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A new H-theorem for age-dependent dynamics

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Abstract. Physical systems with a finite number of connected states are considered. We assume the transition rates between the different states are age dependent. The time evolution of the system is described in terms of an age-state probability density. We prove the validity of a general H-theorem, which shows that the age-state probability density evolves towards a time-persistent form. We try to extend the result to hybrid systems, comprising 'jump' and 'non-jump' stochastic processes.

1. Formulation of the problem

The H-theorems have a long history and play an important role in non-equilibrium statistical mechanics (see, for instance, Van Kampen 1981, Schnakenberg 1976, Kubo 1981).

Here we shall try to derive such a theorem for a class of physical systems with age structure (Vlad *et al* 1984, Vlad and Popa 1986, 1987, Vlad 1987). Our approach has been suggested by several papers dealing with the entropy production due to statistical equilibration in heavy-ion collisions (Csernai and Kapusta 1986, Das *et al* 1986, Hahn and Stöcker 1986, Jingshang and Wolschin 1983, Knoll 1987, Remler 1986).

We consider a system which may exist in a finite number of states $i=1,\ldots,S$ and assume that the transition rates from the state i to other states $j_1, j_2, \ldots$ depend on the age a of the initial state

$$W_{ij}\Delta t = W_{ij}(a)\Delta t \qquad j=j_1,j_2,\ldots. \tag{1}$$

Here, by age a we mean the time interval in which the state of the system was i. As the age is merely the time elapsed from a given reference point, it seems that the age and time are not independent. However, the age depends on a previous random event, a transition to state i from other states; thus the age a is in fact a random variable.

We denote by

$$\mathscr{P}_i = \mathscr{P}_i(a,t) \qquad \sum_{i=1}^{S}\int_0^\infty \mathscr{P}_i(a,t)\,\mathrm{d}a = 1 \tag{2}$$

the age-state probability density at time t. The time evolution of the system is described by means of the balance equations

$$\mathscr{P}_i(a+\Delta t, t+\Delta t)\Delta t = \mathscr{P}_i(a,t)\Delta t\left(1-\sum_j W_{ij}(a)\Delta t\right)$$

$$\mathscr{P}_i(0+\Delta t, t+\Delta t)\Delta t = \sum_j \int_0^\infty W_{ji}(a')\Delta t\mathscr{P}_j(a',t)\,\mathrm{d}a'$$

wherefrom, for $\Delta t \to 0$, we get the so-called age-dependent master equations (ADME) (Vlad *et al* 1984):

$$(\partial_t + \partial_a)\mathcal{P}_i(a, t) = -\mathcal{P}_i(a, t) \sum_j W_{ij}(a) \tag{3}$$

$$\mathcal{P}_i(0, t) = \sum_j \int_0^\infty W_{ji}(a')\mathcal{P}_j(a', t)\, \mathrm{d}a'. \tag{4}$$

Together with the boundary condition

$$\lim_{a \to \infty} \mathcal{P}_i(a, t) = 0 \tag{5}$$

and the initial condition

$$\mathcal{P}_i(a, 0) = \mathcal{P}_i^0(a) \tag{5'}$$

the ADME system describes the time evolution of the age-state probability density $\mathcal{P}_i(a, t)$.

For simplicity, we shall assume that all the S states are connected, i.e. for each pair of states i and j there is at least one sequence of transitions connecting the two states in both directions (Schnakenberg 1976). Our aim is to investigate the asymptotic behaviour of the age-state probability density.

2. Steady states

First we look for a stationary solution of the ADME system:

$$\mathcal{P}_i = \mathcal{P}_i^{\mathrm{st}}(a) = \text{independent of } t. \tag{6}$$

Following Vlad and Popa (1986) we shall express $\mathcal{P}_i^{\mathrm{st}}(a)$ as:

$$\mathcal{P}_i^{\mathrm{st}}(a) = P_i^{\mathrm{st}} R^{\mathrm{st}}(a|i) \tag{7}$$

where

$$P_i^{\mathrm{st}} = \int_0^\infty \mathcal{P}_i^{\mathrm{st}}(a)\, \mathrm{d}a \qquad \sum_i P_i^{\mathrm{st}} = 1 \tag{8}$$

is the stationary-state probability and $R^{\mathrm{st}}(a|i)\, \mathrm{d}a$ is the probability that the age of a given state i is between a and $a + \mathrm{d}a$.

By integrating the ADME system we get (see also Vlad and Popa 1986):

$$R^{\mathrm{st}}(a|i) = \gamma_i(a) \left(\int_0^\infty \gamma_i(a)\, \mathrm{d}a \right)^{-1} \tag{9}$$

where

$$\gamma_i(a) = \exp\left(-\sum_j \int_0^a W_{ij}(a'')\, \mathrm{d}a'' \right) \tag{10}$$

is the probability that in the age interval $(0, a)$ the system remains in the state i. On the other hand, P_i^{st} obeys a phenomenological master equation

$$\sum_j (\tilde{W}_{ij} P_i^{\mathrm{st}} - \tilde{W}_{ji} P_j^{\mathrm{st}}) = 0 \tag{11}$$

where

$$\tilde{W}_{ij} = \int_0^{\infty} W_{ij}(a) R^{st}(a|i)\, da \tag{12}$$

are age-averaged transition rates. We note that as $W_{ij} \geq 0$ we have $\tilde{W}_{ij} \geq 0$. Similarly $W_{ij} > 0$ implies that $\tilde{W}_{ij} > 0$. As all S states are connected, it follows that (11), together with the normalisation condition $\Sigma_i P_i^{st} = 1$, determine a unique set of steady-state probabilities $P_1^{st}, \ldots, P_S^{st}$ (see also Schnakenberg 1976), and thus a unique age-state probability density $\mathcal{P}_i^{st}(a)$, $i = 1, \ldots, S$.

