CONTINUOUS-TIME RANDOM WALK THEORY AND NON-EXPONENTIAL DECAYS OF CORRELATION FUNCTIONS

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1. Introduction

Relaxation, or approach to equilibrium, is customarily associated with a damped exponential time dependence. However, there are notable and interesting exceptions. In spin glasses, for example, the remanent magnetization M(t) exhibits a logarithmic fall-off of the form A-B log (λt). A similar behaviour has long been known in the case of rock magnetism, where it can be understood as originating from the occurrence of randomly dispersed magnetic clusters of varying sizes. The magnetic moments of these clusters face a whole spectrum of activation barriers to their re-orientation. This leads to a continuous superposition of conventional exponential relaxation functions. Thus M(t) takes the form $\int dE\ \rho(E) \exp[-\lambda(E)t]$, where $\rho(E)$ is some weight factor. If the standard Arrhenius form $\lambda_0 \exp(-E/kT)$ is assumed for the relaxation rate $\lambda(E)$, it is easily shown (e.g., by a change of integration variables from E to $\lambda(E)$) that M(t) has a logarithmic decay of the form referred to above.

The emergence of non-exponential relaxation (including power-law decays) from a continuous spectrum of exponentials is a rather general feature, common to numerous physical situations. With the help of the relaxation-response relationship underlying linear response theory, one may trace this back to a similar time-dependence for certain associated two-time correlation functions. The latter are frequently determined most conveniently by stochastic techniques, as this permits modelling closely guided by the physics of the problem (such as the identification of the relevant time scales, etc.) It is of interest, therefore, to identify the circumstances and modifications under which the random processes commonly used in physical applications can display a superposition of 'relaxation' times in their two-time correlation functions. For the sake of clarity, attention will be restricted to a single, scalar, stationary random process x(t), and its autocorrelation function.

This task may be approached in (at least) two different ways. In the first (described in Sec.2), one stays within the framework of Markov processes. After some brief remarks on the situation with respect to continuous Markov processes, we consider the simplest and most commonly employed jump processes (the dichotomic and the Kubo-Anderson process), and lead up to a generalization (the "kangaroo process") that has the desired property. The second approach is in many respects a more powerful and more generally applicable one : continuous-time random walk (CTRW) theory[1]. In Secs. 3 and 4, we describe the essentials of this theory, and show how time dependences of the kind referred to in the foregoing arise very naturally. We also exhibit a step-wise constant random process that is a non-Markovian generalization of the well known Kubo-Anderson process.

It must be mentioned that CTRW theory is a particularly appropriate technique for the investigation of diffusion and related phenomena in disordered materials. An extensive literature exists on this application [2]. A number of interesting questions of a technical nature arises in this connection, including the much-debated one on the correctness or otherwise of incorporating a first-waiting-time distribution that is distinct from the holding time distribution for the CTRW. We shall not be concerned here with any of these aspects. Our discussion should, however, be of some help also as an introduction to the analyses carried out in some of the papers listed under [2].

2. Some special Markov jump processes

It is common practice, on physical grounds, to model physical random variables in terms of Markov processes. In many applications, it is convenient to treat $x(t)$ as a continuous Markov process (a "diffusion" process), specified by the stationary probability density $W(x)$ and the conditional density $P(x,t|x_o)$. The latter obeys a generalized Fokker-Planck equation of the form

$$\frac{\partial}{\partial t} P(x,t|x_o) = -\frac{\partial}{\partial x}[A(x)P] + \frac{\partial^2}{\partial x^2}[B(x)P] \quad , \tag{1}$$

where $A(x)$ and $B(x)$ are the 'drift' and 'diffusion' coefficients, respectively. An extensive literature exists on the properties of such generalized Fokker-Planck equations. For our purpose, it suffices to note that the autocorrelation function

$$\begin{aligned} C(t) &= \langle x(o)\ x(t) \rangle \\ &= \int dx_o \int dx\ W(x_o)\ P(x,t\,|\,x_o)\ x x_o \end{aligned} \tag{2}$$

is a single exponential function provided certain conditions are satisfied [3]; namely, if

$$\lim_{t \downarrow o} P(x,t\,|\,x_o) = W(x) \tag{3}$$

(which is true in the context of systems in equilibrium); and if $B(x)$, $A(x)$ are respectively second and first order polynomials in x, together with the requirement that $B(x)\ W(x)$ vanish at the end points of the range of variation in x, and the condition that

$$\langle x \rangle = \int dx\ W(x)x \ , \quad \langle x^2 \rangle = \int dx\ W(x)x^2 \tag{4}$$

be finite. In other cases, $C(t)$ may be a discrete or partially continuous superposition of exponentials.

