Detailed balance in non-equilibrium systems

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Abstract. We show by explicit construction that any system described by a Markov process having a stationary density may be put in generalized detailed balance adding some odd parameters. A physical interpretation of the construction is given in terms of the different time-scales involved.

1 Introduction

The symmetry of detailed balance (DB) in a Markov process describing a physical system in terms of a set of fluctuating macrovariables has its origin in the time-reversal invariance of the underlying microscopic system. If one includes parameters, the symmetry can be extended to generalized detailed balance (GDB). For systems in thermodynamic equilibrium, one can show that one has DB (or GDB if some external parameter must be changed (van Kampen, 1992)). However, in non-equilibrium situations, this is not the case (van Kampen, 1992) in general and there is no reason to expect this symmetry (Hänggi & Thomas, 1982). On the other hand, Graham (1980) remarked that it is always possible when one has a diffusion process which is not in GDB to construct another process adding one new odd parameter \( \lambda \) which is in GDB (the new process reduces to the original one for \( \lambda = 1 \)). We shall discuss this result here and extend it to a general Markov process in a very direct way using the notion of a reversed process which turns out to be the relevant concept. This is done in Section 2, while in Section 3 we give an interpretation of the previous construction which indicates that one can understand in a very simple way the absence of DB as a problem of different time-scales.
2 Construction of the process in GDB

Macroscopic systems are described by a set of macroscopic variables \( \{X^a, \mu = 1, \ldots, N\} \). If fluctuations are taken into account \( \{X^a\} \) is a stochastic process \( X^a \) is a random variable for each time \( t \) which in many cases of physical interest can be considered as Markovian (van Kampen, 1992). We consider this case here. Let \( P_+(x, t; x', t'; \sigma) \) be the conditional probability density of the Markov process where \( x \) stands for \( (x^1, \ldots, x^N) \), \( \sigma \) for a set of external parameters \( (\sigma^1, \ldots, \sigma^M) \) and the subscript `+' means the advanced conditional probability \( (t \geq t') \). The joint probability densities (van Kampen, 1992),

\[
\omega^{(a)}(x_1, t_1; x_2, t_2; \ldots; x_n, t_n) = \text{prob} \{X(t_1) = x_1, \ldots, X(t_n) = x_n\}
\]

are given by

\[ (t_1 \geq t_2 \geq \ldots > t_n) : \]

\[
P_+(x_1, t_1|x_2, t_2; \sigma)P_+(x_2, t_2|x_3, t_3; \sigma) \ldots P_+(x_{n-1}, t_{n-1}|x_n, t_n; \sigma) \cdot \omega^{(1)}(x_n, t_n; \sigma) \tag{1}\]

We consider Markov processes homogeneous in time, i.e. \( P_+(x, t; x', t'; \sigma) = \tilde{P}_+(x, t-t'; \sigma) \) is a function of \( (t-t') \). We assume that the process has a stationary probability density \( \rho(x, \sigma) \)

\[
\rho(x, \sigma) = \lim_{\tau \to \infty} \tilde{P}_+(x, \tau|x'; \sigma) \tag{2}\]

In the stationary state, one has (see (1)) that \( \omega^{(1)}(x, t; \sigma) = \rho(x, \sigma) \) is time independent and the functions \( \omega^{(a)} \) are functions of the time differences. Writing \( \mathcal{W}^{(a)} \) for the joint probability densities in the stationary state we have

\[
\mathcal{W}^{(a)}(x_1, t_1; x_2, t_2; \ldots; x_n, t_n; \sigma) =
\]

\[
P_+(x_1, t_1|x_2, t_2; \sigma)P_+(x_2, t_2|x_3, t_3; \sigma) \ldots P_+(x_{n-1}, t_{n-1}|x_n, t_n; \sigma) \cdot \rho(x_n, \sigma) \tag{3}\]