3. The *H*-theorem

In order to show that $\mathcal{P}_i^{st}(a)$ describes the large-time behaviour of $\mathcal{P}_i(a, t)$, we shall try to build a function $H(t)$ obeying the following conditions:

(a) for $\mathcal{P}_i(a, t) \neq \mathcal{P}_i^{st}(a)$ $\quad H(t) > 0$ (13)

(b) for $\mathcal{P}_i(a, t) = \mathcal{P}_i^{st}(a)$ $\quad H(t) = 0$ (14)

(c) for $\mathcal{P}_i(a, t) \neq \mathcal{P}_i^{st}(a)$ $\quad dH(t)/dt < 0$ (15)

(d) for $\mathcal{P}_i(a, t) = \mathcal{P}_i^{st}(a)$ $\quad dH(t)/dt = 0.$ (16)

We shall assume that $H(t)$ has the following form:

$$H(t) = \sum_i \int_0^{\infty} \mathcal{P}_i(a, t) \ln[\mathcal{P}_i(a, t)/\mathcal{P}_i^{st}(a)]\, da. \tag{17}$$

Next we shall show that, if

$$\lim_{a \to \infty} (\mathcal{P}_i(a, t)/\mathcal{P}_i^{st}(a)) = \text{finite} \tag{18}$$

then $H(t)$ fulfils the conditions (13)-(16).

First we shall prove that the ADME system conserves the normalisation condition

$$\sum_i \int_0^{\infty} \mathcal{P}_i(a, t)\, da = 1 \tag{19}$$

provided that

$$\sum_i \int_0^{\infty} \mathcal{P}_i(a, 0)\, da = 1. \tag{20}$$

Indeed, summing in (3) over i, integrating over a and using (4) and (5), we get

$$\partial_t \sum_i \int_0^{\infty} \mathcal{P}_i(a, t) da = 0 \tag{21}$$

wherefrom, taking into account (20), we come to (19).

Similarly, we can show that the time-dependent solution of the ADME system is non-negative

$$\mathcal{P}_i(a, t) \geq 0 \qquad i = 1, \ldots, S \tag{22}$$

provided that

$$\mathscr{P}_i(a, 0) \geqslant 0 \qquad i = 1, \ldots, S. \tag{23}$$

Indeed, integrating (3) we obtain

$$\mathscr{P}_i(a, t) = h(t-a)\mathscr{P}_i(0, t-a)\gamma_i(a) + h(a-t)\mathscr{P}_i(a-t, 0)\gamma_i(a)/\gamma_i(a-t) \tag{24}$$

where $h(t)$ is the usual Heaviside function. Inserting (24) into (4) we get a system of linear integral equations for $\mathscr{P}_i(0, t)$:

$$\mathscr{P}_i(0, t) = \sum_j \int_0^t W_{ji}(a)\gamma_j(a)\mathscr{P}_j(0, t-a)\, da$$
$$+ \sum_j \int_t^\infty W_{ji}(a)[\gamma_j(a)/\gamma_j(a-t)]\mathscr{P}_j(a-t, 0)\, da. \tag{25}$$

From (25) we can give a formal series expansion for $\mathscr{P}_i(0, t)$:

$$\mathscr{P}_i(0, t) = \sum_{q=0}^{\infty} \mathscr{P}_i^{(q)}(0, t) \tag{26}$$

where $\mathscr{P}_i^{(q)}(0, t)$ may be computed recursively from

$$\begin{aligned}\mathscr{P}_i^{(0)}(0, t) &= \sum_j \int_t^\infty W_{ji}(a)[\gamma_j(a)/\gamma_j(a-t)]\mathscr{P}_j(a-t, 0)\, da \\ \mathscr{P}_i^{(q+1)}(0, t) &= \sum_{j_q} \int_0^t W_{j_q i}(a)\gamma_{j_q}(a)\mathscr{P}_{j_q}^{(q)}(0, t-a)\, da.\end{aligned} \tag{26'}$$

We observe that all the functions independent of $\mathscr{P}_i(0, t)$ occuring in (25), (26) and (26′) are non-negative ($W_{ji}(a)$, $\gamma_j(a)$, $\gamma_j(a-t, 0)$, $\mathscr{P}_j(a-t, 0) \geqslant 0$). Thus the solving of (25) involves the summation of infinite numbers of non-negative terms, i.e. $\mathscr{P}_i(0, t)$ and thus $\mathscr{P}_i(a, t)$ are non-negative.

