Talkner, *Chem. Phys.* **180**, 199 (1994).

[12] J. Lehmann, P. Reimann, P. Hänggi, *Phys. Rev. Lett.* **84**, 1639 (2000); *Phys. Rev.* **E62**, 6282 (2000).