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Generalized Master Equations for Continuous-Time Random Walks[1]

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An equivalence is established between generalized master equations and continuous-time random walks by means of an explicit relationship between $\psi(t)$, which is the pausing time distribution in the theory of continuous-time random walks, and $\phi(t)$, which represents the memory in the kernel of a generalized master equation. The result of Bedeaux, Lakatos-Lindenburg, and Shuler concerning the equivalence of the Markovian master equation and a continuous-time random walk with an exponential distribution for $\psi(t)$ is recovered immediately. Some explicit examples of $\phi(t)$ and $\psi(t)$ are also presented, including one which leads to the equation of telegraphy.

KEY WORDS: Generalized master equations; random walks; statistical mechanics; transport theory.

1. INTRODUCTION

A standard starting point for the discussion of various random walks and other transport processes is the master equation

$$d\tilde{P}(l,t)/dt = -\alpha\tilde{P}(l,t) + \alpha \sum_{l'\neq l} p(l,l')\,\tilde{P}(l',t) \tag{1}$$

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[1] For continuity, the reader is directed to the article entitled "Random Walks on Lattices. IV. Continuous Time Walks and Influence of Absorbing Boundaries," by E. W. Montroll and H. Scher, which will appear in Volume 9, Number 2, of this journal, and which should precede the following article. Regrettably, the two articles were inadvertently switched during processing.

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where $\tilde{P}(l, t)$ is the probability that a system of interest is in state l at time t and $\alpha p(l, l')$ is the probability per unit time of a transition from l' to l. Equation (1) is of course equivalent to the "gain–loss" form of the master equation

$$d\tilde{P}(l, t)/dt = \alpha \sum_{l'} [p(l, l') \tilde{P}(l', t) - p(l', l) \tilde{P}(l, t)] \tag{2a}$$

since transition probabilities have the normalization

$$\sum_{l'} p(l', l) = 1 \tag{2b}$$

We now interpret the states $\{l\}$ to be lattice points on a periodic space lattice and the system to be a random walker on the lattice. This intepretation is not necessary but it is made to give a direct contact with the results of Ref. 1. It was emphasized there that certain interesting random walks cannot be described by (1).

The basic quantity employed in the preceding paper is the pausing time distribution function $\psi(t)$ (the probability density function for the time t between the arrival of a walker at a given lattice point and the initiation of the next step to another site). All lattice points were postulated to be equivalent (periodic boundary conditions being used) so that $\psi(t)$ can be taken to be universal for all points. The methods of the preceding paper involve the random walk generating function which satisfies the Green's function equation [with $\tilde{P}(l, 0) = \delta_{l,0}$]

$$G(l, z) - z \sum_{l'} p(l - l') G(l', z) = \delta_{l,0} \tag{3a}$$

The form for $G(l, z)$ on a d-dimensional periodic lattice with $N \times N \times N \times \cdots$ lattice points in each direction (with periodic boundary conditions) is

$$G(l, z) = N^{-d} \sum_{\{s_j=1\}}^{N} \cdots \sum e^{ik.l}/[1 - z\lambda(k)] \tag{3b}$$

where $k_j = 2\pi s_j/N$ and $\lambda(k)$ is the so-called structure function

$$\lambda(k) = \sum_{l} p(l) e^{ik.l} \tag{3c}$$

The quantity $\tilde{P}(l, t)$ was shown to be related to $G(l, z)$ through the inverse Laplace transform formula[1,2]

$$P(l, t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{ut} du \{[1 - \psi^*(u)]/u\} G(l, \psi^*(u)) \tag{4}$$

where $\psi^*(u)$ is the Laplace transform of $\psi(t)$.

It was emphasized in Ref. 1 that Eq. (4) can be used to analyze processes which do not lie within the reach of the master equation (1); furthermore it has been shown by Bedeaux *et al.*[3] that when one chooses $\psi(t)$ to be an exponential distribution, expression (4) is identical to the solution of (1) that corresponds to the initial condition $\tilde{P}(l, 0) = \delta_{l,0}$. For no other form of $\psi(t)$ are the two expressions for $\tilde{P}(l, t)$ identical for all $t > 0$.