and from now on we consider this process which is characterized by the functions \( \mathcal{W}^{(a)} \) given by (3). Notice that one can always consider the process defined for all times \( t \in (-\infty, \infty) \) in the stationary state as it can be seen in (3). GDB is a symmetry defined in terms of the functions \( \mathcal{W}^{(a)} \) and with respect to a given time-reversal transformation \( \{x \to \tilde{x}, \sigma \to \tilde{\sigma}\} \) of the variables and parameters which is such that applied twice is the identity, i.e. \( \tilde{\tilde{x}} = x, \tilde{\tilde{\sigma}} = \sigma \). Variables and parameters can be chosen with a well-defined parity with respect to time reversal, in which case \( \tilde{\tilde{x}}^a = \varepsilon(y^a) x^a, \varepsilon(\sigma) = \pm 1, \tilde{\tilde{\sigma}}_j = \varepsilon(j) \sigma_j, \varepsilon(j) = \pm 1 \), and one speaks of even and odd quantities (see van Kampen (1992) and Gardiner (1983) for a discussion of this symmetry). The definition of GDB says that the Markov process with joint probability functions \( \mathcal{W}^{(a)} \) is in GDB with respect to the transformation \( \{x \to \tilde{x}, \sigma \to \tilde{\sigma}\} \) if

\[
\mathcal{W}^{(12)}(x, t; x', t'; \sigma) = \mathcal{W}^{(12)}(x', t; x, t'; \sigma) \tag{4}\]

This relation implies \( \rho(\tilde{x}, \tilde{\sigma}) = \rho(x, \sigma) \) by integration over \( x' \). The conditional probability density obeys an equation of the form (see Hänggi and Thomas (1982) for a discussion)

\[
\partial_\tau P_+(x, t|x', t; \sigma) = \int dy \Gamma(x, y; \sigma) P_+(y, t|x', t; \sigma) \tag{5}\]

with initial condition \( P_+(x, t|x', t; \sigma) = \delta(x-x') \) for \( t \to t' + \). For diffusion processes the kernel \( \Gamma \) is a differential operator and (5) reduces to the Fokker–Planck
equation. One can formally write (5) as an infinite series of the form (Hänggi & Thomas, 1982) (sum over repeated indices should be understood from now on)

\[ \partial_t P_+(x, t|x', t'; \sigma) = \sum_{n \geq 1} \frac{(-1)^n}{n!} \partial_{x_1} \ldots \partial_{x_n} A_{x_1} \ldots A_{x_n} (x, \sigma) \]  

which is the Kramers–Moyal expansion. Consider the case of a jump process with discrete extensive variables \{N^\alpha(\cdot)\}. If the transition rates have the canonical form (van Kampen, 1992) in terms of the intensive variables \( x^\alpha = N^\alpha/\Omega \), where \( \Omega \) is the size of the system, then in (6) the term with \( n \) derivatives has a factor \( \eta^{n-1} \), where \( \eta = \Omega^{-1} \) is a small parameter. GDB can be expressed in terms of the reversed process which we define now. The reversed process consists in looking at the original process in the opposite direction of time and its conditional probability density \( P_+^R(x, t|x', t'; \sigma) = P_-(x, t-t|x', t'; \sigma) \), \( t > t' \) (7)

where \( P_- \) is the retarded conditional probability of the initial process (conditioning is with respect to a future time) corresponding to

\[ P_-(x', t'\mid x', t; \sigma) = \text{prob}\{x(t') = x'|x(t') = x'\}, \quad t < t' \]  

(8)

For \( t > t' \) we have

\[ W^{(2)}(x, t; x, t') = P_+(x, t|x', t'; \sigma) \rho(x', \sigma) = P_-(x', t'|x, t; \sigma) \rho(x, \sigma) \]  

(9)

and from (7)–(9), we obtain

\[ P_+^R(x, t|x', t'; \sigma) = P_-(x', t'|x, t; \sigma) \frac{\rho(x, \sigma)}{\rho(x', \sigma)} \]  

(10)

and we can see, taking the limit \( (t-t') \to \infty \), that the stationary probability of the reversed process is again \( \rho(x, \sigma) \). The joint probability functions \( W_{-R}^{(2)} \) of the reversed process in the stationary state are given by formula (3) replacing \( P_- \) by \( P_+^R \). One can easily check that GDB as defined by (4) with respect to the transformation \( \{x \to \bar{x}, \sigma \to \bar{\sigma}\} \) is equivalent to

\[ P_+^R(x, t|x', t'; \sigma) = P_+(-\bar{x}, t|\bar{x}', t'; \bar{\sigma}) \]  

(11)

From (5), we have that the kernel \( \Gamma \) is given by

\[ \Gamma(x, x'; \sigma) = \lim_{t \to t'} \partial_t P_+(x, t|x', t'; \sigma) \]  

(12)

and from (10) we see that the kernel \( \Gamma^R \) of the reversed process is

\[ \Gamma^R(x, x'; \sigma) = \Gamma(x', x; \sigma) \frac{\rho(x, \sigma)}{\rho(x', \sigma)} \]  

(13)

From (11), we see that in terms of the kernels, (4) is equivalent to

\[ \Gamma^R(x, x'; \sigma) = \Gamma(\bar{x}, \bar{x}'; \bar{\sigma}) \]  

(14)

One should remark here that in order to show the equivalences one must have \( \rho(\bar{x}, \bar{\sigma}) = \rho(x, \sigma) \) which is implied by (11) taking the limit \( (t-t') \to \infty \).