Equations (13) and (14) may be proved starting from the well known relations

$$\begin{aligned} &x \ln x + 1 - x > 0 \qquad \text{for } x > 0 \quad x \neq 1 \\ &x \ln x + 1 - x = 0 \qquad \text{for } x = 1. \end{aligned} \tag{27}$$

Indeed, using (19), equation (17) may be rewritten as

$$H(t) = \sum_i \int_0^\infty [\mathscr{P}_i(a, t) \ln(\mathscr{P}_i(a, t)/\mathscr{P}_i^{\mathrm{st}}(a)) + \mathscr{P}_i^{\mathrm{st}}(a) - \mathscr{P}_i(a, t)]\, da \tag{28}$$

wherefrom, taking account of (27), we get (13) and (14).

Similarly, the proof of (15) and (16) is based on the relations

$$\begin{aligned} &\ln x - x + 1 < 0 \qquad \text{for } x > 0 \quad x \neq 1 \\ &\ln x - x + 1 = 0 \qquad \text{for } x = 1. \end{aligned} \tag{29}$$

By applying (17) and (19) we have

$$\dot{H}(t) = \sum_i \int_0^\infty [\partial_t \mathscr{P}_i(a, t)] \ln[\mathscr{P}_i(a, t)/\mathscr{P}_i^{\mathrm{st}}(a)]\, da. \tag{30}$$

Inserting (3) into (30) and integrating by parts, we come to

$$\dot{H}(t)=\sum_i \int_0^\infty [\partial_a \mathscr{P}_i(a,t)] \ln[\mathscr{P}_i(a,t)/\mathscr{P}_i^{st}(a)]\, da$$

$$-\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t) \ln[\mathscr{P}_i(a,t)/\mathscr{P}_i^{st}(a)]\, da$$

$$=-\sum_i \mathscr{P}_i(a,t) \ln[\mathscr{P}_i(a,t)/\mathscr{P}_i^{st}(a)]\Big|_0^\infty$$

$$+\sum_i \int_0^\infty \mathscr{P}_i(a,t)[(\partial_a \mathscr{P}_i(a,t)/\mathscr{P}_i(a,t))-\partial_a \mathscr{P}_i^{st}(a)/\mathscr{P}_i^{st}(a))]\, da$$

$$-\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t) \ln[\mathscr{P}_i(a,t)/\mathscr{P}_i^{st}(a)]\, da \qquad (31)$$

wherefrom, by using (3), (4), (18) and (19), we get

$$\dot{H}(t)=\sum_i \mathscr{P}_i(0,t) \ln[\mathscr{P}_i(0,t)/\mathscr{P}_i^{st}(0)]$$

$$+\sum_i \int_0^\infty \mathscr{P}_i(a,t)\left[-(\partial_t \mathscr{P}_i(a,t)/\mathscr{P}_i(a,t))-\sum_j W_{ij}(a)+\sum_j W_{ij}(a)\right] da$$

$$-\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t) \ln[\mathscr{P}_i(a,t)/\mathscr{P}_i^{st}(a)]\, da$$

$$=\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t) \ln[\mathscr{P}_j(0,t)\mathscr{P}_i^{st}(a)/\mathscr{P}_i(a,t)\mathscr{P}_j^{st}(0)]\, da. \qquad (32)$$

Applying the inequality (29) to (32), we obtain

$$\dot{H}(t)=\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t) \ln[\mathscr{P}_j(0,t)\mathscr{P}_i^{st}(a)/\mathscr{P}_i(a,t)\mathscr{P}_j^{st}(0)]\, da$$

$$<\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t)[\mathscr{P}_j(0,t)\mathscr{P}_i^{st}(a)/\mathscr{P}_i(a,t)\mathscr{P}_j^{st}(0)-1]\, da$$

$$\text{for } \mathscr{P}_i(a,t)\neq \mathscr{P}_i^{st}(a) \qquad (33)$$

$$\dot{H}(t)=\sum_i \sum_j \int_0^\infty W_{ij}(a)\mathscr{P}_i^{st}(a) \ln 1=0 \qquad \text{for } \mathscr{P}_i(a,t)=\mathscr{P}_i^{st}(a). \qquad (33')$$

Using (4), the relationships (33) and (33′) lead to (15) and (16). We have

$$\dot{H}(t)<\sum_j (\mathscr{P}_j(0,t)/\mathscr{P}_j^{st}(0)) \sum_i \int_0^\infty W_{ij}(a)\mathscr{P}_i^{st}(a)\, da-\sum_j \sum_i \int_0^\infty W_{ij}(a)\mathscr{P}_i(a,t)\, da$$

$$=\sum_j \mathscr{P}_j(0,t)-\sum_j \mathscr{P}_j(0,t)=0 \qquad \text{for } \mathscr{P}_i(a,t)\neq \mathscr{P}_i^{st}(a)$$

i.e.

$$\begin{aligned} &\dot{H}(t)<0 \qquad \text{for } \mathscr{P}_i(a,t)\neq \mathscr{P}_i^{st}(a) \\ &\dot{H}(t)=0 \qquad \text{for } \mathscr{P}_i(a,t)=\mathscr{P}_i^{st}(a). \end{aligned} \qquad (34)$$

4. Hybrid stochastic processes

In the following we shall try to generalise the above results to the more general case of hybrid processes involving both 'jump' and 'non-jump' phenomena. Such processes would be of interest in connection with dissipative nuclear fluid dynamics (Morgenstern and Nörenberg 1988), electrodiffusion (Bak 1959, Iordache 1987), the stochastic theory of line shape (Kubo 1963, 1969), etc.

