Coupled generalized master equations for Brownian motion anisotropically scattered

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The connection between a coupled non-Markovian Chapman-Kolmogorov equation and the coupled generalized master equation is established. In particular the model of coupled random walk is used for the description of correlated Brownian motion with anisotropic scattering.

Starting from a Liouville equation, the projectionoperator technique gives a generalized master equation (GME). This GME is, in general, a non-Markovian equation and all the problems are included in the memory kernel. On the other hand, it is very well known that the continuous-time random walk (CTRW) is connected with a GME,^{1,2} the relation between the memory kernel and the waiting-time density being well understood.

Recently the problem of including internal degrees of freedom into the random walk (RW) has been studied,^{3,4} and the close connection between the CTRW with internal degrees of freedom and GME has been pointed out.³ Nevertheless this problem has only been studied for translationally invariant RW schemes, and a self-averaged (in each mode) waiting time has been used (this must not be confused with the Hartree approximation used by Scher and Lax⁵ which involves a space-averaged version). What we need is an explicit calculation using a modedependent waiting time, for example, in order to understand neutron diffusion in a two-group energy model⁴ or, as in the present paper, to study the Lorentz model where the forward and backward scattering has a different waiting-time distribution (such as due to some internal excitation).

In order to understand the motion of a Brownian particle when the random force is correlated with its velocity (i.e., all scattering centers present an anisotropy in the sense that the direction of the velocity after scattering depends on the direction before it), a set of coupled recurrence relations of the RW type has been studied.^{6,7} Also in this problem, the CTRW theory has been applied to describe more general situations.^{8,9} However in these studies, we have used only a unique averaged waiting time, i.e., we have neglected completely the mode dependence of this function (note that in this case, "the onedimensional Lorentz model," each mode is represented by the direction of its velocity).

What we want to do in this paper is to study the non-Markovian behavior (through its associated coupled GME) which arises as a consequence of the mode dependence of the waiting time. We have called this approach "coupled CTRW," and it is closely related to the CTRW with internal degrees of freedom. The difference between this and related approaches has been discussed.⁴

In this paper we establish the connection between the coupled CTRW and the coupled generalized master equation (coupled GME) associated with it. Particularly the nearest-neighbor persistent RW model is used to study a

non-Markovian Lorentz-gas model (the connection between the persistent RW and the Lorentz-gas model has been shown elsewhere¹⁰).

I. THE COUPLED GME

As it is known in the CTRW theory,¹¹ the basic quantity is the waiting-time density function $\psi(t) \left[\psi(t) dt \right]$ is the probability that the walker makes its jump in the time interval (t, t + dt)]. Owing to the necessity of including a mode dependence we must extend this waiting-time concept to $\psi_{ll'}(t)$, a mode-dependent waiting-time function. This is because we are interested in solving certain classes of coupled recurrence relations between probability functions. We only need to define quantities like $P_l(j,t)$ instead of the transition quantities $P_{ll'}(j,t)$ defined by Landman et al.³ Both probabilities are closely related, but due to the simplicity of work with a vector we shall continue with our description. It follows that, in the coupled CTRW theory, the probability distribution $P_l(j,t)$ (*l* being the mode and j the site) will be found as an average over all the paths accessible to the walker. In what follows we present the connection between the coupled CTRW and the coupled GME for the general case where translational invariance is not demanded and the mode dependence is included. This situation has not been treated up till now.

As in Ref. 4, we start with a general set of coupled CTRW recurrence relations for $P_n^l(j,t)$, the probability of the particle to be at the site *j* with model *l*, at time *t* in the *n*th step:

$$\mathbf{P}_{n+1}(j,t) = \int_0^t \sum_{j'} \vec{\psi}(j,j',t-\tau) \cdot \mathbf{P}_n(j',\tau) d\tau$$
(1)

which can be seen as a set of coupled generalized Chapman-Kolmogorov equations, for non-Markovian situations, for each of the components of the vector $\mathbf{P}_n(j,t)$ (characterizing different "degrees of freedom" or "modes"). The transition matrix $\psi(j, j', t)$ completely characterizes the set of coupled recurrence relations. Also $[\psi(j,j',\tau)]_{ll'}d\tau$ is the probability that arriving at position j' and mode l', the walker makes a transition to a position j and mode l at time $\tau, \tau + d\tau$. Thus, the following normalization conditions are fulfilled:

$$\sum_{j} \sum_{l} \int_{0}^{\infty} [\vec{\psi}(j,j',\tau)]_{ll'} d\tau = 1 .$$
⁽²⁾

