Linear Response in Complex Systems: CTRW and the Fractional Fokker-Planck Equations.

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We consider the linear response of systems modelled by continuous-time random walks (CTRW) and by fractional Fokker-Planck equations under the influence of time-dependent external fields. We calculate the corresponding response functions explicitly. The CTRW curve exhibits aging, i.e. it is not translationally invariant in the time-domain. This is different from what happens under fractional Fokker-Planck conditions.

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I. INTRODUCTION

Many systems, such as polymer chains and networks, proteins, glasses and charge-carriers in semiconductors are characterized by extremely slow relaxation processes. The microscopic mechanisms leading to such slow relaxations differ considerably from system to system, but their microscopic manifestations often correspond to power-laws. A recently introduced approach to slow relaxation is based on fractional Fokker-Planck equations (FFPEs) or on fractional Master equations. The FFPE describing subdiffusive behavior in an external field reads:

$$ \frac{\partial}{\partial t} P(x, t) = D^{1-\gamma}_t \mathcal{L}_{FP} P(x, t), $$

(1)

where $P(x, t)$ is the pdf to find a particle (walker) at point $x$ at time $t$. In Eq. (1) $D^{1-\gamma}_t$ is the fractional Riemann-Liouville operator $\mathcal{L}_{FP}$ is the Fokker-Planck operator,

$$ \mathcal{L}_{FP} = K\Delta - \mu \nabla f(x), $$

(3)

In what follows we concentrate on the case in which the acting force $f(x) = -\nabla U$ is homogeneous and of magnitude $E$. In this case we have $\mathcal{L}_{FP} = K\Delta - \mu E \nabla$.

The fractional Fokker-Planck equation, Eq. (1), has turned out to be useful in describing a broad range of phenomena connected with anomalous diffusion. There are essentially two main mechanisms leading to long-time memory in the behavior of complex systems. One is related to the hierarchical structure of the modes of the system, as is the case for polymer chains and networks, and for rough interfaces. The other is associated with the diffusion in complex, (almost) quenched potential landscapes, which occur in glassy systems (ranging from normal glasses to proteins). A phenomenological description of free relaxation (i.e. the time-evolution of a system which is prepared in a nonequilibrium initial condition and then evolves under time-independent external conditions) in terms of fractional Fokker-Planck equations is reasonable in both situations. Thus, the FFPE, Eq. (1), can be viewed as a phenomenological linear-response theory for a system with long memory in contact with a heat bath. This equation can be derived systematically from the continuous-time random walk (CTRW) scheme using the standard Kramers-Moyal procedure. The equivalence of the two approaches was discussed in [8,9]. Thus, the free relaxation properties of a CTRW system are closely reproduced by Eq. (1) and can be expressed in terms of Mittag-Leffler functions.

In what follows we concentrate on the response of the two models to time-dependent external fields, and discuss the mean current (velocity) and mean polarization (coordinate) as a function of time in systems under pulsed or sinusoidal external fields. We show that the linear response to time-dependent fields predicted by FFPE (which is exactly the same as for hierarchical models) differs strongly from what is expected under CTRW conditions. Thus, the response to time-dependent fields of the systems described by FFPE is mainly influenced by the values of the field at times immediately preceding the observation time $t$, while the memory of the earlier history fades out. On the other hand, in CTRW-systems the response of the current to external fields is local in time, while the corresponding susceptibility decays. In such systems the polarization depends much on the early history of the system.

II. LINEAR RESPONSE WITHIN THE FFPE SCHEME

Let us consider a system whose dynamics is described by a fractional Fokker-Planck equation and concentrate...
on the mean particles’ displacement under the action of an external force. This mean displacement \( \overline{X}(t) \) is given by

\[
\overline{X}(t) = \int_{-\infty}^{\infty} xP(x,t)dx. \tag{4}
\]

Multiplying Eq.(1) by \( x \) and integrating it over the whole space we obtain:

\[
\frac{\partial}{\partial t} \int xP(x,t)dx = 0D_i^{1-\gamma} \left[ K \int x\Delta P(x,t)dx - \mu E(t) \int x\nabla P(x,t)dx \right]. \tag{5}
\]

The left hand side of Eq.(5) is nothing but \( \frac{d}{dt}\overline{X}(t) \), whereas the right hand side can be simplified by integration by parts. Since \( P(x,t) \) and its derivatives with respect to the coordinates vanish at infinity, the first integral vanishes and the second one is unity. Hence

\[
\frac{d}{dt} \overline{X}(t) = 0D_i^{1-\gamma} \mu E(t). \tag{6}
\]

Note that such kind of response is typical for complex and hierarchically built systems, like polymer chains and networks, see [4].