We have then that GDB with respect to the transformation \( x \to \bar{x}, \sigma \to \bar{\sigma} \) can be expressed by (4) or by any of the two equivalent expressions (11) and (14). Thus, we see that GDB can be expressed in a very simple and intuitive way in terms of
the reversed process. We remark that the reversed process we consider here is
defined independently of any time-reversal transformation (see (10) and (13)) and
also that reversing twice takes one back to the initial process which we shall call
the direct process. Let us see the meaning of the direct and reversed process in
terms of realizations. Let \( x^d = \gamma^d(t) \) and \( x^r = \gamma^r(t) = \gamma^d(-t), t \in [-T, T] \) be two
realizations, then one has that the probability of \( \gamma^d(\cdot) \) calculated with the
direct process is equal to the probability of \( \gamma^r(\cdot) \) calculated with the reversed process. If
the direct process is in GDB with respect to the transformation
\( \{ x \to \bar{x} = x, \sigma \to \bar{\sigma} = \sigma \} \), we have that the reversed process coincides with the direct
process (see (11)) and consequently the two curves \( \gamma(\cdot) \) and \( \gamma^r(\cdot) \) have the same
probability.

We shall see now that if we have an initial process with conditional probability
\( P_+(x, t|x', t'; \sigma, \lambda) \) which is not in GDB with respect to the transformation
\( \{ x \to \bar{x} = x, \sigma \to \bar{\sigma} = \sigma \} \) (all variables and parameters are even), we can always
construct a new process with one more odd parameter \( \lambda \) which coincides with the
initial process for \( \lambda = 1 \) and which is in GDB with respect to the previous
transformation plus \( \lambda \to \bar{\lambda} = -\lambda \). The procedure is a generalization of construction
made by Graham (1980) for diffusion processes. The new process will have a conditional probability
\( P_+(x, t|x', t'; \sigma, \lambda) \) satisfying the equation

\[
\partial_t P_+(x, t|x', t'; \sigma, \lambda) = \int dy \, \Gamma(x, y; \sigma, \lambda) P_+(y, t|x', t'; \sigma, \lambda) 
\]

\[ \Gamma(x, y; \sigma, \lambda) \equiv \frac{1}{2} \left[ \Gamma(x, y; \sigma) + \Gamma^R(x, y; \sigma) \right] + \frac{\lambda}{2} \left[ \Gamma(x, y; \sigma) - \Gamma^R(x, y; \sigma) \right] \]  

(15)

(16)

From (16), we see that the new kernel will conserve positivity if \( |\lambda| \leq 1 \) and also that
the new process coincides with the initial one for \( \lambda = 1 \) and with the reversed
process for \( \lambda = -1 \). We remark that the stationary probability of the new process
coincides with the stationary probability \( \rho(x, \sigma) \) of the initial process and its
reversed process since

\[
\int dy \, \Gamma(x, y; \sigma, \lambda) \rho(y, \sigma) = \int dy \, \Gamma^R(x, y; \sigma) \rho(y, \sigma) = 0
\]

(17)

Let us calculate the kernel \( \Gamma^R(x, y; \sigma, \lambda) \) of the reversed process of (15) which is
given by (see (13))

\[
\Gamma^R(x, y'; \sigma, \lambda) = \Gamma(x', x; \sigma, \lambda) \frac{\rho(x, \sigma)}{\rho(x', \sigma)}
\]

(18)

a simple calculation using (16) and (13) shows that

\[
\Gamma^R(x, x'; \sigma, \lambda) = \Gamma(x, x'; \sigma, -\lambda)
\]

(19)

and from (14) we conclude that the process (15) is in GDB with respect to the
transformation \( \{ x \to \bar{x} = x, \sigma \to \bar{\sigma}, \lambda \to \bar{\lambda} = -\lambda \} \).