While continuous Markov processes are mathematically quite complicated to handle in general, in many physical applications it may be quite appropriate to treat $x(t)$ as a jump process that changes discontinuously from one value to another under the triggering action of a random pulse sequence. Let us consider some specific examples [4]. The simplest such process is the telegraph process or the dichotomic Markov process

(DMP). Here the variable $x(t)$ is step-wise constant, and can assume just two values, say $+\xi$ and $-\xi$. It is triggered from one value to another by a stationary Poisson pulse sequence with a (constant) mean pulse rate λ, i.e., the probability that exactly n pulses occur in a time interval t is given by

$$P(n,t) = \frac{(\lambda t)^n}{n!}\exp(-\lambda t) \ . \tag{5}$$

It is easy to see that the conditional density for the process $x(t)$ is given by

$$P(x,t|x_o) = [\delta(x-x_o) \cosh \lambda t + \delta(x+x_o) \sinh \lambda t] \exp(-\lambda t) \ , \tag{6}$$

where the initial value x_o can be either $+\xi$ or $-\xi$. The autocorrelation of x is given by

$$C(t) = \xi^2 \exp(-2\lambda t) \ , \tag{7}$$

a single exponential. A minor generalization of the above DMP allows $x(t)$ to take on the values ξ_1 and ξ_2, with different transition rates λ_{12} and λ_{21}. The condition

$$\lambda_{12}\ \xi_2 + \lambda_{21}\ \xi_1 = o \tag{8}$$

ensures that the mean $\langle x \rangle$ vanishes.

A non-trivial generalization of the DMP leads to the Kubo-Anderson process (KAP). This is again a stepwise constant Markov process, the jumps being triggered by a Poisson pulse sequence as before. However, the variable $x(t)$ is completely 'randomized' at each jump, and can take on any value characterized by a stationary probability density $W(x)$. Since the probability of zero pulses occurring in an interval t is $\exp(-\lambda t)$, it is easily seen that

$$P(x,t|x_o) = \delta(x-x_o) \exp(-\lambda t) + W(x) \quad 1-\exp(-\lambda t) \tag{9}$$

in this case. Hence, if $\langle x \rangle = o$, we again find the exponential behaviour

$$C(t) = \langle x^2 \rangle \exp(-\lambda t) \ . \tag{10}$$

To obtain a superposition of exponentials for $C(t)$, a further generalization of the KAP (still within the framework of stationary Markov processes) is needed. The transition-causing pulse rate λ may itself be a function of the current value of the random variable. If x happens to be far out in the tail of the distribution $W(x)$, for instance, one may intuitively expect the pulse rate $\lambda(x)$ to be considerably larger than its mean value, so as to bring x back towards more probable values more rapidly. The transition rate equation for such a Markov process reads

$$P_{tr}(x, \Delta t|x_o, o) = \delta(x-x_o) [1- \lambda(x_o) \Delta t] + \tilde{W}(x) \quad \lambda(x_o) \Delta t + 0 [(\Delta t)^2] . \tag{11}$$

Here $\tilde{W}(x)$ is a probability distribution that is distinct from, but related to, the distribution $W(x)$, as we shall see below. Equation (11) yields the master equation

$$\frac{\partial}{\partial t} P(x,t \mid x_o) = \lim_{\Delta t \downarrow o} \int dx_1 \left\{ P_{tr} \ (x,t + \Delta t \mid x_1, t) \ P(x_1, t \mid x_o) \right.$$

$$- P_{tr} (x_{1}, t + \Delta t | x,t) \; P(x,t|x_o) \Big\}$$

$$= - \lambda(x) \; P(x,t|x_o) + \tilde{W}(x) \int dx_1 \; P(x_1, t|x_o) \; \lambda(x_1) \; . \tag{12}$$

