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On an interpolation model for the transition operator for Markov and non-Markov processes

V BALAKRISHNAN
Reactor Research Centre, Kalpakkam 603 102

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Abstract. A phenomenological interpolation model for the transition operator of a stationary Markov process is shown to be equivalent to the simplest difference approximation in the master equation for the conditional density. Comparison with the formal solution of the Fokker-Planck equation yields a criterion for the choice of the correlation time in the approximate solution. The interpolation model is shown to be form-invariant under an iteration-cum-rescaling scheme. Next, we go beyond Markov processes to find the effective time-development operator (the counterpart of the conditional density) in the following very general situation: the stochastic interruption of the systematic evolution of a variable by an arbitrary stationary sequence of randomizing pulses. Continuous-time random walk theory with a distinct first-waiting-time distribution is used, along with the interpolation model for the transition operator, to obtain the solution. Convenient closed-form expressions for the 'averaged' time-development operator and the autocorrelation function are presented in various special cases. These include (i) no systematic evolution, but correlated pulses; (ii) systematic evolution interrupted by an uncorrelated (Poisson) sequence of pulses.

Keywords. Markov processes; transition operator; interpolation model; continuous-time random walk; pulse sequences; non-Markov processes.

1. Introduction

The effects of random fluctuations in a very large variety of physical problems are studied by modelling the fluctuations in terms of Markov processes. A vast literature exists on the latter subject (see, e.g., Stratonovich 1963). In this paper we demonstrate certain interesting and useful properties of a very convenient approximate solution to the master equation for the conditional probability density of a Markov process. Subsequently, we construct also the conditional density for non-Markov processes (i.e., those with memory) corresponding to the same form of the transition operator as in the earlier instance. For notational simplicity, we consider a single-component, stationary random process $\xi(t)$.

If $\xi(t)$ is a stationary Markov process, it is characterised by its two-point conditional probability density $P(\xi, t \mid \xi_0)$. This quantity obeys the well-known Chapman-Kolmogorov equation

$$P(\xi, t \mid \xi_0) = \int d\xi_1 \, P(\xi, t-t_1 \mid \xi_1) \, P(\xi_1, t_1 \mid \xi_0), \; (0 < t_1 < t), \tag{1}$$

a summation instead of integration being understood in the case of a discrete random variable. In terms of $w(\xi \mid \xi_1)$, the transition probability per unit time for the random

variable to jump from the value ξ_1 to the value ξ, the Markov property is embodied in the master equation

$$\frac{\partial}{\partial t} P(\xi, t \mid \xi_0) = \int d\xi_1 [w(\xi \mid \xi_1) P(\xi_1, t \mid \xi_0) - w(\xi_1 \mid \xi) P(\xi, t \mid \xi_0)]. \tag{2}$$

In many applications involving a continuous variable ξ, it is customary to convert (2) to a partial differential equation with the aid of a systematic Kramers-Moyal expansion (Kramers 1940; Moyal 1949; Van Kampen 1961, 1977; Pawula 1967; Haken 1975). With the identification of a proper expansion parameter, it is possible to justify the truncation of the Kramers-Moyal series at the second term, and a generalised Fokker-Planck equation for P results. (ξ is then called a *continuous* Markov process). Attention then shifts to the solution of this equation.

Returning to the general equations (1) and (2), it is often convenient to use an operator notation of the following sort: let $\mid \xi)$ denote a ' stochastic state ' corresponding to the fact that the random variable has a value ξ, so that $P(\xi, t \mid \xi_0)$ is simply the matrix element of a time-dependent operator $\mathscr{P}(t)$:

$$P(\xi, t \mid \xi_0) \equiv (\xi \mid \mathscr{P}(t) \mid \xi_0). \tag{3}$$

Equation (2) is then transcribed as

$$\partial \mathscr{P}(t)/\partial t = W \mathscr{P}(t), \tag{4}$$

with the formal solution

$$\mathscr{P}(t) = \exp(Wt) \tag{5}$$

corresponding to the initial $P(\xi, 0 \mid \xi_0) = \delta(\xi - \xi_0)$. The operator W is sometimes called the ' relaxation matrix ', especially in the context of line-shape problems (Anderson 1954; Kubo 1954). Physical arguments enable one to model W directly in many instances, and hence obtain what is essentially a stochastic Liouville operator describing the evolution of the sub-system of interest when the latter is coupled to a ' bath ' comprised of a very large number of degrees of freedom. Depending on the specific situation, a satisfactory approximation to the effective time-development operator $\mathscr{P}(t)$ may be found thus, without necessarily solving what may be a complicated Fokker-Planck equation. Such approximations are familiar, for instance, in the theory of the collision broadening of spectral lines (see Rautian and Sobel'man 1967; Ben Reuven 1966, 1975 and references therein; Dattagupta 1977), extended rotational diffusion models for molecular motions in liquids (Gordon 1966), etc.