3 Interpretation of the construction

The construction of Section 2 involved the addition of a new odd parameter \( \lambda \).
Physically, a macroscopic parameter can be interpreted as a variable varying in a
very slow time-scale with respect to the characteristic times of the system. Let us
consider a diffusion process in which case the kernel \( \Gamma \) in (5) is the kernel of a second-order differential operator and \( P_+(x, t|x', t') \) obeys a Fokker–Planck equation (\( \partial_\mu \equiv \partial/\partial x_\mu \)):

\[
\partial_\mu P_+(x, t|x', t') = \partial_\mu \left( -A^\mu(x) + \frac{\eta}{2} \partial_\nu g^{\mu\nu}(x) \right) P_+(x, t|x', t')
\]  

(20)

which corresponds to the Langevin equation (interpreted in the Ito (1979) sense)

\[
x_\mu = A_\mu(x) + \sqrt{\eta} \sigma_\mu \xi_j(t), \quad \mu = 1, \ldots, n
\]  

(21)

where \( \xi_j, j = 1, \ldots, m \) are Gaussian white noises with zero mean value and correlation \( \langle \xi_j(t) \xi_k(t') \rangle = \delta(t-t'). \) One has

\[
g^{\mu\nu}(x) = \sigma_\mu(x) \sigma_\nu(x)
\]  

(22)

We suppose that this process is not in DB for the transformation \( \{x \to \tilde{x} = x\} \) and we shall make the construction of the previous section. The reversed process of (20) will again be a diffusion process with conditional probability density (Barra et al., 1995) \( P^R_+ \) satisfying

\[
\partial_\mu P^R_+(x, t|x', t') = \partial_\mu \left[ -A^R_\mu(x, \eta) + \frac{\eta}{2} \partial_\nu g^{R\nu}(x) \right] P^R_+(x, t|x', t')
\]  

(23)

\[
A^R_\mu(x, \eta) = -A_\mu(x) + \eta \partial_\nu g^{\nu\mu} - g^{\nu\mu} \partial_\nu \phi(x, \eta)
\]  

(24)

where the common stationary probability of the direct and the reversed process is \( \rho(x) = \exp(-\eta \phi(x, \eta)). \) Defining

\[
D_\mu = \frac{1}{2}(A_\mu + A^R_\mu), \quad R_\mu = \frac{1}{2}(A_\mu - A^R_\mu)
\]

the process in GDB of Section 2 will have a conditional probability density \( P_+(x, t|x'; \lambda) \) which satisfies the equation

\[
\partial_\mu P_+(x, t|x', t'; \lambda) = \partial_\mu \left[ -B_\mu(x, \lambda) + \frac{\eta}{2} \partial_\nu g^{R\nu}(x) \right] P_+(x, t|x', t'; \lambda)
\]

(25)

\[
B_\mu(x, \lambda) \equiv D_\mu(x) + \lambda R_\mu(x), \quad 1 \leq \mu \leq n
\]

(26)

The stationary probability \( \rho(x, \lambda) = \exp(-\phi(x, \eta)) \) of the process defined by (25), (26) is independent of \( \lambda \) and coincides with the stationary probability of the original process (21). We consider now that \( \lambda \) is a new variable \( \lambda(t) \) varying slowly and obeying an equation

\[
\dot{\lambda} = B_{n+1}(\lambda) + \sqrt{\eta} \zeta^{m+1}(t)
\]

(27)

where \( \zeta^{m+1}(t) \) is a Gaussian white noise with zero mean and uncorrelated with \( \zeta^1(t) \ldots \zeta^m(t) \). Putting

\[
\langle \xi_j(t) \xi_k(t') \rangle = \epsilon^j_k \delta(t-t'), \quad 1 \leq j, k \leq m+1
\]

(28)

one has \( \epsilon^k = c^k \) for \( 1 \leq j, k \leq m, \zeta^{m+1,j} = \delta_{m+1,j} \). The function \( B_{n+1}(\lambda) = -B_{n+1}(-\lambda) \) is odd and we consider two cases

\[
B_{n+1}(\lambda) = -\frac{1}{T} \lambda
\]

(29)
\[ B_{n+1}(\lambda) = \frac{1}{T}(\lambda - \lambda^3) \] (30)