More specifically, we shall assume that the state of the system is described by the discrete states index i, by the age a of state i as well as by other continuous state variables

$$\boldsymbol{X} = (X^1, X^2, \ldots). \tag{35}$$

We shall suppose that between two jumps the evolution of the system is Markovian and may be described in terms of a Fokker-Planck equation

$$\partial_t G_i(\boldsymbol{X}|\boldsymbol{X}'; t) = \mathbb{L}_i G(\boldsymbol{X}|\boldsymbol{X}'; t) \tag{36}$$

with the initial condition

$$G_i(\boldsymbol{X}|\boldsymbol{X}'; 0) = \delta(\boldsymbol{X} - \boldsymbol{X}') \tag{36$'$}$$

where $G_i(\boldsymbol{X}|\boldsymbol{X}'; t)\,\mathrm{d}\boldsymbol{X}$ is the probability that for a discrete state index, i, at time t, the continuous variables have values between X^α and $X^\alpha + \mathrm{d}X^\alpha$, provided that for $t=0$ the continuous state variables had the values X'^α, $\alpha = 1, 2, \ldots$; $\mathbb{L}_i$ are the Fokker-Planck operators corresponding to different labels $i = 1, 2, \ldots$

$$\mathbb{L}_i(\ldots) = -\partial_{X^\alpha}(K_i^\alpha(\boldsymbol{X})\ldots) + \partial^2_{X^\alpha X^\beta}(D_i^{\alpha\beta}(\boldsymbol{X})\ldots) \tag{37}$$

and $K_i^\alpha(\boldsymbol{X})$ and $D_i^{\alpha\beta}(\boldsymbol{X})$ are drift and diffusion coefficients. Here and in the following we shall use the summation convention over pairs of two equal Greek indices.

The conservation of normalisation

$$\int_{\boldsymbol{X}} G_i(\boldsymbol{X}|\boldsymbol{X}'; t)\,\mathrm{d}\boldsymbol{X} = 1 \tag{38}$$

requires that

$$\int_{\boldsymbol{X}} \mathrm{d}\boldsymbol{X}\,\mathbb{L}_i G_i = 0. \tag{39}$$

We shall introduce the probability

$$\mathscr{B}_i(a, \boldsymbol{X}, t)\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X} \qquad \sum_i \int_0^\infty \int_{\boldsymbol{X}} \mathscr{B}_i(a, \boldsymbol{X}, t)\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X} = 1 \tag{40}$$

that at time t the discrete state index is i, the age of state i is between a and $a + \mathrm{d}a$ and the continuous variables have values between X^α and $X^\alpha + \mathrm{d}X^\alpha$. The evolution equations (3) and (4) become

$$(\partial_t + \partial_a - \mathbb{L}_i)\mathscr{B}_i(a, \boldsymbol{X}, t) = -\mathscr{B}_i(a, \boldsymbol{X}, t)\sum_j W_{ij}(a, \boldsymbol{X}) \tag{41}$$

$$\mathscr{B}_i(0, \boldsymbol{X}, t) = \sum_j \int_0^\infty W_{ji}(a, \boldsymbol{X})\mathscr{B}_j(a, \boldsymbol{X}, t)\,\mathrm{d}a \tag{42}$$

with the boundary conditions

$$\lim_{a\to\infty} \mathscr{B}_i(a, \boldsymbol{X}, t) = 0 \tag{43}$$

$$\mathscr{B}_i(a, \boldsymbol{X} = \boldsymbol{X}_{\mathrm{boundary}}, t) = 0 \tag{44}$$

and the initial condition

$$\mathscr{B}_i(a, \boldsymbol{X}, t=0) = \mathscr{B}_i^0(a, \boldsymbol{X}). \tag{45}$$

Here we assume that the transition rates may depend on the discrete state labels, on the age as well as on the continuous state variables. As in the case of pure jump processes, we shall suppose that all the possible states $(i, \boldsymbol{X})$ are connected, i.e. all the points $(i, \boldsymbol{X})$ are accessible.

Looking for a stationary solution of (41) and (42)

$$\mathscr{B}_i = \mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) = \text{independent of } t \tag{46}$$

we come to (see appendix 1):

$$\mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) = \int_{\boldsymbol{X}'} \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', 0)\mathscr{B}_i^{\mathrm{st}}(0, \boldsymbol{X}')\, \mathrm{d}\boldsymbol{X}' \tag{47}$$

where

$$\mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', a') = \tau \exp\left[\int_{a'}^{a} (\mathbb{L}_i - \sum_j W_{ij}(a'', \boldsymbol{X}))\, \mathrm{d}a''\right] \delta(\boldsymbol{X}-\boldsymbol{X}') \tag{48}$$

are Green functions obeying the equations

$$\partial_t \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', a') = \left[\mathbb{L}_i - \sum_j W_{ij}(a, \boldsymbol{X})\right] \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', a') \tag{49}$$

$$\mathscr{G}_i(\boldsymbol{X}, a'|\boldsymbol{X}', a') = \delta(\boldsymbol{X}-\boldsymbol{X}'). \tag{50}$$