First, the random process is regarded as a chain made up of primary events or ' collisions ' (i.e., a Poisson sequence of pulses) occurring at a mean rate λ, so that

$$W = \lambda(\mathscr{T} - \mathbf{1}) \tag{6}$$

where $\mathbf{1}$ is the unit operator and $\mathscr{T}$ is called the collision or transition operator that changes the stochastic state. Conservation of probability implies that

$$\int d\xi (\xi \mid \mathscr{T} \mid \xi_0) = 1. \tag{7}$$

Further, detailed balance requires that

$$p(\xi_0)\,(\xi|\mathcal{T}|\xi_0) = p(\xi)\,(\xi_0|\mathcal{T}|\xi), \tag{8}$$

where $p(\xi)$ is the stationary probability density corresponding to the random variable ξ. In the context of systems in equilibrium, we have also

$$\lim_{t\to\infty} P(\xi, t|\xi_0) = p(\xi). \tag{9}$$

(In many cases of physical interest, ξ is also a Gaussian process. In the familiar instance of a free Brownian particle, for example, ξ is the velocity of the particle, $p(\xi)$ is the Maxwellian distribution with zero mean and variance $k_B T/m$, and is the asymptotic limit of the solution of the simplest Fokker-Planck equation—namely, the Ornstein-Uhlenbeck process—Ornstein and Uhlenbeck 1930; Wang and Uhlenbeck 1945.) In the no-collision *limit*, $\mathcal{T}$ is simply the unit operator. Next comes the weak-collision *approximation*, in which each collision is assumed to alter the pre-collision value of ξ only infinitesimally. This leads to the Fokker-Planck equation for $P(\xi,t|\xi_0)$, with the initial condition as already stated. At the other extreme is the '*strong-collision approximation*', in which it is assumed that the distribution 'equilibriates' so rapidly that it loses all memory of the pre-collision value of the variable: in other words,

$$(\xi|\mathcal{T}|\xi_0) \simeq p(\xi), \tag{10}$$

the right-hand side being the only ξ_0-independent function that satisfies (8). Substituting in (6) and carrying out the exponentiation required by (5), the solution obtained is

$$P(\xi, t|\xi_0) = \delta(\xi-\xi_0)\exp(-\lambda t) + p(\xi)\,[1-\exp(-\lambda t)]. \tag{11}$$

It is evident (from the exponential form of (5) itself) that this expression satisfies the Chapman-Kolmogorov equation (1). It is also the simplest functional form expressing the decay of the initial 'state' and the simultaneous approach to the equilibrium distribution. An improvement over the approximation (10) is afforded by the class of *interpolation models* (Fixman and Rider 1969; Dattagupta and Sood 1979), in which one assumes that

$$(\xi|\mathcal{T}|\xi_0) = \gamma p(\xi) + (1-\gamma)\,\delta(\xi-\xi_0),\ (0<\gamma<1). \tag{12}$$

Thus the primary transition operator *itself* is taken to be an interpolation between the initial and asymptotic distributions. The interesting point is that the corresponding conditional probability works out now to

$$P(\xi, t|\xi_0) = \delta(\xi-\xi_0)\exp(-\gamma\lambda t) + p(\xi)\,[1-\exp(-\gamma\lambda t)]. \tag{13}$$

This means that the interpolation (12) has merely rescaled the effective correlation time to a larger value, from λ^{-1} to $(\lambda\gamma)^{-1}$. Though simple, this device often turns out

to be effective when confronted with experimental data in various applications, such as those referred to in the foregoing.

This paper is concerned with the following formal aspects. First, we show how the interpolation model (equations (12) and (13)) amounts to nothing more than the simplest possible difference approximation in an appropriate version of the master equation. We comment on the nature of the solution *vis-a-vis* the solution of the Fokker-Planck equation, and point out that the interpolation model can be understood also as a certain weighted averaging over all the ' relaxation modes ' of the system. Second, we demonstrate in two alternative pictures an invariance of the interpolation model under iteration and rescaling. Next, we go beyond Markov processes and consider a general problem: if the variable $\xi(t)$ evolves deterministically, but with stochastic interruptions by a (possibly correlated) sequence of pulses that randomise the value of the variable, what is the effective time-development operator equal to? An answer is obtained by means of a continuous-time random walk method. For correlated (non-Poisson) pulse sequences, a distinct first-waiting-time distribution must be used; this is taken care of. The case of a purely random process (no deterministic evolution) is a special case of the general result. So is the case when the pulse sequence is an uncorrelated one. In this instance we present also expressions of practical utility for the ' averaged ' time-development operator and the autocorrelation function. Finally, we explain why the interpolation model does not correspond to a mere rescaling of the pulse rate in the strong collision model in most cases of physical interest.

2. The interpolation model as a difference approximation

In general, the master equation (4) describes the evolution from a given initial distribution to an asymptotic stationary distribution. The 'relaxation' may occur with a whole set of characteristic time scales. On the other hand, if we change variables from t to $z=\exp(-\mu t)$, Re $\mu>0$, the physical range of variation of t is made compact (the end points are $z=0$, 1). Denoting the operator $\mathscr{P}(t)$ by $Q(z)$, it is then tempting to make the extremely simple difference approximation*

$$\partial Q(z)/\partial z \approx Q(1) - Q(0), \tag{14}$$

regardless of what the right-hand side of (4) is (it will of course decide the best value of μ). The interpolation model is just this! Integration of (14) trivially yields

$$Q(z) = (1-z)\, Q(0) + z\, Q(1). \tag{15}$$

Reverting to the variable t, and taking appropriate matrix elements, this is equivalent to

$$P(\xi, t \mid \xi_0) = \delta(\xi-\xi_0) \exp(-\mu t) + p(\xi)\,[1-\exp(-\mu t)]. \tag{16}$$

*Since $\partial/\partial t \to -\mu z\, \partial/\partial z$, note that the z-independence of the right-hand side in (14) will not immediately lead to an inconsistency. For any other mapping of the range $t \geqslant 0$ to the interval [0, 1] —e.g., by a change of variables to $\tanh \mu t$—this will no longer be the case. This practically dictates the choice $z=\exp(-\mu t)$.