The set of Langevin equations \((y_n = x_\mu, 1 \leq \mu \leq n, y_{n+1} = \lambda)\)

\[ y_r = R_\mu(y, \lambda) + \sqrt{\eta} \sum_{j=0}^{m+1} \tilde{\sigma}_j(y) \xi^j_r(t), \quad 1 \leq r \leq n + 1 \] (31)

with \(\tilde{\sigma}_j = \sigma_\mu, 1 \leq j \leq n, 1 \leq \mu \leq m,\) and \(\tilde{\sigma}^{n+1}_j = \tilde{\delta}_{n+1,j}\) interpreted in the Ito sense define a diffusion process with conditional probability density \(P_+ (y, t|y', t') = P_+(x, \lambda, t|x', \lambda', t')\) satisfying \((\partial_r = \partial_\lambda)\)

\[ \partial_r P_+(y, t|y', t') = \partial_\lambda \left[ -B_\mu(x, \lambda) + \frac{\eta}{2} \tilde{\sigma}_\mu \tilde{\sigma}_\mu^\pi(x) \right] P_+(y, t|y', t') \] (32)

\[ \tilde{\sigma}^\pi(x) + \sum_{j=1}^{m+1} \tilde{\sigma}_j \tilde{\sigma}_j^\pi \] (33)

One has \(\tilde{\sigma}^\pi = \tilde{\sigma}^\pi, 1 \leq r, s \leq n\) and \(\tilde{\sigma}^{n+1,1} = \tilde{\delta}_{n+1,1}\). The conditional probability \(P^h_+ (y, t|y', t')\) of the reversed process will satisfy equation (32) with \(B_\mu(y)\) replaced by \(B^h_\mu(y)\) given by

\[ B^h_\mu = -B_\mu(y) + \eta \tilde{\sigma}_\mu \tilde{\sigma}_\mu^\pi(y) - \tilde{\sigma}^\pi(y) \partial_r \Psi \] (34)

\[ \tilde{\sigma}^\pi(y) = \exp \left( -\frac{1}{\eta} \Psi (y, x, \eta) \right) \] (35)

where \(\tilde{\sigma}^\pi(y)\) is the stationary probability of the process defined by (32). One easily checks that

\[ \Psi (y, x, \eta) = \phi(x, \eta) + \tilde{\phi}(\lambda) \] (36)

\[ \tilde{\phi}(\lambda) = -2 \int_0^\lambda du B_{n+1}(u) \] (37)

The condition for the process (32) to be in DB with respect to the transformation \(y_n = y_\mu, \epsilon(1) = \ldots = \epsilon(n) = 1, \epsilon(n+1) = -1\) is \(P^h_+ (y, t|y', t') = P^h_+(y, t|y', t')\) which is equivalent to \(B^h_\mu(y) = \epsilon(\mu) B_\mu(y), 1 \leq s \leq n + 1\). This last relation is verified using (34) and the process (31) is then in DB without changing any parameter but in the stationary state corresponding to the stationary probability (see (35)):

\[ \tilde{\sigma}^\pi(y) = \exp \left( -\frac{1}{\eta} \phi(x, \eta) \right) \exp \left( -\frac{1}{\eta} \tilde{\phi}(\lambda) \right) \] (38)

In the case (29), one has \(\tilde{\phi}(\lambda) = \lambda^3/T\) and then the most probable value of \(\lambda\) is zero and from (26) we understand why the system is now in DB for times \(t 

\[ A_\mu(x) = D_\mu(x) + R_\mu(x), \quad 1 \leq \mu \leq n \] (39)