Here τ is the Dyson's time-ordering operator, the functions $\mathscr{B}_i^{\mathrm{st}}(0, \boldsymbol{X})$ satisfy the integral equations

$$\mathscr{B}_i^{\mathrm{st}}(0, \boldsymbol{X}) = \sum_j \int_{\boldsymbol{X}'} \Gamma_{ji}(\boldsymbol{X}' \to \boldsymbol{X})\mathscr{B}_j^{\mathrm{st}}(0, \boldsymbol{X}')\, \mathrm{d}\boldsymbol{X}' \tag{51}$$

the normalisation condition is

$$\sum_i \int_{\boldsymbol{X}'} \Xi_i(\boldsymbol{X}')\mathscr{B}_i^{\mathrm{st}}(0, \boldsymbol{X}')\mathrm{d}\boldsymbol{X}' = 1 \tag{52}$$

and the kernels $\Gamma_{ji}(\boldsymbol{X}' \to \boldsymbol{X})$ and $\Xi_i(\boldsymbol{X})$ are given by

$$\Gamma_{ji}(\boldsymbol{X}' \to \boldsymbol{X}) = \int_0^\infty W_{ji}(a, \boldsymbol{X})\mathscr{G}_j(\boldsymbol{X}, a|\boldsymbol{X}', 0)\, \mathrm{d}a \tag{53}$$

$$\Xi_i(\boldsymbol{X}') = \int_0^\infty \int_{\boldsymbol{X}} \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', 0)\, \mathrm{d}a\, \mathrm{d}\boldsymbol{X}. \tag{54}$$

The time-dependent solution of (41) and (42) may be expressed in a similar way. We get (see appendix 1):

$$\begin{aligned}\mathscr{B}_i(a, \boldsymbol{X}, t) = h(t-a) &\int_{\boldsymbol{X}'} \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}', 0)\mathscr{B}_i(0, \boldsymbol{X}', t-a)\, \mathrm{d}\boldsymbol{X}' \\ &+ h(a-t) \int_{\boldsymbol{X}'} \mathscr{G}_i(\boldsymbol{X}, a|\boldsymbol{X}_0, a-t)\mathscr{B}_i(a-t, \boldsymbol{X}_0, 0)\, \mathrm{d}\boldsymbol{X}_0\end{aligned} \tag{55}$$

where the functions $\mathscr{B}_i(0, \boldsymbol{X}, t)$ satisfy the integral equations

$$\mathscr{B}_i(0, \boldsymbol{X}, t) = \sum_j \int_0^t \int_{\boldsymbol{X}'} W_{ji}(a, \boldsymbol{X}) \mathscr{G}_j(\boldsymbol{X}, a|\boldsymbol{X}', 0) \mathscr{B}_j(0, \boldsymbol{X}', t-a) \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X}' + \sum_j \int_t^\infty \int_{\boldsymbol{X}_0} W_{ji}(a, \boldsymbol{X}) \mathscr{G}_j(\boldsymbol{X}, a|\boldsymbol{X}_0, a-t) \mathscr{B}_j(a-t, \boldsymbol{X}_0, 0) \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X}_0. \tag{56}$$

As in the case of pure jump processes, we can prove that the initial condition

$$I(0) = \sum_i \int_0^\infty \int_{\boldsymbol{X}} \mathscr{B}_i(a, \boldsymbol{X}, 0) \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X} = 1 \tag{57}$$

implies the validity of the normalisation condition

$$I(t) = \sum_i \int_0^\infty \int_{\boldsymbol{X}} \mathscr{B}_i(a, \boldsymbol{X}, t) \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X} = 1 \tag{58}$$

for any time. Indeed, integrating (41) over a, $\boldsymbol{X}$, performing a partial integration with respect to $\boldsymbol{X}$ in which the boundary terms vanish, and taking into account (42), we come to

$$\partial_t \sum_i \int_0^\infty \mathscr{B}_i(a, \boldsymbol{X}, t) \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X} = 0 \tag{59}$$

i.e.

$$I(t) = I(0) = 1. \tag{60}$$

Unfortunately, in this case the uniqueness of $\mathscr{B}_i^{\mathrm{st}}$ and the positivity of $\mathscr{B}_i^{\mathrm{st}}$ and $\mathscr{B}_i$ cannot be proved in a simple way. Only in a particular case we can give a partial proof of these assertions (see appendix 2).

5. A generalised *H*-function

Assuming that the uniqueness of $\mathscr{B}_i^{\mathrm{st}}$ and the positivity of $\mathscr{B}_i^{\mathrm{st}}$ and $\mathscr{B}_i$ are physically plausible, we shall try to show that the expression

$$H(t) = \sum_i \int_0^\infty \int_{\boldsymbol{X}} \mathscr{B}_i(a, \boldsymbol{X}, t) \ln[\mathscr{B}_i(a, \boldsymbol{X}, t)/\mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X})] \, \mathrm{d}a \, \mathrm{d}\boldsymbol{X} \tag{61}$$

fulfils the requirements of an H-function.

First the proof of the conditions

$$H(t) > 0 \qquad \text{for } \mathscr{B}_i(a, \boldsymbol{X}, t) \neq \mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) \tag{62}$$

$$H(t) = 0 \qquad \text{for } \mathscr{B}_i(a, \boldsymbol{X}, t) = \mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) \tag{63}$$

is straightforward and is based on the relationships (27), (58) and (61).