As a simple example let us consider a chain of \( N \gg 1 \) beads connected by harmonic springs and immersed in a viscous fluid (a Rouse-chain). We assume the first bead of the chain to be tagged (say, charged) and experience the external field \( E \). The motion of the beads is governed by the equation

\[
\zeta \frac{dx_0}{dt} = -k(x_0 - x_1) + E(t) + f_0(t) \tag{7}
\]

for the first bead (bearing number 0),

\[
\zeta \frac{dx_N}{dt} = -k(x_N - x_{N-1}) + f_N(t) \tag{8}
\]

for the last one and

\[
\zeta \frac{dx_i}{dt} = k(x_{i+1} - x_{i-1} - 2x_i) + f_i(t) \tag{9}
\]

for all other beads, \( 0 < i < N \). In Eqs.(7) to (9), \( f_i(t) \) are Gaussian, \( \delta \)-correlated forces with zero mean. Note that due to the linearity of Eqs.(7) to (9) the mean positions and velocities of the beads (averaged over the realizations of the \( f_i(t) \)) follow equations similar in form, but where the random forces \( f_i(t) \) are omitted. Let us suppose that the velocity response of the first bead of the chain (averaged over the realizations of the random forces \( f_i(t) \)) is described by the memory function \( M(t) \). Supposing that the initial mean velocities of the beads vanish, this leads after a Laplace transformation to

\[
v_0(\lambda) = \lambda x_0(\lambda) = M(\lambda)E(\lambda). \tag{10}
\]

If \( N \) is very large, \( N \to \infty \), the chain can be considered as infinite; then the subchain starting with bead 1 has the same linear response properties as the entire chain starting with bead 0. Thus, \( M(t) \) can be found using Eq.(10) and noting that the equation of motion for bead 1 has the same form, Eq.(10), with the acting force now being \( F = k(x_0 - x_1) \) instead of \( E \). The Laplace-representation of the equation of motion for the first bead reads:

\[
v_0(\lambda) = -k \left[ \frac{v_0(\lambda)}{\lambda} - \frac{v_1(\lambda)}{\lambda} \right] + E(\lambda) \tag{11}
\]

(where we set \( x_0(\lambda) = v_0(\lambda)/\lambda \) and \( x_1 = v_1(\lambda)/\lambda \)). Moreover, the analog of Eq.(11) for the velocity of the bead 1 reads:

\[
v_1(\lambda) = M(\lambda)k \left[ \frac{v_0(\lambda)}{\lambda} - \frac{v_1(\lambda)}{\lambda} \right]. \tag{12}
\]

The solution of Eqs.(11) to (12) gives \( M(\lambda) = -\lambda/2k + \sqrt{\lambda^2/4k^2 + \lambda/\zeta k} \). Thus, for \( \lambda \to 0 \), \( M(\lambda) \approx \tau_0^{1/2}\lambda \) with \( \tau_0 = 1/\zeta k \), which is exactly the Laplace-representation of a semi-derivative, \( \tau_0^{1/2}0D_i^{1-\gamma} \) with \( \gamma = 1/2 \) in Eq.(5).

This is the value which we will use in our numerical examples in what follows.

In the case where the friction coefficients \( \zeta \) and/or the spring constants \( k_i \) differ from site to site, other values of \( \gamma \) may be obtained [4]. The same holds also for more complex (higher-dimensional, fractal or tree-like) structures. For example, the case when a tagged monomer is attached to a membrane corresponds to \( \gamma = 2/3 \) [10].

III. LINEAR RESPONSE OF A CTRW SYSTEM

Let us now turn to the linear response in the framework of the CTRW model introduced by Montroll and Weiss [1]. This model was extremely successful in the explanation of dispersive transport in amorphous semiconductors [12]; see [13,14] for reviews. As is usual in CTRW, we envisage an ensemble of noninteracting particles which may be influenced by external fields (say, the particles are charged). The particles follow then CTRWs, i.e. sequences of jumps. The time intervals \( t_i \) between the jumps are uncorrelated. Of interest are waiting times which follow power-law distributions, i.e.

\[
\psi(t) = t/(1 + t/\tau_0)^{1+\gamma}, \quad \text{with} \quad 0 < \gamma < 1. \tag{13}
\]

The physical motivation for such \( \psi(t) \)-forms may be rationalized using random traps whose energy distribution is exponential [15]. In what follows we put \( \tau_0 = 1 \) and work in dimensionless time units.