was considered by Jauslin (1985) in his classification of Fokker–Planck models and we can see now that it corresponds to a decomposition of the drift in an irreversible
and a reversible part since the drift of the reversed process \( \lambda = -1 \) in (26)) is
\[
A_\mu^R(x) = D_\mu(x) - R_\mu(x)
\]
In the case (30), one has
\[
\bar{\phi}(\lambda) = \frac{1}{T} - \lambda^2 + \lambda^4
\]
and the stationary probability \( \exp(-1/\eta \bar{\phi}(\lambda)) \) of the variable \( \lambda \) now has two peaks at \( \lambda = \pm 1 \). A typical realization, \( \lambda(t) \), will then fluctuate around \( \lambda(t) \approx 1 \) for a time of the order of the exit time \( \tau = \pi T \exp(1/2\eta T) \) of the attractor \( \lambda = 1 \) and then jump to \( \lambda(t) = -1 \) and so on. For times \( t \gg \tau \), the process (31) will be in DB with respect to \( x \to \tilde{x} = x, \lambda \to \tilde{\lambda} = -\lambda \), but with the stationary probability (38) which implies \( \langle \lambda(t) \rangle \sim = 0 \). The original process (25), where \( \lambda \) is a parameter with the value \( \lambda = 1 \), appears in the process defined by (32), where \( \lambda \) is now a variable \( \lambda(t) \), as a metastable state in which the system remains for a time \( O(\tau) \), and is of course not in DB. The property of DB (parameters do not change by the time-reversal transformation) is known to have important consequences for a Markov process (Graham, 1980; Risken, 1984) and one can ask if our construction of the process defined by (32) which is in DB can be useful through the implications of DB. The answer is that (32) is in DB with respect to the stationary state (38) and all consequences of DB apply to this situation and not directly to the metastable state in which \( \lambda(t) \) fluctuates around one which corresponds to the original system. We have seen that in our construction the decomposition (39) of the drift \( A_\mu(x) \) of the diffusion process plays a central role. Consider the curves \( \gamma^{(1)} \)
\[
x_\mu = y^{(1)}_\mu(t), y^{(1)}_\mu(t_0) = Q_\mu^{(0)}, y^{(1)}_\mu(T) = Q_\mu^{(0)} + t_0, t_0 \leq t \leq T,
\]
and \( \gamma^{(2)} \):
\[
x_\mu = y^{(2)}_\mu(t) = y^{(1)}_\mu(T + t_0 - t).\]
Both curves are related by a time-reversal transformation (with all \( x_\mu \) even). We recall that for the process defined by (20) we take \( g^{(\mu)} = \delta^{(\mu)} \) which involves no loss of generality when the metric defined by \( g^{(\mu)}(x) \) has vanishing curvature) the probability of a curve \( \gamma: x_\mu = y_\mu(t) \) with fixed end-points is given by (Langouche et al., 1978)
\[
\text{prob}[\gamma(\cdot)] \approx \exp\left(-\frac{1}{\eta} \int_0^T dt L(y(t), y'(t))\right)
\]
\[
L(y(t), y'(t)) = \sum_{\mu=1}^n \left[ \frac{1}{2} \left( y_\mu(t) + y'(t) \right)^2 - y_\mu(t) A_\mu(y) + \frac{\eta}{2} \tilde{\phi}_\mu A_\mu(y) \right]
\]
Then the ratio \( R \) of the probabilities of the two curves \( \gamma^{(1)} \) and \( \gamma^{(2)} \) is
\[
R = \frac{\text{prob}[\gamma^{(1)}]}{\text{prob}[\gamma^{(2)}]} = \exp\left( \frac{2}{\eta} \int_{\gamma_t^{(1)}} A_\mu(x) \, dx_\mu \right)
\]
we consider now a closed curve \( \gamma^{(1)}_t \) (\( Q^{(0)} = \hat{Q} \) in the previous formulae). Since \( A_\mu = D_\mu + R_\mu \) with \( D_\mu(x) \) given by (see (24))
\[
D_\mu(x) = -\frac{1}{2} g^{(\mu)} \tilde{\phi}_\mu \phi(x, \eta)
\]
one has that (42) reduces to (Barra et al., 1995)
\[
R = \frac{\text{prob}[\gamma^{(1)}]}{\text{prob}[\gamma^{(2)}]} = \exp\left( \frac{2}{\eta} \int_{\gamma_t^{(1)}} R_\mu(x) \, dx_\mu \right)
\]
Since \( \gamma^{(2)} \) is the realization of the process obtained by time reversal, one has that the probability \( \text{prob}[\gamma^{(2)}, R] \) of this curve calculated with the reversed process equals the probability \( \text{prob}[\gamma^{(1)}, R] \) calculated with the direct process of the curve \( \gamma^{(1)} \) (see Section 2) and (44) can also be written as

\[
R = \text{prob}[\gamma^{(2)}, D] / \text{prob}[\gamma^{(1)}, R] = \exp \left( \frac{2}{\eta} \int_{\gamma^{(1)}} R_\mu(x) \, dx_\mu \right)
\]  

(45)

and we can see that this quotient will be one only when the process is in DB with respect to \( x_\mu \rightarrow \tilde{x}_\mu = x_\mu \) i.e. when \( R_\mu = 0 \), in which case the reversed process coincides with the direct process (see Barra et al. (1995) for a discussion). On the other hand, in Ryter (1987) the decomposition (39) of the drift arises through the definition for a diffusion process of an associated system. This last system is the reversed process considered here and this fact gives a very intuitive understanding of the results in Jauslin, 1985; Ryter, 1987.