It is then not difficult to use (5) and (6) to show that the corresponding $\mathcal{T}$-matrix element is

$$(\xi \mid \mathcal{T} \mid \xi_0) = (\mu/\lambda)\, p(\xi) + (1-\mu/\lambda)\, \delta(\xi-\xi_0), \tag{17}$$

which is essentially (12). In the form of the ansatz (14), there is no mystery left in this approximation.

At this juncture it is pertinent to dispose of a question that arises. We have already said that the expression (16) satisfies the Chapman-Kolmogorov equation (1). Further, if $\langle \xi \rangle = 0$, it is trivially verified from (16) that

$$\langle \xi(t)\, \xi(t+\tau) \rangle = \langle \xi^2 \rangle \exp(-\mu\, \tau). \tag{18}$$

One might therefore wonder whether there is a conflict with Doob's theorem (Doob 1942): a (one-dimensional) stationary, Gaussian-Markov process is necessarily exponentially correlated, as in (18), and the corresponding $P(\xi, t \mid \xi_0)$ *must* be the Ornstein-Uhlenbeck distribution, which (16) clearly is not. The answer is that the approximation of the interpolation model makes the random process non-Gaussian. In addition, mere inspection shows that the inclusion of $\delta(\xi - \xi_0)$ in the density itself (and not merely as a boundary value as $t \to 0$) takes us out of the class of twice-differentiable density functions.

How is μ related to W? For a continuous Markov process, the answer is easy to find. We may compare the simple functional form in (16) with the exact solution of the Fokker-Planck equation. The latter depends on the boundary conditions relevant to the problem concerned, but in many cases it can be expressed in the form (Stratonovich 1963)

$$P(\xi, t \mid \xi_0) = (1/p(\xi_0)) \sum_{n=0}^{\infty} X_n(\xi) X_n(\xi_0) \exp(-\lambda_n t). \tag{19}$$

Here $\{\lambda_n\}$ are the eigenvalues and $\{X_n(\xi)\}$ are the eigenfunctions, orthonormalised with weight $1/p(\xi)$, of the second-order differential operator representing W. Further, the eigenfunction corresponding to the eigenvalue $\lambda_0 = 0$ is $X_0(\xi) = p(\xi)$. Now the interpolation model (i.e., (16)) is nothing other than the replacement of

$$\sum_{n=1}^{\infty} X_n(\xi)\, X_n(\xi_0) \exp(-\lambda_n\, t) \text{ by } \exp(-\mu t) \sum_{n=1}^{\infty} X_n(\xi) X_n(\xi_0), \tag{20}$$

as can be verified with the help of the completeness relation for $\{X_n\}$. In a sense, (20) may be regarded as an averaging* over the non-zero eigenvalues of W, to obtain an

*Ignoring some technicalities, one may note that, if $\lambda_n \propto n$, the prescription

$$\sum_1^{\infty} c_n \exp(-nx) \Big/ \sum_1^{\infty} c_n \to \exp(-\mu x) \text{ is equivalent to saying that}$$

$$\sum_1^{\infty} c_n\, n^{-a} \Big/ \sum_1^{\infty} c_n \to \mu^{-a} \ (\mathrm{Re}\, a > -1),$$

which gives an ' average ' value of the *index* n.

effective eigenvalue μ. Of course (20) is no more than an *approximation*; it is *not* an equation between two different functions of t, ξ and ξ_0. However, it is possible to specify an appropriate value for μ if we are primarily concerned with the random process upto the level of its autocorrelation function. The correlation time of the random process is μ^{-1} in the interpolation model. Equating this to the exact correlation time for the Markov process described by (19), we get the following criterion for the choice of μ:

$$1/\mu = \sum_{n=1}^{\infty} (h_n^2/\lambda_n) \Big/ \sum_{n=1}^{\infty} h_n^2 , \tag{21}$$

where $$h_n = \int d\xi \, X_n(\xi)\xi . \tag{22}$$

For the ordinary Fokker-Planck equation satisfied by the conditional density of the velocity of a Brownian particle in one dimension, $\lambda_n = n\beta$, where β is the drift coefficient or friction constant. Also $h_n=0$ for $n \geqslant 2$ in this case, so that the choice $\mu=\beta$ is the correct one.

3. Form invariance of the interpolation model

3.1. *One form of the invariance*

We have already seen that a transition operator with matrix elements

$$(\xi \mid \mathcal{T} \mid \xi_0) = \gamma p(\xi) + (1-\gamma)\, \delta(\xi - \xi_0), \tag{12}$$

when ' pulsed ' at a rate λ leads to a Markov process with conditional density

$$(\xi \mid \mathcal{P}(t) \mid \xi_0) = \delta(\xi - \xi_0) \exp(-\mu t) + p(\xi)[1 - \exp(-\mu t)], \tag{16}$$

where $\mu=\gamma\lambda$. The correlation time for this process is $\tau_c=\mu^{-1}$. Now let us effect a coarse graining as follows. We shall use the $\mathcal{P}(t)$ of (16) to construct a new Markov process with a scaled-up correlation time $q\tau_c$. The quantity $(\xi \mid \mathcal{P}(t=q\tau_c) \mid \xi_0)/q\tau_c$ is to be regarded as the matrix element of a second transition operator $\mathcal{T}'$ which, pulsed at the scaled-down rate λ/q, will lead to the required process. That is, we make the identification

$$(\lambda/q)(\xi \mid \mathcal{T}' \mid \xi_0) = (\xi \mid \mathcal{P}(t=q\tau_c) \mid \xi_0)/q\tau_c. \tag{23}$$