Using the limit (3) in Eq.(12), we obtain

$$\tilde{W}(x) = \lambda(x) \; W(x) \; / \langle \lambda \rangle \; , \tag{13}$$

where the mean rate $\langle \lambda \rangle$ is defined as

$$\langle \lambda \rangle = \int dx \; W(x) \;\; \lambda(x) \; . \tag{14}$$

It is also clear from Eq.(12) why one could not have simply written $W(x)$ instead of $\tilde{W}(x)$ in Eq.(11). The process described by Eq.(11) or Eq.(12) is called a "kangaroo process" (KP). It reduces trivially to the KAP if $\lambda(x) = \lambda$, a constant. The solution of Eq.(12) has the Laplace transform

$$\tilde{P}(x,s|x_o) = \frac{\delta(x-x_o)}{s+ \lambda(x)} + \frac{\lambda(x_o) \; \lambda(x) \; W(x)}{s(s+ \lambda(x_o))(s+ \lambda(x)) \; \langle \lambda(s+\lambda)^{-1} \rangle} \tag{15}$$

where

$$\langle \lambda(s+\lambda)^{-1} \rangle = \int dx \; W(x) \;\; \lambda(x) / [s+ \; \lambda(x)] \; . \tag{16}$$

For simplicity, let us assume that the range of x is $(- \infty , \infty)$, and that $\lambda(x)$, $W(x)$ are even functions of x. Then Eq.(15) leads to

$$C(t) = \int dx \; W(x) \; x^2 \; \exp \quad - \lambda(x) t \quad . \tag{17}$$

This is to be compared with Eq.(10) for a KAP. A change of integration variables from x to $\lambda(x)$ in Eq.(17), shows that a KP has a continuous superposition of 'relaxation times' in general. Among the physical applications of KP's, we may mention in particular the case of wave propagation in random media.

In most cases of practical interest, one works at the level of the first two moments, i.e., the mean and the autocorrelation function. The Markov assumption is therefore not very crucial. It can be sacrified in favour of a tractable generalization (such as CTRW) that provides greater flexibility in modelling in order to accommodate the underlying physics.

3. The continuous-time random walk method : construction of the pulse sequence

CTRW theory is useful whenever the random process of interest can be regarded as a stochastic sequence that is an ongoing 'renewal' process. Let us first obtain the statistics of the underlying pulse sequence, i.e., the probability $P(n,t)$ of n transition-causing pulses occurring in time t. In general, of course, this is not given by Eq.(5).

The holding time distribution $P(t)$ may be regarded as the fundamental quantity in a CTRW. This is the following conditional probability : given that a transition (jump) has just occurred at some epoch t_o, $p(t)$ is the probability that no further jumps have occurred till epoch t_o+t. Evidently, $p(o)\equiv 1$, $p(t_2)\leqslant p(t_1)$ if $t_2>t_1$, and $p(\infty)\to o$. The corresponding (conditional) transition probability that a jump does occur between (t_o+t) and (t_o+t+dt) is easily seen to be equal to $-\dot{p}(t)dt$. Further, the mean life-time of a 'state' of the random variable, i.e., the mean time between pulses or jumps, is therefore given by

$$\tau = \int_0^\infty dt\; t\,[-\dot{p}(t)] \,/ \int_0^\infty dt\,[-\dot{p}(t)] \;=\; \int_0^\infty dt\; p(t) \qquad (18)$$

Before the required distribution $P(n,t)$ can be constructed in terms of $p(t)$, it is necessary to take care of the first-waiting-time complication. The origin of time in the quantity $P(n,t)$ is arbitrary. Hence it would be incorrect to suppose that the probability for the first pulse (after the clock is started at this arbitrary origin, labelled $t=o$) to occur at epoch t is given by $-\dot{p}(t)dt$, for the latter is a <u>conditional</u> probability. It pre-supposes that the preceding pulse occurred exactly at $t = o$, whereas we have no way of knowing the precise epoch $t_o(\leqslant o)$ at which it did occur. As far as the first pulse in $P(n,t)$ is concerned, therefore, we require the <u>unconditional</u> counterpart of $-\dot{p}(t)$. Let us denote this transition probability by $-\dot{p}_o(t)$, in anticipation of the fact that its integral $p_o(t)$ is just the first-waiting-time distribution-the unconditional counterpart of $p(t)$. One can find $-\dot{p}_o(t)$ as follows. Let a pulse have occurred at epoch $t_o($ $o)$, and let the next pulse occur at epoch $t($ $o)$. The corresponding transition probability is $-\dot{p}(t-t_o)dt$. On the other hand, one may view the event as a two-step process, with an associated probability $p(-t_o)$ $-\dot{p}_o(t)dt$. The two quantities may be equated, provided we sum over all possible values of the epoch t_o. Thus

$$\int_{-\infty}^{0} dt_o\; [-\dot{p}(t-t_o)] = \int_{-\infty}^{0} dt_o\; p(-t_o)\;\; [-\dot{p}_o(t)] \quad , \qquad (19)$$