If we define the vector generating function by

$$\mathbf{R}(j,t,z) = \sum_{n=0}^{\infty} z^{n} \mathbf{P}_{n}(j,t)$$
(3)

and assume that the initial condition for the vector probability distribution is

$$\mathbf{P}_{0}(j,t) = \delta_{j,0} \delta_{t,0}(\alpha_{1},\alpha_{2},\ldots) , \qquad (4)$$

where α_i are the initial normalizations for each mode, we can write a matrix equation for $\mathbf{R}(j,t,z)$. Upon multiplication of Eq. (1) by z^n , summation over all n, and use of the initial condition Eq. (4), we obtain

$$\widetilde{\mathbf{R}}(j,u,z) = z \sum_{j'} \vec{\psi}(j,j',u) \cdot \widetilde{\mathbf{R}}(j',u,z) + \mathbf{P}_0(j) , \qquad (5)$$

where the overhead tilde (\sim) indicates the Laplace $(t \rightarrow u)$ transformation. Defining $\widetilde{\mathbf{R}}(j,u) \equiv \widetilde{\mathbf{R}}(j,u,z=1)$, Eq. (5) reads

$$\widetilde{\mathbf{R}}(j,u) = \sum_{j'} \vec{\widetilde{\psi}}(j,j',u) \cdot \widetilde{\mathbf{R}}(j',u) + \mathbf{P}_0(j) .$$
(6)

This equation connects the matrix $\overline{\psi}(j,j',\tau)$ with the vector $\mathbf{R}(j,\tau)$, the probability per unit time to reach j in time τ independent of the number of steps to arrive at j. This is the starting point to obtain the relation between the coupled CTRW Eq. (1) and the coupled GME.

As an extension of the Montroll¹¹ relation between the probability distribution P(j,t) and the generating function R(j,t) we assume, as in Ref. 4, the following relation between the vectors P(j,t) and R(j,t):

$$P_{l}(j,t) = \sum_{l'} \int_{0}^{t} [\vec{\phi}(t-\tau,j)]_{ll'} R_{l'}(j,t) d\tau , \qquad (7)$$

where $\vec{\phi}(\tau)$ is a diagonal matrix, which is a natural generalization of the function $\phi(\tau)$ of Montroll. In the Laplace representation this is given by

$$[\vec{\widetilde{\phi}}(u,j)]_{ll'} = \frac{1 - \sum_{j'} \sum_{l''} [\widetilde{\psi}(j',j,u)]_{l''l}}{u} \delta_{ll'} .$$
(8)

After Laplace transforming, Eq. (7) can be rewritten in matrix form as

$$\widetilde{\mathbf{P}}(j,u) = \overleftarrow{\phi}(u,j) \cdot \widetilde{\mathbf{R}}(j,u) .$$
(9a)

In order to solve Eq. (6) as a master equation for the vector probability, we use the inverse of Eq. (9a),

$$\widetilde{\mathbf{R}}(j,u) = [\vec{\phi}(u,j)]^{-1} \cdot \widetilde{\mathbf{P}}(j,u)$$
(9b)

which replaced in Eq. (6) gives

$$[\vec{\phi}(u,j)]^{-1} \cdot \widetilde{\mathbf{P}}(j,u) = \sum_{j'} \vec{\psi}(j,j',u) \cdot [\vec{\phi}(u,j')]^{-1} \cdot \widetilde{\mathbf{P}}(j',u) + \mathbf{P}_0(j) .$$
(10)