Using $\lambda\tau_c = 1/\gamma$, we get

$$(\xi \mid \mathcal{T}' \mid \xi_0) = \gamma p(\xi)\, [1 - \exp(-q)] + \gamma\delta(\xi - \xi_0) \exp(-q) \tag{24}$$

To absorb the factor γ on the right-hand side, we must simultaneously rescale the

random variable ξ according to $\xi' = \xi/\gamma$, or $|\ \xi') = \sqrt{\gamma}\ |\ \xi)$. The form invariance of the interpolation model is then explicit, for we have

$$(\xi'\ |\ \mathcal{T}'\ |\ \xi_0') = \gamma' p'(\xi') + (1-\gamma')\ \delta\ (\xi'-\xi'_0), \tag{25}$$

where $$\gamma' = 1-\exp\ (-q) \tag{26}$$

and further*

$$p'(\xi') = p'(\xi/\gamma) \equiv \gamma p(\xi). \tag{27}$$

We may now construct the operator

$$\mathcal{P}'(t) = \exp\ [\lambda(\mathcal{T}'-1)/q], \tag{28}$$

describing a Markov process with correlation time $\tau'_c = q\tau_c$. This process can be repeated, and we find

$$(\xi^{(n)}\ |\ \mathcal{T}^{(n)}\ |\ \xi_0^{(n)}) = \gamma^{(n)}\ p^{(n)}\ (\xi^{(n)}) + (1-\gamma^{(n)})\ \delta(\xi^{(n)}-\xi_0^{(n)}), \tag{29}$$

where $$\xi^{(n)} = \xi^{(n-1)}/\gamma^{(n-1)},\ p^{(n)}(\xi^{(n)}) = \gamma^{(n-1)}\ p^{(n-1)}\ (\xi^{(n-1)}),$$

but $$\gamma^{(n)} = \gamma^{(n-1)} = \ldots = \gamma'' = \gamma' = 1-\exp\ (-q). \tag{30}$$

Thus, whatever the value of γ one begins with, the interpolation model is invariant in the sense described above. Indeed, the starting point (12) is itself quite likely to be an intermediate stage in the coarse graining or iteration of some primitive transition operator, in which case γ ought to be identified with $[1-\exp\ (-q)]$, where q is the scaling factor.

3.2. *An alternative form of the invariance*

The invariance exhibited in the foregoing shows that there is nothing fundamental about the particular value of γ that we may happen to start with in writing down $\mathcal{T}$ in the interpolation model. On the other hand, the pulsing rate λ is evidently connected closely to the dynamical properties of the specific system under consideration. To name a few instances, it is directly related to the mean rate of molecular reorientations, or velocity changes, or frequency modulation, or jumps in jump diffusion, and so on. Therefore one may argue that it is λ^{-1} which ought to be regarded as the basic correlation time τ_c, instead of $(\lambda\gamma)^{-1}$. If this point of view is adopted, the iteration scheme of § 3.1 gets modified. Equations (12), (16) and (23) remain unaltered; however, (23) now leads to

$$(\xi\ |\ \mathcal{T}'\ |\ \xi_0) = \gamma' p(\xi) + (1-\gamma')\ \delta\ (\xi-\xi_0), \tag{31}$$

*The prime in p' does not denote a derivative, of course. Note that if the range of ξ is $(-\infty, \infty)$ and $p(\xi) = (2\pi\sigma^2)^{-1/2}\ \exp\ (-\xi^2/2\sigma^2)$, then $p'(\xi')$ is again a Gaussian in ξ', with a rescaled variance σ^2/γ^2. For a general $p(\xi)$, (27) follows from the normalisation of the distribution.

where, in contrast to (26),

$$\gamma' = 1 - \exp(-\gamma q), \tag{32}$$

γ being the initial interpolation parameter and q the scaling factor, as before. Hence (31) is already in the interpolation-model form, no further re-scaling of ξ being necessary. Repeating the procedure, we obtain

$$(\lambda/q^2)(\xi \mid \mathcal{T}'' \mid \xi_0) = (\xi \mid \mathscr{P}'(t=q^2\tau_c) \mid \xi_0)/q^2\tau_c, \tag{33}$$

or

$$(\xi \mid \mathcal{T}'' \mid \xi_0) = \gamma'' p(\xi) + (1-\gamma'')\delta(\xi - \xi_0), \tag{34}$$

where

$$\gamma'' = 1 - \exp(-\gamma' q). \tag{35}$$

Repeated iteration of the construction therefore yields an effective interpolation parameter that obeys the recursion relation

$$\gamma^{(n+1)} = 1 - \exp(-q\gamma^{(n)}), \quad \gamma^{(0)} \equiv \gamma. \tag{36}$$

The fixed-point solution of this transformation is given by

$$\gamma^* = 1 - \exp(-q\gamma^*). \tag{37}$$

This is an interesting result. If the scaling factor $q=1$, we have $\gamma^*=0$, i.e., we approach the no-collision limit. For $1<q<\infty$, there exists a definite limiting value γ^* such that $0<\gamma^*<1$, and which is the optimal value to use in a phenomenological analysis involving macroscopic or coarse-grained variables, provided q is specified by other considerations. If $q\to\infty$, $\gamma^*\to 1$, i.e., the strong collision limit is attained.