We consider now a general Markov process with conditional probability density \( P_+(x, t|x', t') \) obeying (5) (we omit \( \sigma \) from now on since it plays no role). In Section 2, we constructed a new process with conditional probability \( P_+(x_\mu, t|x', t; \lambda) \) obeying (15) which was in GDB with respect to \( x \rightarrow \tilde{x} = x_\mu \lambda \rightarrow \tilde{\lambda} = -\lambda \). The kernel (see (16)) of this process was (we now write \( \Gamma(x|y) \) instead of \( \Gamma(x,y) \))

\[
\Gamma(x|y; \lambda) = \frac{1}{2} \left[ \Gamma(x|y) + \Gamma^R(x|y) \right] + \frac{1}{2} \left[ \Gamma(x|y) - \Gamma^R(x|y) \right]
\]

(46)

Let \( \tilde{\Gamma} \) be the stochastic matrix

\[
\begin{pmatrix}
-\alpha & \alpha \\
\alpha & -\alpha
\end{pmatrix}, \quad 1 > \alpha > 0
\]

(47)

and \( \lambda(j) \) the function \( \lambda(1) = 1, \lambda(2) = -1 \). We define the kernel

\[
\Gamma(x,j|y;k) = \delta_{jk} \Gamma(x|y; \lambda(j)) + \delta(x-y) \Gamma_{jk}
\]

(48)

where \( j \) and \( k \) take values in \( \{1, 2\} \) and \( \Gamma_{jk} \) are the matrix elements of \( \tilde{\Gamma} \). This kernel defines by

\[
\frac{\partial}{\partial t} P_+(x,j,t|x',j',t') = \sum_{k=1}^{2} \int \Gamma(x,j|y,k) P_+(y,k,t|x',j',t')
\]

(49)

a Markov process with state space \( (x,j) \) where \( x \) is a vector in \( \mathbb{R}^d \) and \( j \) take integer values in \( \{1, 2\} \). The stationary probability of this process will be \( \rho(x,j) = \rho_1(x) \rho_2(j) \) where \( \rho_1(x) \) is the stationary probability of the initial process with kernel \( \tilde{\Gamma}(x|y) \) and \( \rho_2(1) = \rho_2(2) = \frac{1}{2} \) (\( \rho_2(j) \) is the stationary probability of the Markov process taking discrete values which is defined by the kernel \( \Gamma_{jk} \)). We define the time-reversal transformation of the discrete variable \( j \) as \( (1 \rightarrow 1, 2 \rightarrow 2) \) which implies \( \lambda(j) = -\lambda(j) \). It is easy to check that the reversed process \( P_{R}(x,j,t|x',j',t') \) will have the kernel

\[
\Gamma^R(x,j|y,k) = \delta_{jk} \Gamma(x|y; -\lambda(j)) + \delta(x-y) \Gamma_{jk}
\]

(50)

which satisfies \( \Gamma^R(x,j|y,k) = \Gamma(x,j|y,k) \) and then the process (49) is in DB with respect to \( (x \rightarrow \tilde{x} = x_\mu, 1 \rightarrow 2, 2 \rightarrow 1) \). We now have an interpretation of the construction of the process with kernel \( \Gamma(x,j,y; \lambda) \) given by (46) in terms of \( P_+(x,j,t|x',j',t) \) defined by (49) which tells us that if we start in (49) with an initial condition \( j = 1 \) (then \( \lambda(j) \) in (48) is 1) the system will evolve for a time \( O(t \approx x^{-1}) \)
as the initial system with kernel $\Gamma(x|y)$ (see (46)), then $j$ will jump to $j=2$, $\lambda(j=2) = -1$, and the system will evolve with $\Gamma^k(x|y)$ for a time $O(\tau)$ and so on. If $\tau$ is much greater than the characteristic times of the initial system with kernel $\Gamma(x|y)$, the process (49) will be in a metastable state with $\lambda = 1$, i.e. it will behave as the initial system and arrive to a pseudo-stationary state with stationary probability $\rho_1(x)$, before $j$ jumps to $j=2$. The complete process (49) is in DB but with respect to the stationary probability $\rho(x,j) = \rho_1(x)\rho_2(j) = \frac{1}{2}\rho_1(x)$, which means in particular $\langle \lambda(t) \rangle^n = 0$ and we are in the same situation we have described for diffusion processes when we added equation (27) for $\lambda(t)$ with $B_{\lambda+1}(\lambda)$ given by (30).