Owing the diagonality of the matrix $[\vec{\phi}(u,j')]^{-1}$, we can write for the *l*th component,

$$\frac{u}{F_{l}(j,u)}\widetilde{P}_{l}(j,u) = \sum_{j'} \sum_{l''} [\widetilde{\psi}(j,j',u)]_{ll''} \frac{u}{F_{l''}(j',u)} \widetilde{P}_{l''}(j',u) + [\mathbf{P}_{0}(j)]_{l}, \qquad (11a)$$

where for the inverse $[\vec{\phi}(u,j')]^{-1}$ we have used Eq. (8) and defined

$$F_{l}(j,u) = 1 - \sum_{j'} \sum_{l'} [\vec{\psi}(j',j,u)]_{l'l} .$$
(11b)

Adding and subtracting $\sum_{l'} u \tilde{P}_{l'}(j,u) \delta_{l'l}$ in Eq. (11a) we get

$$\sum_{l'} u \widetilde{P}_{l'}(j, u) \delta_{ll'} - [P_0(j)]_l$$

$$= \sum_{j'} \sum_{l''} [\vec{\psi}(j, j', u)]_{ll''} \frac{u}{F_{l''}(j', u)} \widetilde{P}_{l''}(j', u)$$

$$- \sum_{l'} u \frac{[1 - F_{l'}(j, u)]}{F_{l'}(j, u)} \widetilde{P}_{l'}(j, u) \delta_{ll'} . \qquad (12)$$

Finally, using Eq. (11b) and making the inverse Laplace transform of Eq. (12), we find the *l*th component of the coupled GME we are seeking:

$$\frac{\partial}{\partial t}P_{l}(j,t) = \sum_{j''}\sum_{l''}\int_{0}^{t} [\vec{\Lambda}(j,j'',t-\tau)]_{ll''}P_{l''}(j'',\tau)d\tau$$
$$-\int_{0}^{t}P_{l}(j,\tau)\sum_{j''}\sum_{l''} [\vec{\Lambda}(j'',j,t-\tau)]_{l''l}d\tau ,$$
(13a)

where the memory kernel is

$$[\vec{\Lambda}(j,j',u)]_{ll'} = \frac{u [\tilde{\psi}(j,j',u)]_{ll'}}{F_{l'}(j',u)} .$$
(13b)

This coupled GME is a generalization of the treatment of Landman *et al.*³ for the general situation indicated above. At this level Eq. (13) offers a formidable task if we want to solve it. In fact the memory kernel $\vec{\Lambda}$ is a fourth-rank tensor and if the space domain is bounded to [-N,N] the dimension of each matrix $[\vec{\Lambda}(j,j',u)]_{ll'}$ will be $2N \times 2N$.

Nevertheless if a decoupled space-temporal model is used, a simplification is obtained. Then as a special case of coupled GME [Eq. (13)] we can use a decoupled space-temporal matrix $\psi(j,j,\tau)$, that is,

$$[\overline{\psi}(j,j',\tau)]_{ll'} = W_{ll'}(j,j')\psi_{ll'}(\tau) , \qquad (14a)$$

where $\psi_{ll'}(\tau)$ must satisfy the normalization condition

$$\int_{0}^{\infty} \psi_{ll'}(\tau) d\tau = 1 .$$
 (14b)

Thus, using the normalization condition Eq. (2), for (14a), we obtain

$$\sum_{l} \sum_{j} W_{ll'}(j,j') = \sum_{l} Q_{ll'}(j') = 1 .$$
 (14c)

Then the definition of functions $F_{l'}(j',u)$ [Eq. (11b)] gives us the possibility of writing the memory kernel as

$$[\widetilde{\Lambda}(j,j',u)]_{ll'} = \widetilde{\Omega}_{ll'}(u,j')W_{ll'}(j,j') , \qquad (15a)$$

where the temporal memory function $\widetilde{\Omega}_{ll'}(u, j')$ is given by

$$\widetilde{\Omega}_{ll'}(u,j') = \frac{u\psi_{ll'}(u)}{1 - \sum_{l''} \widetilde{\psi}_{l'l'l'}(u)Q_{l'l'l}(j')} .$$
(15b)