Starting from the other end, if we *begin* with $\gamma=1$ (i.e., the strong collision approximation), the iteration or coarse graining causes a ' mellowing down ' of the approximation, and we are led to an interpolation form with the parameter γ^* as in (37). In either instance, the precise value of the scaling factor q has to be *selected*, presumably, on physical grounds appropriate to the particular problem under consideration.

4. Non-Markov processes

4.1. *Continuous-time random walk method*

In many applications, it is necessary to incorporate memory effects (also called probability after-effects), thus going beyond Markov processes. Higher conditional densities are no longer expressible entirely in terms of $P(\xi, t \mid \xi_0)$, but the latter quantity continues to be of importance—manifestly so at the level of the autocorrelation. However, the master equation (4) and its solution (5) no longer hold good. The question therefore arises: given a primitive transition operator $\mathcal{T}$, how does one construct the time development operator $\mathscr{P}(t)$, i.e., the conditional density?

A direct and powerful method of solving this problem is to use the continuous-

time random walk theory (Montroll and Weiss 1965; Montroll and Scher 1973; see also Stratonovich 1963). We shall use these ideas to set up the expression for $\mathscr{P}(t)$, omit the algebra, and quote the final answers. The Markovian result will emerge as a special case. The basic idea is to break up the time interval $(0, t)$ into sub-intervals specified by the points $t_1, t_2, \ldots, t_n$ at which the transition operator acts to change the stochastic state from one intermediate state to another, and to sum over all such chains possible. We shall also take into account the correct first-waiting-time distribution (Tunaley 1976). This is a crucial detail, as the pulse sequences $(t_1, \ldots, t_n)$ may not in all cases be uncorrelated.

If the stochastic state $|\ \xi)$ has just come into being at $t=0$, let $\phi(t)$ be the probability that the same state persists at time t. Thus $\phi(0)\equiv 1$ and $-\dot{\phi}(t)dt$ is the probability that a transition to some other state occurs in the interval $(t, t+dt)$. The first waiting time distribution is then given by (Feller 1966)

$$\phi_1(t) = \phi(t) \Big/ \int_0^\infty dt'\, \phi\,(t'), \tag{38}$$

while the probability of no transition occurring at all in the time interval from the randomly chosen origin of time up to the instant t is

$$\Phi\,(t) = 1 - \int_0^t dt'\, \phi_1\,(t'). \tag{39}$$

The conditional density may be developed then as the series

$$(\xi\,|\,\mathscr{P}(t)\,|\,\xi_0) = \Phi\,(t)\,\delta\,(\xi - \xi_0) + \sum_{n=1}^{\infty} \int_0^t dt_n \ldots \int_0^{t_2} dt_1\,(-1)^{n-1}\,\phi(t-t_n)\cdot$$

$$\dot{\phi}\,(t_n - t_{n-1}) \ldots \dot{\phi}\,(t_2 - t_1)\,\phi_1\,(t_1)\,(\xi\,|\,\mathfrak{I}^n\,|\,\xi_0). \tag{40}$$

It is natural to consider the Laplace transform of (40), because of its convoluted form (a consequence of the stationarity of the process). The summation over n can then be carried out and a formal operator solution for $\mathscr{P}(t)$ obtained (see, for example, Kehr and Haus 1978). We are interested, however, in the special case when $\mathfrak{I}$ is given by the interpolation model, equation (12). It is convenient to note that the operator $(\mathfrak{I}-1)$ can also be written then in the form

$$(\mathfrak{I} - 1) = \gamma\,(\mathfrak{I}_1 - 1), \tag{41}$$

where $\mathfrak{I}_1$ is the idempotent operator with matrix element

$$(\xi\,|\,\mathfrak{I}_1\,|\,\xi_0) = p\,(\xi)\,(\forall\ \xi_0). \tag{42}$$

Carrying out the algebra, we find finally that the Laplace transform of the required conditional probability density reads

$$(P\,(\xi, t\,|\,\xi_0))_s = (1/s)\,[1 - F(s)]\,\delta\,(\xi - \xi_0) + (1/s)\,F(s)\,p\,(\xi), \tag{43}$$

where $$F(s) = \gamma \tilde{\phi}(s) / \tilde{\phi}(0) \{\gamma + (1 - \gamma) s \tilde{\phi}(s)\}. \tag{44}$$

Here s is the transform variable and $\tilde{\phi}(s)$ is the Laplace transform of $\phi(t)$. Equations (43) and (44) represent the solution to our problem.

$\mathscr{P}(t)$ describes a Markov process when the pulses occurring at $t_1, t_2, \ldots, t_n$ constitute an uncorrelated Poisson sequence—*equivalently*, when $\phi(t)$ itself satisfies the equation $\phi(t) = \phi(t-t_1)\,\phi(t_1)$ for all $0 < t_1 < t$. In other words, when

$$\phi(t) = \exp(-\lambda t). \tag{45}$$

The symbol λ is used here advisedly, for it is exactly the same quantity as occurs in (6)*ff*. When (45) is used in (43) and (44), we find precisely the result quoted earlier for the Markovian case, namely, equation (13),

$$P(\xi, t \mid \xi_0) = \delta(\xi - \xi_0) \exp(-\gamma\lambda t) + p(\xi)\,[1 - \exp(-\gamma\lambda t)].$$