The proof of

$$\dot{H}(t) < 0 \qquad \text{for } \mathscr{B}_i(a, \boldsymbol{X}, t) \neq \mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) \tag{64}$$

$$\dot{H}(t) = 0 \qquad \text{for } \mathscr{B}_i(a, \boldsymbol{X}, t) = \mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) \tag{65}$$

is more difficult. To prove these conditions we shall assume the validity of the following restrictions:

(a) the matrix of the diffusion coefficients $\|D_i^{\alpha\beta}(\boldsymbol{X})\|$ is positive definite, i.e.

$$Y_\alpha Y_\beta D_i^{\alpha\beta}(\boldsymbol{X}) > 0 \qquad \forall\, Y_\alpha,\ Y_\beta \neq 0 \text{ and real} \tag{66}$$

(b)

$$\lim_{a \to \infty} \mathscr{B}_i(a, \boldsymbol{X}, t)/\mathscr{B}_i^{\mathrm{st}}(a, \boldsymbol{X}) = \text{finite}. \tag{67}$$

We note that (66) is commonly used in Markovian dynamics (Lebowitz and Bergmann 1957, Graham 1978, Risken 1984). On the other hand, (67) is similar to (18).

The proof proceeds in many steps. First, combining (41), (58) and (61), we get

$$\begin{aligned}\dot{H}(t)&=\sum_i\int_0^\infty\int_X[\partial_t\mathscr{B}_i(a,X,t)]\ln[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\,\mathrm{d}a\,\mathrm{d}X\\&=\sum_i\int_0^\infty\int_X[\mathbb{L}_i\mathscr{B}_i(a,X,t)]\ln[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\,\mathrm{d}a\,\mathrm{d}X\\&\quad-\sum_i\sum_j\int_0^\infty\int_X W_{ij}(a,X)\mathscr{B}_i(a,X,t)\ln[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\,\mathrm{d}a\,\mathrm{d}X\\&\quad+C(t)\end{aligned}\tag{68}$$

where

$$C(t)=-\sum_i\int_0^\infty\int_X[\partial_a\mathscr{B}_i(a,X,t)]\ln[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\,\mathrm{d}a\,\mathrm{d}X.\tag{69}$$

Performing a partial integration with respect to a and taking account of (43) and (67), equation (69) becomes

$$\begin{aligned}C(t)&=-\sum_i\int_X\mathscr{B}_i(a,X,t)\ln[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\Big|_0^\infty\mathrm{d}X\\&\quad+\sum_i\int_0^\infty\int_X\{\partial_a\mathscr{B}_i(a,X,t)-[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\partial_a\mathscr{B}_i^{st}(a,X)\}\,\mathrm{d}a\,\mathrm{d}X\\&=\sum_i\int_X\mathscr{B}_i(0,X,t)\ln[\mathscr{B}_i(0,X,t)/\mathscr{B}_i^{st}(0,X)]\,\mathrm{d}X+\sum_i\int_X\mathscr{B}_i(a,X,t)\Big|_0^\infty\mathrm{d}X\\&\quad-\sum_i\int_0^\infty\int_X[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\partial_a\mathscr{B}_i^{st}(a,X)\,\mathrm{d}a\,\mathrm{d}X.\end{aligned}\tag{70}$$

Inserting $\mathscr{B}_i(0,X,t)$ from (42) and expressing the term $\partial_a\mathscr{B}_i^{st}(a,X)$ from (41) applied for $\mathscr{B}_i=\mathscr{B}_i^{st}(a,X)$ we come to

$$\begin{aligned}C(t)&=\sum_i\sum_j\int_0^\infty\int_X W_{ji}(a,X)\mathscr{B}_j(a,X,t)\ln[\mathscr{B}_i(0,X,t)/\mathscr{B}_i^{st}(0,X)]\,\mathrm{d}a\,\mathrm{d}X\\&\quad-\sum_i\sum_j\int_0^\infty\int_X W_{ji}(a,X)\mathscr{B}_j(a,X,t)\,\mathrm{d}a\,\mathrm{d}X\\&\quad-\sum_i\int_0^\infty\int_X[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)]\\&\quad\times\Big\{[\mathbb{L}_i\mathscr{B}_i^{st}(a,X)]-\sum_j W_{ij}(a,X)\mathscr{B}_i^{st}(a,X)\Big\}\,\mathrm{d}a\,\mathrm{d}X\end{aligned}\tag{71}$$

$$\begin{aligned}&=-\sum_i\int_0^\infty\int_X[\mathscr{B}_i(a,X,t)/\mathscr{B}_i^{st}(a,X)][\mathbb{L}_i\mathscr{B}_i^{st}(a,X)]\,\mathrm{d}a\,\mathrm{d}X\\&\quad+\sum_i\sum_j\int_0^\infty\int_X W_{ji}(a,X)\mathscr{B}_j(a,X,t)\ln[\mathscr{B}_i(0,X,t)/\mathscr{B}_i^{st}(0,X)]\,\mathrm{d}a\,\mathrm{d}X.\end{aligned}\tag{72}$$