Generalized master equations have appeared naturally for non-Markovian processes associated with nonequilibrium phenomena.[4] They have the form

$$d\tilde{P}(l, t)/dt = \int_0^t d\tau \sum_j [K_{lj}(t-\tau)\,\tilde{P}(j, \tau) - K_{jl}(t-\tau)\,\tilde{P}(l, \tau)] \tag{5}$$

In the theory of nonequilibrium statistical mechanics the kernels $\{K_{lj}(t)\}$ are derived from dynamics. We shall not be concerned with those results but merely consider Eq. (5) to characterize certain stochastic processes.

The main result of this note is to establish an equivalence between generalized master equations such as (5) and continuous-time random walks characterized by (4).

2. THE EQUIVALENCE

Since in the special lattice walk with which we are concerned all lattice points are equivalent, the form of (5) appropriate for our walk would have kernels of the following type:

$$K_{lj}(t) \equiv \phi(t)\, p(l-j) \tag{6}$$

where $p(l)$ is just the transition probability which appears in (3a). Then (5) becomes

$$d\tilde{P}(l, t)/dt = \int_0^t \phi(t-\tau)[-\tilde{P}(l, \tau) + \sum_{l'}{}' p(l-l')\,\tilde{P}(l', \tau)]\, d\tau \tag{7}$$

where we have used the conservation of probability equation

$$\sum_{l'} p(l'-l) = 1$$

If initially the walker is at the origin so that $\tilde{P}_l(0) = \delta_{l,0}$, it is easily shown by taking Laplace transforms of (7) and comparing the resulting equation with (3) that, $\phi^*(u)$ being the Laplace transform of $\phi(t)$,

$$\tilde{P}(l, t) = (1/2\pi i) \int_{c-i\infty}^{c+i\infty} e^{ut}\, du\, \{[u + \phi^*(u)]^{-1}\, G(l, \phi^*/[u + \phi^*])\} \tag{8}$$

By comparing (8) and (4), it is evident that Eq. (7) is an appropriate characterization of the random walks described in Ref. 1 provided that one sets

$$\phi^*(u) = u\psi^*(u)/[1 - \psi^*(u)] \tag{9a}$$

which is equivalent to

$$\psi^*(u) = \phi^*(u)/[u + \phi^*(u)] \tag{9b}$$

If one sets $u = i\omega$, $\phi^*(u)$ is closely related to the frequency-dependent diffusion constant.[5] The reciprocal of $\phi^*(u)$ also appears naturally in the application of linear response theory to random walk transport.[6]

Note that $\psi(t)$ and $\phi(t)$ are related by the integrodifferential equation

$$d\psi/dt + 2\,\delta(t)\,\psi(0) = \phi(t) - \int_0^t \phi(\tau)\,\psi(t-\tau)\,d\tau \tag{10}$$

Note that the random walks described in Ref. 1 can also be characterized through the following equation provided $l \neq 0$:

$$\tilde{P}(l, t) = \int_0^t d\tau\,\psi(t-\tau)\sum_{l'} p(l-l')\,\tilde{P}(l', \tau) \tag{11}$$

This form of the equation can be easily established with the help of the preceding analysis and it shows how the introduction of the pausing time distribution function $\psi(t)$ brings about a generalization of the Chapman–Kolmogorov equation to non-Markovian situations.

3. SOME SPECIAL EXAMPLES

We now consider several special examples of the pausing time distribution function and find the differential equations appropriate to those $\psi(t)$. The first example will be chosen to yield the Markovian master equation (1). Let

$$\psi(t) = \alpha e^{-\alpha t} \tag{12a}$$

Then by taking Laplace transforms and applying (9), we find

$$\psi^*(u) = \alpha/(\alpha + u) \qquad \text{and} \qquad \phi^*(u) = \alpha \tag{12b}$$

so that

$$\phi(t) = 2\alpha\delta(t) \tag{12c}$$

When this expression is substituted into (7) the simple master equation is obtained. In light of the relation between the $\psi(t)$ and $\phi(t)$ established in this paper, the analysis of Ref. 3 which leads to this conclusion is seen to be exactly equivalent to the remark that (7) leads to (1) when $\phi(t)$ is a delta function.