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The coupled GME then takes the form

$$\frac{\partial}{\partial t} P_l(j,t) = \int_0^t \sum_{j''} \sum_{l''} \Omega_{ll''}(t-\tau,j'') W_{ll''}(j,j'') P_{l''}(j'',\tau) d\tau - \int_0^t P_l(j,\tau) \sum_{l''} \Omega_{l''l}(t-\tau,j) Q_{l''l}(j) d\tau .$$
(16a)

Also for this case the temporal memory functions $\Omega_{ll''}(t,j'')$ are space dependent (through the index j'') and thus the simple contraction of the $2N \times 2N$ matrix $W_{ll'}$ and the 2N dimensional vector $P_l(t)$ cannot be decoupled from the temporal memory function.

A big simplification arises if we study a translationally invariant case. Since the quantities $F_l(j',u)$ will be space independent, i.e., we must replace

$$W_{ll'}(j,j') \rightarrow W_{ll'}(j-j') ,$$

$$Q_{ll'}(j) \rightarrow Q_{ll'} ,$$

$$\Omega_{ll'}(j,u) \rightarrow \Omega_{ll'}(u) .$$

Then the coupled GME will be

$$\frac{\partial}{\partial t} P_{l}(j,t) = \int_{0}^{t} \sum_{l''} \Omega_{ll''}(t-\tau) \sum_{j''} W_{ll''}(j-j'') P_{l''}(j'',\tau) d\tau - \int_{0}^{t} P_{l}(j,\tau) \sum_{l''} \Omega_{l''l}(t-\tau) Q_{l''l} d\tau .$$
(16b)

But this temporal memory function $\Omega_{ll'}(t)$ can depend on the structure of the lattice, as will be shown in what follows.

The simplest four temporal memory functions that can be obtained, with different mode dependence for the waiting time are as follows.

(1) Independent of mode: $\widetilde{\psi}_{ll}(u) \rightarrow \widetilde{\psi}(u)$, then

$$\widetilde{\Omega}_{ll'}(u) \to \widetilde{\Omega}(u) = \frac{u\psi(u)}{1 - \widetilde{\psi}(u)}$$
(17a)

which is the well-known case of Montroll.¹

(2) Dependent on the initial mode: $\tilde{\psi}_{ll'}(u) \rightarrow \tilde{\psi}_{l'}(u)$, then

$$\widetilde{\Omega}_{II'}(u) \longrightarrow \widetilde{\Omega}_{I'}(u) = \frac{u\psi_{I'}(u)}{1 - \widetilde{\psi}_{I'}(u)}$$
(17b)

which shows us that different temporal decays appear in each mode, independent of the lattice-structure function, this is the self-averaged (in each mode) waiting time that we pointed out before which has been used by Ladman $et al.^3$

(3) Dependent on the final mode: $\tilde{\psi}_{ll'}(u) \rightarrow \tilde{\psi}_l(u)$, then

$$\widetilde{\Omega}_{II'}(u) \longrightarrow \frac{u\psi_I(u)}{1 - \sum_{I''} Q_{I''I'} \widetilde{\psi}_{I''}(u)}$$
(17c)

showing that, in this case, the temporal memory function depends on the lattice-structure function through the coefficient $Q_{II'}$, a result which does not appear in the Montroll or Landman descriptions.

The coefficients $Q_{ll'}$ are a generalization of the latticestructure functions, which are used when there is translational invariance. Then the normalization condition using Eqs. (2) and (14b) can be written as

$$\sum_{l} W_{ll'}^{*}(k=0) = \sum_{l} Q_{ll'} = 1 .$$
(17d)

Obviously in this case if we want to have a δ -Dirac memory we must solve an eigenvalue problem, where the coefficients Q_{ll} have an important role.