Combining (68) and (71), we observe that $\dot{H}(t)$ may be expressed as the sum of three terms

$$\dot{H}(t)=\dot{H}_1(t)+\dot{H}_2(t)+\dot{H}_3(t) \tag{73}$$

with

$$\dot{H}_1(t)=\sum_i\sum_j\int_0^\infty\int_{\boldsymbol{X}} W_{ji}(a,\boldsymbol{X})\mathscr{B}_j(a,\boldsymbol{X},t) \times\ln[\mathscr{B}_i(0,\boldsymbol{X},t)\mathscr{B}_j^{\text{st}}(a,\boldsymbol{X})/\mathscr{B}_j(a,\boldsymbol{X},t)\mathscr{B}_i^{\text{st}}(0,\boldsymbol{X})]\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X} \tag{74}$$

$$\dot{H}_2(t)=-\sum_i\int_0^\infty\int_{\boldsymbol{X}}[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})][\mathbb{L}_i\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X} \tag{75}$$

$$\dot{H}_3(t)=\sum_i\int_0^\infty\int_{\boldsymbol{X}}[\mathbb{L}_i\mathscr{B}_i(a,\boldsymbol{X},t)]\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X}. \tag{76}$$

We observe that (74) is similar to (33). By applying the method presented in § 3 it is easy to show that

$$\dot{H}_1(t)<0 \qquad \text{for } \mathscr{B}_i(a,\boldsymbol{X},t)\neq\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X}) \tag{77}$$

$$\dot{H}_1(t)=0 \qquad \text{for } \mathscr{B}_i(a,\boldsymbol{X},t)=\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X}). \tag{78}$$

Thus the proof of (64) and (65) may be reduced to the proof of

$$\dot{H}_2(t)+\dot{H}_3(t)<0 \qquad \text{for } \mathscr{B}_i(a,\boldsymbol{X},t)\neq\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X}) \tag{79}$$

$$\dot{H}_2(t)+\dot{H}_3(t)=0 \qquad \text{for } \mathscr{B}_i(a,\boldsymbol{X},t)=\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X}). \tag{80}$$

Performing in (75) a partial integration with respect to $\boldsymbol{X}$ and taking into account that the boundary terms vanish, we obtain

$$\begin{aligned}\dot{H}_2(t)&=\sum_i\int_0^\infty\int_{\boldsymbol{X}}[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\partial_{X_\alpha}\{K_i^\alpha(\boldsymbol{X})\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})\\&\quad-[\partial_{X^\beta}D_i^{\alpha\beta}(\boldsymbol{X})]\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})-D_i^{\alpha\beta}(\boldsymbol{X})[\partial_{X^\beta}\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\,\mathrm{d}\boldsymbol{X}\\&=-\sum_i\int_0^\infty\int_{\boldsymbol{X}}\mathscr{B}_i(a,\boldsymbol{X},t)\{\partial_{X^\alpha}\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\\&\quad\times\{K_i^\alpha(\boldsymbol{X})-[\partial_{X^\beta}D_i^{\alpha\beta}(\boldsymbol{X})]-D_i^{\alpha\beta}(\boldsymbol{X})\partial_{X^\beta}[\ln\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X}.\end{aligned} \tag{81}$$

The term $\dot{H}_3(t)$ may be expressed in a similar way:

$$\begin{aligned}\dot{H}_3(t)&=\sum_i\int_0^\infty\int_{\boldsymbol{X}}\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\partial_{X^\alpha}\{-K_i^\alpha(\boldsymbol{X})\mathscr{B}_i(a,\boldsymbol{X},t)\\&\quad+[\partial_{X^\beta}D_i^{\alpha\beta}(\boldsymbol{X})]\mathscr{B}_i(a,\boldsymbol{X},t)+D_i^{\alpha\beta}(\boldsymbol{X})[\partial_{X^\beta}\mathscr{B}_i(a,\boldsymbol{X},t)]\}\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X}\\&=\sum_i\int_0^\infty\int_{\boldsymbol{X}}\mathscr{B}_i(a,\boldsymbol{X},t)\{\partial_{X^\alpha}\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\\&\quad\times\{K_i^\alpha(\boldsymbol{X})-[\partial_{X^\beta}D_i^{\alpha\beta}(\boldsymbol{X})]-D_i^{\alpha\beta}(\boldsymbol{X})\partial_{X^\beta}[\ln\mathscr{B}_i(a,\boldsymbol{X},t)]\}\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X}\end{aligned} \tag{82}$$

and thus

$$\begin{aligned}&\dot{H}_2(t)+\dot{H}_3(t)\\&\quad=-\sum_i\int_0^\infty\int_{\boldsymbol{X}}\mathscr{B}_i(a,\boldsymbol{X},t)D_i^{\alpha\beta}(\boldsymbol{X})\{\partial_{X^\alpha}\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\\&\quad\quad\times\{\partial_{X^\beta}\ln[\mathscr{B}_i(a,\boldsymbol{X},t)/\mathscr{B}_i^{\text{st}}(a,\boldsymbol{X})]\}\,\mathrm{d}a\,\mathrm{d}\boldsymbol{X}.\end{aligned} \tag{83}$$

Combining (66) and (83) we get the relationships (79) and (80).

6. Discussion

The ADME formalism has been introduced in order to describe the memory effects. Gartner (1989), Vlad (1987) and Vlad and Pop (1989) proved that the ADME formalism is related to the continuous-time random walks theory (CTRW) (Montroll and West 1979), as well as to the generalised master equation (GME) (Montroll and West 1979). Unfortunately, within the framework of the CTRW or GME theories the H-theorem cannot accomodate arbitrary waiting-time distribution functions (Rajagopal *et al* 1983). The ADME formalism may be used to circumvent this difficulty. The success of our approach is due to the fact that we have considered the age of a state as an additional random variable.