Bedeaux *et al.*[3] have also shown that when the moments

$$\mu_n \equiv \int_0^\infty t^n \psi(t)\, dt \tag{13}$$

are all finite, the master equation is appropriate for a description of a random walk at times which are large compared with

$$t^* = \sup[\mu_n/n!]^{1/n} \tag{14}$$

Our second example is chosen to derive an equation which at early times after the walk has started yields results which are quite different from those that would follow from (1) and yet which at large times become equivalent to them.

Let us consider (with $\lambda^2 > 4a$)

$$\psi(t) = 2a(\lambda^2 - 4a)^{-1/2}\, e^{-\lambda t/2} \sinh[\tfrac{1}{2}t(\lambda^2 - 4a)^{1/2}] \tag{15}$$

which is equivalent to the difference between two exponentials. The corresponding expression for $\phi(t)$ is

$$\phi(t) = ae^{-\lambda t} \tag{16}$$

When (7) is differentiated with respect to t and (16) is substituted into the resulting expression the ensuing equation is

$$P_{tt}(l, t) + \lambda P_t(l, t) = a\left[-P(l, t) + \sum_{l'} p(l - l')\, P(l', t)\right] \tag{17}$$

If steps are taken to nearest-neighbor points only and if the lattice spacings are made very small, then by proceeding to the continuum limit this equation takes the form of the telegrapher's equation (with $P_t \equiv \partial P/\partial t$, etc.)

$$a^{-1}P_{tt} + (\lambda/a)\, P_t = DP_{xx} + kP_x \tag{18}$$

the D and λ being appropriately defined. It is known that at early times an initial pulse propagates as a wave, while at later times it propagates as a diffusion packet. This phenomenon was observed in the early days of telegraphy.[7] Signal diffusion reduced the data rate in long cables such as the early Atlantic cable. More recent applications of (17) or (18) have been to propagation of impulses in nerves and to exciton transport in photosynthetic units.[8]

The concept of the pausing time associated with a nondelta $\phi(t)$ or a nonexponential $\psi(t)$ is particularly physical in the problem of exciton transport in photosynthetic units. (An exciton hops from site to site but pauses at each site. Lattice vibrations provide a relaxation mechanism which yields a pausing time of the order of 10^{-12} sec.) The traditional theory of exciton transport postulates a Markovian random walk which corresponds to an exponential $\psi(t)$ and therefore a deltalike $\phi(t)$. However, this represents an instantaneous relaxation of the exciton at every site. A general theory which takes into account the actual non-Markovian nature of the process and the finite magnitude (10^{-12} sec) of the relaxation time has been developed recently.[8] Equations like (7) and (17) have been used[9] to analyze the oscillatory approach to equilibrium observed in a study of certain models in nonequilibrium statistical mechanics.

Since it was pointed out in Ref. 1 that there is some evidence in transient photoconductivity experiments that $\psi(t)$ may not have any finite moments, we close our discussion with a consideration of one of the forms of $\psi(t)$ without moments which was presented there. We choose

$$\psi(t) = 4a^2[\exp(ta^2)]\, i^2 \operatorname{erfc}(at^{1/2}) \tag{19a}$$

Since

$$\psi^*(u) = [1 + (u^{1/2}/a)]^{-2} \tag{19b}$$

$$\phi^*(u) = a^2\{1 - [1 + (u^{1/2}/2a)]^{-1}\} \tag{19c}$$

whose Laplace transform is

$$\phi(t) = 2a^2\delta(t) - 2a^3(\pi t)^{-1/2} + 4a^4[\exp(4ta^2)] \operatorname{erfc}(2at^{1/2}) \tag{20}$$

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