The solution (43) can be written also as a master equation involving a memory function. Again omitting the intermediate steps, we get

$$\frac{1}{\gamma}\frac{\partial}{\partial t} P(\xi, t \mid \xi_0) = \frac{p(\xi)}{\int_0^\infty dt'\,\phi(t')} - f(t)\,\delta(\xi - \xi_0)$$

$$- \int_0^t dt'\, K(t - t')\, P(\xi, t' \mid \xi_0), \tag{46}$$

where $f(t)$ is the inverse Laplace transform of

$$\tilde{f}(s) = [\tilde{\phi}(s) - \tilde{\phi}(0) + s\tilde{\phi}(0)\,\tilde{\phi}(s)]/s\tilde{\phi}(0)\,\tilde{\phi}(s), \tag{47}$$

and the kernel $K(t)$ is the inverse transform of

$$\tilde{K}(s) = [1 - s\tilde{\phi}(s)]/\tilde{\phi}(s). \tag{48}$$

Again, for $\phi(t)$ as in (45), $f(t)$ vanishes, while $K(t) = \lambda\delta(t)$, and the process becomes Markovian.

In the strong collision approximation, $\gamma = 1$, and the general solution (43) simplifies considerably. The result is expressed most compactly, and in an intuitively obvious form, in terms of the no-transition probability $\Phi(t)$ defined in (38) and (39). We find

$$P(\xi, t \mid \xi_0) = \delta(\xi - \xi_0)\,\Phi(t) + p(\xi)\,[1 - \Phi(t)], \tag{49}$$

where (for ready reference)

$$\Phi(t) = \int_t^\infty dt'\, \phi(t') \Big/ \int_0^\infty dt'\, \phi(t'). \tag{50}$$

The integration involved in going from the original waiting time distribution $\phi(t)$ to the no-transition probability $\Phi(t)$ ' smooths out ' the switching from the initial density $\delta(\xi-\xi_0)$ to the final one, $p(\xi)$. For the compact functions

$$\phi(t) = (1-\lambda t)^n\, \theta(1-\lambda t)\ (n = 0, 1, \ldots), \tag{51}$$

defined for $t \geqslant 0$, it is easy to show that

$$\Phi(t) = (1-\lambda t)^{n+1}\, \theta(1-\lambda t). \tag{52}$$

Thus we have (in the strong collision approximation)

$$P(\xi, t \mid \xi_0) = \begin{cases} \delta(\xi-\xi_0)\,(1-\lambda t)^{n+1} + p(\xi)\,[1-(1-\lambda t)^{n+1}], & (\lambda t<1) \\ p(\xi), & (\lambda t>1). \end{cases} \tag{53}$$

For the Gaussian distribution

$$\phi(t) = \exp(-\lambda^2 t^2), \tag{54}$$

one obtains similarly

$$P(\xi, t \mid \xi_0) = \delta(\xi-\xi_0)\ \mathrm{erfc}(\lambda t) + p(\xi)\ \mathrm{erf}(\lambda t). \tag{55}$$

When $\gamma < 1$, the corresponding expressions become considerably more complicated.

4.2. *Generalisation—Randomly interrupted systematic evolution*

The situation encountered most frequently in physical applications is a generalisation of the case considered in § 4.1. The variable $\xi(t)$ evolves deterministically, but with interruptions that alter its value in a random manner. The problem is to find the effective time-development operator $\mathscr{P}(t)$. Once again, the continuous-time random walk method provides the solution. We shall first give the formal solution in the general case, and then present some further results in the special case of uncorrelated interruptions.

Let the systematic (or deterministic) evolution of the variable $\xi(t)$ be governed by the Liouville operator L, so that a state at $t=0$ evolves in time t to

$$U(t) \mid \xi) \equiv \exp(iLt) \mid \xi). \tag{56}$$

Now suppose this evolution is stochastically interrupted by a pulse sequence with

waiting time distribution $\phi(t)$ and transition operator $\mathcal{T}$. The effective time-development operator is then a generalisation of (40) that reads

$$\mathcal{P}(t) = \Phi(t)\, U(t) + \sum_{n=1}^{\infty} \int_0^t dt_n \ldots \int_0^{t_2} dt_1\, (-1)^{n-1}\, \phi(t-t_n)\, U(t-t_n) \times$$

$$\times\, \dot{\phi}(t_n - t_{n-1})\, \mathcal{T} U(t_n - t_{n-1}) \ldots \dot{\phi}(t_2 - t_1)\, \mathcal{T} U(t_2 - t_1)\, \phi_1(t_1)\, \mathcal{T} U(t_1). \quad (57)$$

The formal solution for $\mathcal{P}(t)$ is compactly expressible in terms of its Laplace transform,

$$\tilde{\mathcal{P}}(s) = (\Phi U)_s + (\phi U)_s\, [1 + (\dot{\phi}\, \mathcal{T} U)_s]^{-1}\, (\phi_1\, \mathcal{T} U)_s, \quad (58)$$

where $$(\phi U)_s = \int_0^{\infty} dt\, \phi(t)\, U(t) \exp(-st), \text{ etc.} \quad (59)$$

Equation (58) is the desired result. Of course $[\mathcal{T}, U] \neq 0$ in general. It is not difficult to verify that the earlier result (43) is a special case of (58) that is obtained on setting $U(t) = 1$ and using the interpolation model for $\mathcal{T}$.