which yields the result

$$-\dot{p}_o(t) = (1/\tau)\; p(t) \quad . \qquad (20)$$

The associated first-waiting-time distribution is therefore

$$p_o(t) = (1/\tau) \int_t^\infty dt'\; p(t') \; . \qquad (21)$$

We are now in a position to write down the distribution $P(n,t)$ for the pulse sequence. Obviously,

$$P(o,t) \equiv p_o(t) \; . \qquad (22)$$

Further (and this clarifies the meaning of the term 'renewal' process), for $n \geqslant 1$,

$$P(n,t) = \int_0^t dt_n \ldots \int_0^{t_2} dt_1 (-1)^n\; p(t-t_n)\; \dot{p}(t_n-t_{n-1}) \ldots \dot{p}(t_2-t_1)\,\dot{p}_o(t_1) \; . \qquad (23)$$

It is immediately evident that if $p(t) = \exp(-\lambda t)$, we have $p_o(t) \equiv p(t)$. The first-waiting-time distribution is identical with the holding time distribution in this case. Further, Eq.(23) simplifies to yield the Poisson sequence of Eq.(5). While such an explicit reduction of $P(n,t)$ is not possible in general, it is easy to see that a compact expression obtains for the Laplace transform of $P(n,t)$, and for its generating function

$$H(z,t) = \sum_{n=0}^{\infty} P(n,t)\, z^n . \tag{24}$$

We find

$$\tilde{H}(z,s) = \frac{1}{s} + \frac{(z-1)\,\tilde{p}(s)}{s\,\tau[1 - z\{1 - s\tilde{p}(s)\}]} , \tag{25}$$

where $\tilde{p}(s)$ is the Laplace transform of $p(t)$. This completes the specification of the pulse sequence.

4. Jump processes in the CTRW formalism

With Eq.(25) at hand, an entire class of stepwise constant random processes can be investigated. It is convenient to use an operator notation : let $\mathcal{J}$ be the "collision" operator that changes the value of the random variable at each pulse. The matrix element $\mathcal{J}_{x \to x'}$ represents the transition probability for the variable to jump from the value x to the value x' under the action of a pulse. Similarly, let $\mathcal{P}(t)$ denote the effective time development operator whose matrix element $[\mathcal{P}(t)]_{x_o \to x}$ is simply the conditional density $P(x,t|x_o)$. Inserting the operator $\mathcal{J}$ at each pulse in the multiple integral of Eq.(23), one can construct $\mathcal{P}(t)$. It is evident that the formal operator solution for $\mathcal{P}(t)$ is just the inverse Laplace transform of

$$\tilde{\mathcal{P}}(s) = \tilde{H}(\mathcal{J}, s) , \tag{26}$$

i.e. one replaces z by the operator $\mathcal{J}$ in the expression quoted in Eq.(25). This solution is indeed one of considerable generality, given the flexibility in the choice of both $p(t)$ and $\mathcal{J}$.

A plausible, simple model for $\mathcal{J}$ is as follows. Instead of assuming that each pulse completely randomizes the variable $x(t)$, and throws it from its pre-pulse value x_o to an arbitrary, x_o-independent value in the stationary distribution $W(x)$, let us suppose that

$$\mathcal{J}_{x_o \to x} = \gamma W(x) + (1-\gamma)\ \delta(x-x_o), (o \leqslant \gamma \leqslant 1) . \tag{27}$$

In other words, this model interpolates [5,6] between a strong collision limit ($\gamma = 1$) that is in the spirit of the KAP and KP considered in the foregoing, and a weak collision limit ($\gamma = 0$) that does not alter the pre-pulse value. The required operator inversion can be carried out in this model for $\mathcal{J}$, and one obtains finally [6]

$$\tilde{P}(x,s|x_o) = \delta(x-x_o)\ \frac{[1-\tilde{F}(s)]}{s} + W(x)\ \frac{\tilde{F}(s)}{s} , \tag{28}$$

where

$$\tilde{F}(s) = \gamma\tilde{p}(s)/\tau[\gamma + (1-\gamma)\ s\tilde{p}(s)] . \tag{29}$$

Equation (28) is to be compared with Eq.(15) for a KP (and its special case, Eq.(9), for a KAP). Of course, Eq.(28) does not refer to a Markov process in general. Assuming as before that $\langle x \rangle = 0$, we now find for the autocorrelation function

$$C(t) = \langle x^2 \rangle [1 - \int_0^t F(t')\, dt'] = \langle x^2 \rangle \int_t^\infty dt'\, F(t') \quad , \tag{30}$$

where F(t) is the inverse Laplace transform of $\tilde{F}(s)$. This compact expression encompasses a very wide range of possible decays of C(t).