(4) Symmetric 2×2 model: if

$$\psi_{ll'} = \psi_{l'l} = \psi_1, \quad l \neq l'$$

$$\psi_{ll} = \psi_2; \quad \forall l$$

we have for the 2×2 temporal memory matrix, the following elements:

$$\Omega_{ll}(u) = \frac{u\psi_{2}(u)}{1 - [\psi_{2}(u)Q_{ll} + \psi_{1}(u)Q_{l'l}]}; \quad \forall l$$

$$\Omega_{ll'}(u) = \frac{u\psi_{1}(u)}{1 - [\psi_{2}(u)Q_{l'l'} + \psi_{1}(u)Q_{ll'}]}; \quad l \neq l'.$$
(17e)

It can be seen that for this special case (4), if we want to have a δ -Dirac memory [i.e., $\Omega_{ll'}(t) \rightarrow v_{ll'}\delta(t)$] we must use a Poisson density of time intervals between distinct events. This corresponds to an exponential waiting-time function $\psi_{ll'}(t)$ but in which the characteristic mean time value $\langle t \rangle_{ll'} = \int_0^\infty t \psi_{ll'}(t) dt$ depends on the lattice structure through the coefficient $Q_{ll'}$.

II. EXAMPLE: A NON-MARKOVIAN LORENTZ-GAS MODEL

In order to exemplify this approach we can show the two-mode case for the description of the motion of a onedimensional Brownian particle with anisotropic random force. The Lorentz-gas model has been used in order to study several problems and long-time tail phenomena. This has been carried out incorporating in the model effects of disorder at the scatterer¹² or fractal dimensional effects.¹³ In this example we want to study a slight generalization of the simple persistent RW;^{6-8,14} then we must use a coupled CTRW theory where the waiting time will be mode dependent.

Following the same notation as used in Refs. 6 and 8, $P(j,t) = (P^R(j,t), P^L(j,t))$ being the vector probability previously defined, where $P^R(j,t)$ or $P^L(j,t)$ are the conditional probabilities of finding a particle at site j and time t moving to the right or left direction, respectively, subject to the initial condition

$$\mathbf{P}(j, t=0) = (\alpha_1, \alpha_2) \delta_{j,0} \delta_{t,0} .$$
(18)

If we assume case (4) for the waiting time (i.e., a process, where the time elapsed in each step is different depending on the type of scattering that will occur), $\psi_{RL}(t) = \psi_{LR}(t) = \psi_1(t); \ \psi_{RR}(t) = \psi_{LL}(t) = \psi_2(t)$. This situation is well understood if we take into account that forward and backward scattering are symmetric with respect to the velocity direction of our Brownian particle:

$$P^{R}(j,t) \xrightarrow{\left[\substack{\text{scattering}\\\psi_{LR},w_{LR}}\right]} P^{L}(j't') , \qquad (19)$$

 $P^{R}(j,t) \xrightarrow{\left[\psi_{RR}, w_{RR}\right]} P^{R}(j',t') ,$

where by symmetry we must take

$$\psi_{RR}(t) = \psi_{LL}(t); \quad \psi_{RL}(t) = \psi_{LR}(t)$$

Using the exponential model, characterized by v_i in each one, we can write

$$\psi_{LL}(t) = \psi_{RR}(t) = v_2 e^{-v_2 t} ,$$

$$\psi_{LR}(t) = \psi_{RL}(t) = v_1 e^{-v_1 t}$$
(20)

which implies a Markovian behavior in each mode if there is no coupling among them [i.e., $W_{l'l}(j-j')=0$; $l'\neq l$].

To complete our description we must make an assumption for the lattice structure. Analyzing the case of nearest-neighbor model we must use a translationally invariant single-step transition-probability tensor of fourth rank,

$$\vec{W}(j-j') = \begin{pmatrix} W_{RR}(j-j') & W_{RL}(j-j') \\ W_{LR}(j-j') & W_{LL}(j-j') \end{pmatrix}, \quad (21a)$$

where we have used the index "R" and "L" to characterize each mode; the matrices $W_{ll'}(j-j')$ are given in the following way:

$$W_{RR}(j-j') = [W_{LL}(j-j')]^{T} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ p & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & q & \cdot \\ 0 & 0 & q & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & q \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & 0 & 0 & 0$$