It is most interesting to see what happens in the case $\phi(t) = \exp(-\lambda t)$, i.e., when the deterministic evolution is interrupted by an uncorrelated randomising pulse sequence. One expects, intuitively, that the effective time-development operator will take the form $\exp(iL + W)\, t$. This is indeed borne out. Writing $(U(t))_s = \tilde{U}(s)$, we find that (58) reduces to

$$\tilde{\mathcal{P}}(s) = \tilde{U}(s + \lambda)\, [1 - \lambda\, \mathcal{T}\, \tilde{U}(s + \lambda)]^{-1},$$

$$= [1 - \lambda\, \mathcal{T}\, \tilde{U}(s + \lambda)]^{-1}\, \tilde{U}(s + \lambda), \quad (60)$$

where $$\tilde{U}(s + \lambda) = (s + \lambda - iL)^{-1}. \quad (61)$$

Therefore $$\tilde{\mathcal{P}}(s) = (s - W - iL)^{-1}, \text{ and } \mathcal{P}(t) = \exp(iL + W)\, t, \quad (62)$$

as conjectured, with $W = \lambda(\mathcal{T} - 1)$ as in (6). This result reproduces that of Clauser and Blume (1971).

Let us now insert the interpolation model for $\mathcal{T}$ in (60) or (62). In order to evaluate correlation functions, etc., in a form that is of practical utility, it is helpful to re-express (60) as follows. Now it is the $\mathcal{T}_1$ part of $\mathcal{T}$ that decouples the final and initial states in its matrix elements. One therefore aims at writing a Dyson equation for $\tilde{\mathcal{P}}$ in which $\mathcal{T}_1$ is the final factor on the right in the kernel. This is easily done, because

$$\tilde{\mathcal{P}}(s) = [\tilde{U}^{-1}(s+\lambda) - \lambda \mathcal{T}]^{-1},$$

$$= [\tilde{U}^{-1}(s+\lambda) - \lambda(1-\gamma)\mathbf{1} - \lambda\gamma\mathcal{T}_1]^{-1},$$

$$= [\tilde{U}^{-1}(s+\lambda\gamma) - \lambda\gamma\mathcal{T}_1]^{-1}. \quad (63)$$

It follows immediately that

$$\tilde{\mathscr{P}}(s)=\tilde{U}(s+\lambda\gamma)+\tilde{U}(s+\lambda\gamma)\lambda\gamma\mathfrak{I}_1\tilde{\mathscr{P}}(s), \tag{64}$$

the required operator equation. Note that if matrix elements are taken in (64), the operator $\mathfrak{I}_1$ on the right decouples the matrix element of $\tilde{\mathscr{P}}(s)$ from the other factors. This is the property of relevance in explicit calculations. As illustrations, let us present expressions for two objects that are required most often.

In certain applications, one asks for the ' averaged time-development operator ', or the quantity $\int d\xi\int d\xi_0(\xi|\mathscr{P}(t)|\xi_0)p(\xi_0)$. A common way in which this circumstance arises is as follows. Suppose the auto-correlation of a random variable $\zeta(t)$ is required, and that the stochastic properties of $\zeta(t)$ are specified by those of another, related process $\xi(t)$ as well as a (random) initial value $\zeta(0)$ that is independent of $\xi(t)$. For example, $\zeta(t)$ may be an angle (or a function of this angle), and $\xi(t)$ the corresponding angular velocity whose stochastic properties are given. This situation occurs in rotational diffusion (see, e.g., Dattagupta and Sood 1979). Another instance is the stochastic Liouville equation $\dot{x}(t)=i\omega(t)x(t)$ (Kubo 1963; Mori 1965) where the statistical properties of $\omega(t)$ are specified. (Example: Brownian motion of an oscillator treated as a problem in random frequency modulation.) Here ζ and ξ are to be identified with x and ω respectively. In all such instances, one may write

$$\langle\zeta(0)\,\zeta(t)\rangle=\langle\zeta(0)\,\mathscr{P}(t)\,\zeta(0)\rangle=(\zeta^2(0))_{\mathrm{av}}\,\langle\mathscr{P}(t)\rangle, \tag{65}$$

where the angular brackets on the right-hand side refer to a stochastic averge pertaining to the independent or underlying variable $\xi(t)$, whose randomness drives that in $\zeta(t)$. We can get a convenient formula for $\langle\mathscr{P}(t)\rangle$, or rather, its Laplace transform, from (64). Let $\tilde{U}_{\xi\xi'}$ denote $(\xi|\tilde{U}|\xi')$. Then

$$\begin{aligned}\langle\tilde{\mathscr{P}}(s)\rangle &\equiv \int d\xi\int d\xi_0\,(\xi|\tilde{\mathscr{P}}(s)|\xi_0)\,p\,(\xi_0),\\ &=\int d\xi\int d\xi_0\tilde{U}_{\xi\xi_0}(s+\gamma\lambda)\,p(\xi_0)/[1-\lambda\gamma\int d\xi\int d\xi_0\tilde{U}_{\xi\xi_0}(s+\lambda\gamma)p(\xi_0)].\end{aligned} \tag{66}$$

Next, let us give a formula for another frequently-sought quantity, the auto-correlation function

$$\langle\xi(0)\xi(t)\rangle\equiv\int d\xi\int d\xi_0\xi\xi_0(\xi|\mathscr{P}(t)|\xi_0)p(\xi_0). \tag{67}$$