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References


Appendix

We shall see here that if the system with conditional probability $P_\sigma(x, t|x', t'; \sigma)$ is not in GDB with respect to the time-reversal transformation $(x \rightarrow x \neq x, \sigma \rightarrow \delta \neq \sigma)$, it is again possible to construct a new process in GDB adding odd parameters. This is a generalization of Section 2 where the transformation was the identity (all variables and parameters were even). We consider first the case where $(\rho(x, \sigma)$ is the stationary probability)

$$\rho(x, \sigma) = \rho(x, \delta)$$  (A1)

and define a second reversed process with conditional probability

$$P_{\delta}(x, t|x', t'; \sigma) \equiv P_\sigma(x, -t|x', -t'; \sigma)$$  (A2)

which implies

$$P_{\delta}(x, t|x', t'; \sigma) = P_\sigma(x', t|x, t'; \delta) \frac{\rho(x, \sigma)}{\rho(x', \sigma)}$$  (A3)
the kernel is
\[ \Gamma^R(x, x'; \sigma) = \Gamma(x', x; \sigma) \frac{\rho(x, \sigma)}{\rho(x', \sigma)} \] (A4)
using \( \Gamma^R \) we construct now a new process with kernel
\[ \Gamma(x, x'; \sigma, \lambda) = \frac{1}{2}(\Gamma(x, x'; \sigma) + \Gamma^R(x, x'; \sigma)) + \lambda \left( \Gamma(x, x'; \sigma) - \Gamma^R(x, x'; \sigma) \right) \] (A5)
where \( \lambda \) is an odd parameter under time reversal. If one now calculates the first reversed process of (A5) (the one defined in Section 2) one checks that
\[ \Gamma^K(x, x'; \sigma, \lambda) = \Gamma(x, x; \sigma, \lambda) \] (A6)
and then the process is in GDB (see (14)) with respect to \( (x \to x, \sigma \to \sigma, \lambda \to -\lambda) \).
We consider now the case where (A1) is not verified, i.e. \( \rho(x, \sigma) \neq \rho(x, \sigma) \). We separate the variables \( (x_1, \ldots, x_n) = (x_1, \ldots, x_p, x_{p+1}, \ldots, x_n) \) with \( \{x_j, j = 1, \ldots, p\} \) odd and the rest even, and for the parameters \( (\sigma_1, \ldots, \sigma_p, \sigma_{k+1}, \ldots, \sigma_n) \) we take the first \( k \) as odd and the rest even. The next step is to look at the minimal number of odd variables and parameters which one would have to make even in order to have \( \rho(x, \sigma) = \rho(x, \sigma) \). Let \( (x_1, \ldots, x_p) \) and \( (\sigma_1, \ldots, \sigma_m) \), \( q \leq p, m \leq k \), be these variables and parameters (the choice is not necessarily unique). We then introduce \( q + m \) odd parameters \( (\lambda_1, \ldots, \lambda_q, \mu_1, \ldots, \mu_m) \) and we define
\[ \tilde{P}_+(x, t|x', t'; \sigma, \{\lambda_j\}, \{\mu_j\}) = \prod \left[ \lambda_j \right] P_+(\lambda_1 x_1, \ldots, \lambda_q x_q, x_{q+1}, \ldots, x_n, \right. \\
\left. t|\lambda_1 x_1', \ldots, \lambda_q x_q', x_{q+1}', \ldots, x_n', t'; \mu_1 \sigma_1, \ldots, \mu_m \sigma_m, \sigma_{m+1}, \ldots, \sigma_1) \] (A7)
If \( \tilde{\rho}(x, \sigma, \lambda, \mu) \) is the stationary probability corresponding to \( \tilde{P}_+ \) obtained taking the limit \( (t \to \infty) \) one has that (A1) is now verified since by construction
\[ \tilde{\rho}(x, \sigma, \lambda, \mu) = \tilde{\rho}(x, \sigma, \lambda, \mu) \]
and we can then proceed as before adding one more odd parameter \( \lambda \) as in (A5).