Comparison with the results for the KAP and the KP is facilitated by going over to the strong collision limit, $\gamma = 1$, in the above. As stated earlier, this is in keeping with the assumption inherent in the KAP and the KP. Equations (28) and (29) simplify in this limit, to yield

$$P(x,t|x_0) = \delta(x-x_0)\, p_0(t) + W(x)\, [1-p_0(t)] \quad . \tag{31}$$

If $p(t) = \exp(-\lambda t)$, i.e., if the pulse sequence is Poissonian, we recover the KAP. In other cases, one may regard Eq. (31) as a non-Markovian generalization of the KAP. The autocorrelation function becomes

$$C(t) = \langle x^2 \rangle p_0(t) = \langle x^2 \rangle (1/\tau) \int_t^\infty p(t')\, dt' \quad . \tag{32}$$

In particular, suppose the holding time distribution is a (continuous) superposition of exponentials :

$$p(t) = \int_0^\infty d\nu\, \sigma(\nu)\, \exp(-\nu t) \quad . \tag{33}$$

While this may arise in some cases from a distribution of activation barriers (as already mentioned), it is worth bearing in mind that Eq.(33) is in fact a fairly general representation, valid for a wide class of functions p(t). Using this representation in Eq.(32), we obtain

$$C(t) = \langle x^2 \rangle \int_0^\infty \frac{d\nu}{\nu}\, \sigma(\nu)\, \exp(-\nu t) \Big/ \int_0^\infty \frac{d\nu}{\nu}\, \sigma(\nu) \quad . \tag{34}$$

This is a (continuous) superposition of exponentials, as promised earlier. The actual t-dependence of C(t) is governed by the distribution $\sigma(\nu)$. The latter is directly amenable to physical modelling, perhaps more so than the rate $\lambda(x)$ in Eq. (17), with which the above result is to be compared. Indeed, at the level of the autocorrelation function, the non-Markov process described by Eq.(31) and the KP may be regarded as equivalent in some sense; and the distribution $\sigma(\nu)$ of Eq.(34) can be related to the functional $x^2\, W[x] / \lambda'[x]$, where $\lambda(x) = \nu$.

It remains to observe that the non-analytic (e.g., power law) behaviour that is frequently associated with a continuous range of relaxation times as in Eq. (34) is actually a general feature, independent of the model for the transition operator $\mathcal{T}$. In fact, the random process need not even be stepwise constant. To see this heuristically, consider Eq.(25) for the generating function of the pulse sequence. If the Laplace transform of the representation (33) is inserted for $\tilde{p}(s)$ in that equation, one obtains

$$\tilde{H}(z,s) = \frac{1}{s} + \frac{(z-1)\int_0^\infty \frac{d\nu\,\sigma(\nu)}{(s+\nu)}}{s\,\tau\left[1-z\int_0^\infty d\nu \frac{\sigma(\nu)}{(s+\nu)}\right]}, \tag{35}$$

where

$$\tau = \int_0^\infty d\nu\,\sigma(\nu)/\nu\ . \tag{36}$$

The integrals in Eq.(35) immediately suggest that $\tilde{H}(z,s)$ is singular at s=o . This is a consequence of the possible non-analyticity of $\tilde{p}(s)$ at the same point. More detailed remarks may be made if the properties of the distribution $\sigma(\nu)$ are specified. For instance, if $\int d\nu\,\sigma(\nu)/\nu^3$ diverges, then the small s expansion of $\tilde{p}(s)$ reads

$$\tilde{p}(s) \sim \tau + c_1\,s + c_2\,s^{\alpha} + \ldots\ldots\ldots, \tag{37}$$

where $1 < \alpha < 2$. Among other consequences, this sort of behaviour leads to a $1/f^{\alpha}$ current noise due to the random hopping of carriers in a disordered medium [7].

The simple formalism described above can be generalized in various directions. Some of these are : randomly interrupted deterministic evolution; multi-state renewal processes; quantum mechanical (operator) complications; etc. We conclude with the following comment. The emergence of "non-analytic behaviour" (e.g., power-law decays of correlations, critical exponents, cusps, singularities, and so on) from an underlying continuous spectrum in the problem is a rather universal phenomenon. Examples may be cited from Regge poles to rock magnetism. This "search for non-analyticity", in one form or another, may indeed be regarded as one of the central themes of contemporary theoretical physics.

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