To outline the particularities of our method we mention that within the framework of CTRW or GME theories we are tempted to build the H-function in terms of the state probability $P_i(t)$:

$$H^*(t)=\sum_i P_i(t)\ln(P_i(t)/P_i^{\rm st}) \tag{84}$$

or in terms of the state probability density $B_i(\boldsymbol{X}, t)$:

$$H^{**}(t)=\sum_i \int_{\boldsymbol{X}} B_i(\boldsymbol{X}, t)\ln[B_i(\boldsymbol{X}, t)/B_i^{\rm st}(\boldsymbol{X})]\,{\rm d}\boldsymbol{X} \tag{85}$$

where

$$B_i(\boldsymbol{X}, t)=\int_0^\infty \mathscr{B}_i(a, \boldsymbol{X}, t)\,{\rm d}a \qquad B_i^{\rm st}(\boldsymbol{X})=\int_0^\infty \mathscr{B}_i^{\rm st}(a, \boldsymbol{X})\,{\rm d}a. \tag{86}$$

We note that $H^*(t)$ and $H^{**}(t)$ are different from the H-functions defined by (17) and (61).

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Appendix 1

For steady states, (41) and (42) become

$$(\partial_a-\mathbb{L}_i)\mathscr{B}_i^{\rm st}(a, \boldsymbol{X})=-\mathscr{B}_i^{\rm st}(a, \boldsymbol{X})\sum_j W_{ij}(a, \boldsymbol{X}) \tag{A1.1}$$

$$\mathscr{B}_i^{\rm st}(0, \boldsymbol{X})=\sum_j \int_0^\infty W_{ji}(a, \boldsymbol{X})\mathscr{B}_j^{\rm st}(a, \boldsymbol{X})\,{\rm d}a. \tag{A1.2}$$

Taking (48)-(50) into account, the integration of (A1.1) leads to (47). Inserting (47) into (A1.2) we get the integral equations (51). Combining (47) with the normalisation condition

$$\sum_i \int_0^\infty \int_{\boldsymbol{X}} \mathscr{B}_i^{\rm st}(a, \boldsymbol{X})\,{\rm d}a\,{\rm d}\boldsymbol{X}=1 \tag{A1.3}$$

gives (52).

Integrating (41) along the characteristics and using (48)-(50), we get (55). Substituting (55) into (42) we come to (56).

Appendix 2

The transition rates $W_{ij}(a, \boldsymbol{X})$ may be expressed in the following form:

$$W_{ij}(a, \boldsymbol{X}) = \Omega_i(a, \boldsymbol{X}) T_{ij}(a, \boldsymbol{X}) \tag{A2.1}$$

where $\Omega_i(a, \boldsymbol{X})$ is the overall transition rate from state $(i, \boldsymbol{X})$ to other states, and $T_{ij_1}(a, \boldsymbol{X})$, $T_{ij_2}(a, \boldsymbol{X}), \ldots$ are the transition probabilities from the state $(i, \boldsymbol{X})$ to the states $(j_1, \boldsymbol{X})$, $(j_2, \boldsymbol{X}), \ldots$ for a given age a:

$$\Omega_i(a, \boldsymbol{X}) = \sum_j W_{ij}(a, \boldsymbol{X}) \tag{A2.2}$$

$$T_{ij}(a, \boldsymbol{X}) = W_{ij}(a, \boldsymbol{X}) \left(\sum_j W_{ij}(a, \boldsymbol{X}) \right)^{-1}. \tag{A2.3}$$

We shall consider a particular case

$$\Omega_i = \Omega_i(a) = \text{independent of } \boldsymbol{X}. \tag{A2.4}$$

In this case $\mathbb{L}_i$ and $\Sigma_j W_{ij}$ commute

$$\mathbb{L}_i \Omega_i = \Omega_i \mathbb{L}_i \tag{A2.5}$$

and thus the Green function $\mathscr{G}_i(\boldsymbol{X}, a | \boldsymbol{X}', a')$ can be expressed in terms of $G_i(\boldsymbol{X} | \boldsymbol{X}'; t)$:

$$\mathscr{G}_i(\boldsymbol{X}, a | \boldsymbol{X}', a') = G_i(\boldsymbol{X} | \boldsymbol{X}'; a - a') \gamma_i(a) / \gamma_i(a') \tag{A2.6}$$

where

$$\gamma_i(a) = \exp\left(- \int_0^a \Omega_i(a'') \, \mathrm{d}a'' \right) \tag{A2.7}$$

is the probability that in the age interval $(0, a)$ the discrete state index was i. As G_i and γ_i are probabilities it follows that they are non-negative. From (A2.6) it turns out that the same is true for $\mathscr{G}_i$:

$$\mathscr{G}_i(\boldsymbol{X}, a | \boldsymbol{X}', a') \geqslant 0. \tag{A2.8}$$

Equation (A2.8) allows one to apply the method used in § 3 for proving that $\mathscr{B}_i(a, \boldsymbol{X}, t)$ is non-negative.

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