The notation T indicates the transposed matrix, and p (or q) are the probability of forward (or backward) scattering relative to the flight direction before scattering (p+q=1). Using Eq. (21b) we can calculate the coefficients $Q_{ll'}$ given by Eqs. (14c) or (17d) as follows:

$$Q_{RR} = Q_{LL} = \sum_{j} W_{RR}(j - j') = p ,$$

$$Q_{LR} = Q_{RL} = \sum_{j} W_{LR}(j - j') = q .$$
(22)

Then the temporal memory matrix will be

$$\vec{\widetilde{\Omega}}(u) = \begin{bmatrix} \Omega_{RR}(u) & \Omega_{RL}(u) \\ \Omega_{LR}(u) & \Omega_{LL}(u) \end{bmatrix}, \qquad (23a)$$

where

$$\widetilde{\Omega}_{RR}(u) = \widetilde{\Omega}_{LL}(u) = \frac{u\psi_2(u)}{1 - [\widetilde{\psi}_2(u)p + \widetilde{\psi}_1(u)q]} , \qquad (23b)$$

$$\widetilde{\Omega}_{RL}(u) = \widetilde{\Omega}_{LR}(u) = \frac{u\psi_1(u)}{1 - [\widetilde{\psi}_2(u)p + \widetilde{\psi}_1(u)q]} .$$
(23c)

Note that each element has the same Laplace structure, which can be easily antitransformed. As it was expected it gives a δ dependence together with a transient non-Markovian description:

$$\Omega_{LL}(t) = \nu_2[\delta(t) + q(\nu_1 - \nu_2)e^{-(\nu_1 p + \nu_2 q)t}], \qquad (24a)$$

$$\Omega_{RL}(t) = v_1[\delta(t) + p(v_2 - v_2)e^{-(v_1p + v_2q)t}].$$
(24b)

It can be easily seen from Eq. (16b) and using (24a) and (24b) that for the case $v_2 = v_1$ we recover the Markoviancoupled ME description, i.e., the master equation for the simplest one-dimensional stochastic Lorentz model.^{6,12}

This is so because when we put $v_1 = v_2$ we are averaging the waiting-time functions $\psi_{ll'}(t)$ over all the modes; then we get the Montroll case for the temporary memory function [Eq. (17a)] independent of the mode. Because we have used an exponential waiting-time model we get a δ -Dirac memory function as is well known. Then the coupled GME will be Markovian.¹⁴ If we preserve $v_1 \neq v_2$, non-Markovian effects arise; this is so because the modes are coupled together. Physically our model of modedependent exponential waiting time is closely connected with a non-Markovian description between each step. In other words there are different correlations between the changes of velocity directions of our Brownian particle.

The coupled GME will be

$$\partial_{t} P_{R}(j,t) = v_{2} p P_{R}(j-1,t) + v_{1} q P_{L}(j-1,t) - (v_{2} p + v_{1} q) P_{R}(j,t) + \mathscr{A}(j,t) ,$$

$$\partial_{t} P_{L}(j,t) = v_{2} p P_{L}(j+1,t) + v_{1} q P_{R}(j+1,t) - (v_{2} p + v_{1} q) P_{L}(j,t) + \mathscr{B}(j,t) ,$$
(25)

where the non-Markovian term $\mathcal{A}(j,t)$ is

$$\mathscr{A}(j,t) = \int_{0}^{t} v_{2} p q (v_{1} - v_{2}) e^{-(v_{1}p + v_{2}q)(t-\tau)} P_{R}(j-1,\tau) d\tau + \int_{0}^{t} v_{1} p q (v_{2} - v_{1}) e^{-(v_{1}p + v_{2}q)(t-\tau)} P_{L}(j-1,\tau) d\tau - \int_{0}^{t} [-pq (v_{1} - v_{2})^{2}] e^{-(v_{1}p + v_{2}q)(t-\tau)} P_{R}(j,\tau) d\tau$$
(26a)

and a completely similar expression for the non-Markovian term $\mathscr{B}(j,t)$ can be obtained by making

$$P_{R}(j-1,\tau) \rightarrow P_{L}(j+1,\tau) ,$$

$$P_{L}(j-1,\tau) \rightarrow P_{R}(j+1,\tau) ,$$

$$P_{R}(j,\tau) \rightarrow P_{L}(j,\tau) .$$
(26b)