We find for the corresponding Laplace transform the answer $(\langle\xi(0)\xi(t)\rangle)_s=A+B$,

where $$A=\int d\xi\int d\xi_0\xi\xi_0\tilde{U}_{\xi\xi_0}\,(s+\lambda\gamma)\,p(\xi_0),$$

$$B=\frac{\lambda\gamma[\int d\xi\int d\xi_0\xi\tilde{U}_{\xi\xi_0}(s+\lambda\gamma)p(\xi_0)]\,[\int d\xi\int d\xi_0\xi_0\tilde{U}_{\xi\xi_0}(s+\lambda\gamma)p(\xi_0)]}{1-\lambda\gamma\int d\xi\int d\xi_0\tilde{U}_{\xi\xi_0}(s+\lambda\gamma)p(\xi_0)}. \tag{68}$$

It is straightforward to generate similar formulas for other quantities of interest from (64). To name just one example, diffusion in a periodic potential is a problem

where such expressions are very helpful. A detailed theory of this phenomenon using random walk techniques will be presented separately.

An important remark is in order before we conclude this section. Since $W=\lambda(\mathfrak{J}-1)$ $=\lambda\gamma(\mathfrak{J}_1-1)$ (see (41)), one might get the impression that the interpolation model ($\gamma<1$) is *nothing more than a trivial re-scaling* ($\lambda\to\lambda\gamma$) of the strong collision model ($\gamma=1$). This impression is bolstered by the appearance of $\tilde{U}(s+\lambda\gamma)$ in (63) and all that follows subsequently. This conclusion is correct, provided *both* of the following sufficiency conditions are met: (1) The properties of the sub-system of interest are specified entirely by the single variable $\xi(t)$. (ii) The randomising pulse sequence is uncorrelated, i.e., $\phi(t)=\exp(-\lambda t)$. The latter condition is readily comprehended, in view of the complex possibilities buried in the general result (58). The former bears some explanation. In most physical problems, more than a single variable is involved. These may be directly or indirectly coupled, a fact which is reflected in the structure of the Liouville operator. Operations with respect to one variable may engender a change in the structure of the operator $\tilde{U}$ pertaining to *another* variable, such that it is no longer of the form (61), *even though the corresponding randomising pulses may yet be uncorrelated.* The final line in (63) does not then follow from the preceding one, i.e.,

$$\tilde{U}^{-1}(s+\gamma) - \lambda(1-\gamma)\,\mathbf{1} \neq \tilde{U}^{-1}(s+\lambda\gamma) \tag{69}$$

in such cases. A concrete example is essential. In the rotational diffusion problem referred to earlier (Dattagupta and Sood 1979), ξ corresponds to an angular velocity ω. However, the Liouville operator L has the structure ΩJ_y, where Ω is the part that acts in the ω-space, while J_y is a certain angular momentum operator acting in a vector space spanned by the set $\{|m\rangle\}$ of eigenstates of J_z. It turns out that only the diagonal, $m=0$, matrix elements of the various operators are of concern. Therefore the operator $\tilde{U}(s+\lambda)$ of relevance to the random variable ω is not $(s+\lambda-i\Omega J_y)^{-1}$, but rather $\langle 0|(s+\lambda-i\Omega J_y)^{-1}|0\rangle$. It is immediately evident that (69) applies in this case. How, then, does one proceed? The resolution is formally simple. It suffices to define an operator $\tilde{V}(s;\lambda,\gamma)$ according to

$$\tilde{V}^{-1}(s;\lambda,\gamma) = \tilde{U}^{-1}(s+\lambda) - \lambda(1-\gamma)\,\mathbf{1}. \tag{70}$$

All formulas from (63) to (68) then remain valid, with the replacement of $\tilde{U}(s+\lambda\gamma)$ by $\tilde{V}(s;\lambda,\gamma)$. It is evident that the interpolation model in this situation is no longer the mere replacement of λ by $\lambda\gamma$, even though the form $\phi(t)=\exp(-\lambda t)$ has been assumed.

5. Concluding remarks

We have identified the interpolation model as a simple difference approximation in the master equation, compared it with the exact solution of the generalised Fokker-Planck equation, and suggested a formal criterion for the choice of the effective relaxation time characterizing the model. We have also demonstrated the form

invariance of the solution under a certain scale transformation. Subsequently, a continuous-time random walk technique has been used to find the effective time-development operator (the counterpart of the conditional density) in the following general situation: the deterministic evolution of a variable interrupted by a stationary but otherwise arbitrary sequence of randomising pulses. Special cases such as no deterministic evolution, uncorrelated pulse sequences, etc. have been extracted from the general result. The formalism developed here suggests several avenues for further exploration, such as: improvements on the original difference approximation; integration of the difference approximation along complex paths in the z-plane instead of the real axis to obtain other types of effective time-development operators $\mathscr{P}(t)$; possible application of the scaling properties exhibited in § 3 to specific problems involving the successive enlargement of the degrees of freedom included in the 'sub-system' of interest; and a systematic extension of the theory in § 4 to multivariate case, incorporating also the interrupted evolution of the components via coupled deterministic equations. Finally, it is tempting to speculate on the utility of the interpolation model in the context of problems involving non-standard Fokker-Planck equations, such as optical bistability and chemical desorption. Progress in these instances has been restricted largely to the determination and study of the asymptotic distribution $p(\xi)$. Even a single parameter characterisation of the time-dependent solution, with an appropriately chosen value of the parameter μ, should bring out interesting properties of the systems concerned.

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