We can see from Eq. (26a) that the non-Markovian effect is a causal convolution of $P_l(j,\tau)$ with $\exp[-(t-\tau)/\tau_c]$, where $\tau_c = (v_1p + v_2q)^{-1}$ is a characteristic time, which can be used in order to define a transient non-Markovian regime. Consequently we can infer from the knowledge of τ_c , as a function of backward and forward probabilities (q,p), the characteristic quantities v_1, v_2 which specify our simple non-Markovian Lorentz-gas model.

If we study this system for times $t \gg \tau_c$ we can approximate the coupled GME by one of Markovian type. The non-Markovian terms can be approximated by

This contribution must be added to the Markovian term [Eq. (25)] in order to write the final coupled GME which control our systems for times $t \gg \tau_c$. We can see from Eq. (26) that the non-Markovian effect has been quenched off for sufficiently long times and only effective factors appear in each gain-loss term of the coupled Markovian master equation.

Finally we can remark that in this simple description for $t \gg \tau_c$ the effective loss-term factor will be smaller than for the Markovian approach. This is so because the mode-dependent waiting time introduces a delay in the loss contribution if we want to write a master equation.

On the other hand, for the gain term the sign provided from the non-Markovian contribution will depend on the model: $v_1 > v_2$ or $v_1 < v_2$. We can see, that in the limit of pseudodiffusive phase⁶ $q \rightarrow 0$, the non-Markovian terms disappear. This is due to the fact that if we take this limit the coupling between modes disappear [i.e., $w_{ll'}(j-j')=0l \neq l'$].

In the opposite case, the limit of counterdiffusive phase⁶ $p \rightarrow 0$, the non-Markovian terms disappear also. But in this case it is due to the normalization condition

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(p+q=1) and the model of $\psi_1(t) [\Omega_{ll'}(t) \rightarrow v_1 \delta(t)$ if $l \neq l'$, and $w_{ll}(j-j')=0$]. Then for the limit "one-side RW" we never will have a non-Markovian description. But for the "collapsed RW" the non-Markovian description is directly related to the model for the waiting time $\psi_{RL}(t)$ (the backward process).

Then Eqs. (26a) and (26b) give us useful information on the behavior of the non-Markovian memory function for the description of Brownian motion correlated with anisotropic scattering. As it has been shown before⁴ the formal solution of the RW equivalent problem, can be expressed by means of the coupled CTRW theory [in the Fourier $(j \rightarrow k)$ and Laplace $(t \rightarrow u)$ space] by

$$\widetilde{\mathbf{P}}^{*}(k,u) = \overleftrightarrow{\Phi}^{*}(u) \cdot [1 - \overleftrightarrow{\psi}^{*}(k,u)]^{-1} \cdot \mathbf{P}_{0}^{*} , \qquad (28)$$

where the matrices $\tilde{\psi}, \Phi$ are well defined through Eqs. (14a), (20), (21), and (8), respectively. The probabilistic argument contained in solution (28) is that we have made an average procedure by adding up with their weights all the paths accessible to the walker. In fact the memory function Eq. (24) allows us to use an alternative procedure and study how the non-Markovian description will be relevant to the description of this problem.

In this paper, we have established the connection between the coupled CTRW and the coupled GME, for the general not translationally invariant case, when the mode dependence is taken into account. This is an alternative framework to study the evolution of the coupled CTRW while it is in progress. Also we have analyzed the non-Markovian behavior of a correlated Lorentz-gas model in the framework of the coupled CTRW theory by means of its associated coupled GME, using a mode-dependent exponential waiting time. A study with another modedependent waiting-time function is in progress. Furthermore a variety of physical problems for nonequilibrium processes, other than scattering anisotropy, where a coupled recurrence relation of the form (1) between different modes is relevant, can be encompassed by a description via a coupled GME as given by Eq. (13), or for the decoupled space-temporal model by Eqs. (16a) or (16b).

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