A basic quantity in the CTRW formalism is \( \chi_n(t) \), the probability to make exactly \( n \) steps up to time \( t \). In the standard, decoupled CTRW picture (in which the spatial transition probabilities between the lattice sites are independent of the waiting-times) under time-independent
field the probability distribution \( P(x, t) \) of finding a particle at \( r \) at time \( t \) given that is started at \( 0 \) at time 0 obeys \[ P_n(x, t) = \sum_{i=0}^{\infty} P_n(x)\chi_n(t), \] (14)

where \( P_n(x) \) is the probability to reach \( x \) from \( 0 \) in \( n \) steps. We note that Eq.\((14)\) states that the CTRW is a random process subordinated to simple random walks under the operational time given by the \( \chi_n(t) \)-distribution. Note that exactly this property is the starting point for the derivation of FFPE in Ref.\[13\]. Let us now turn to the case of time-dependent fields. In this case the simple subordination relation, Eq.\((14)\) breaks down, since \( P_n(x) \) starts to depend on the actual value of external field at time \( n \) instants of steps, and thus on the actual times of steps, and not only on their number. On the other hand, the mean velocity or mean displacement of the particles can still be easily found.

Let us discuss the linear response of an ensemble of random walkers performing CTRWs to a changing external field. We consider some physically short time interval \( dt \). Let \( dN \) be the mean number of steps performed during \( dt \). The mean displacement during \( dt \) is \( \Delta x = x dN \) where \( x \) is the mean displacement per step depending on the actual value of the external field \( E \):

\[ x = \mu E = \sum_i x_i \frac{(x_i \cdot E)}{k_B T}. \] (15)

Here \( \mu \) is the mobility tensor. The sum in the second expression runs over all nearest neighbors vectors, \( k_B \) is the Boltzmann constant and \( T \) is the temperature. We obtain now

\[ \frac{\Delta x}{dt} = \mu E(t) dN, \] (16)

where \( dN = N(t+dt) - N(t) \approx dt \sum_{i=0}^{\infty} n \frac{d}{dt}\chi_n(t) \). Thus, the typical particles’ velocity (which is proportional to the particles’ current) is given by:

\[ \frac{\Delta x}{dt} = f(t) \mu E(t). \] (17)

where

\[ f(t) = \sum_{i=0}^{\infty} n \frac{d}{dt}\chi_n(t). \] (18)

Now the current density is \( J(t) = ne\frac{\Delta x}{dt} \), where \( n \) is the density of charge carriers (assumed to be homogeneous) and \( e \) is their charge; the analogue of Eq.\((17)\) holds also for the current,

\[ J(t) = f(t) \sigma E(t), \] (19)

where \( \sigma = ne\mu \) is the conductivity tensor.

According to the theory of CTRW, \( \chi_n(\lambda) \), the Laplace-transform of \( \chi_n(t) \), reads \( \chi_n(\lambda) = \psi(\lambda)^n [1 - \psi(\lambda)] / \lambda \), Ref.\[14\]. From Eq.\((18)\) we now have that the Laplace-transform of \( f(t) \) reads:

\[ f(\lambda) = \frac{\psi(\lambda)}{1 - \psi(\lambda)} \] (20)

The Laplace transform of \( \psi(t) \), Eq.\((13)\), for small \( \lambda \) is known to be \( \psi(\lambda) = 1 - \lambda t \Gamma(1 - \gamma) \). The inverse Laplace-transform of Eq.\((20)\) (for longer times) thus reads:

\[ f(t) = \frac{\sin \pi \gamma}{\pi} t^{\gamma - 1}. \] (21)

Note that the convergence to the behavior given by Eq.\((21)\) can be very fast. Moreover, effective interpolating forms valid both at short and at longer times can be obtained. As an example let us consider the case when \( \psi(t) \) is a one-sided (extreme) Lévy-law, \( \psi(t) = L(t, \gamma, -\gamma) \) (with \( 0 < \gamma < 1 \)), whose Laplace-transform is a stretched exponential \( \psi(u) = \exp(-\lambda u) \). This leads to \( f(\lambda) = [\exp(\lambda^{\gamma} - 1)]^{-1} \). Note that the behavior for large \( \lambda \), i.e. short \( t \), corresponds to that of \( \psi(t) \), since the denominator of \( f(\lambda) \) is dominated by the exponential term. For small \( \lambda \) the asymptotic behavior given by Eq.\((21)\) sets in. The transition between the two types of behaviors takes place at \( t \approx 1 \), and thus at longer times Eq.\((21)\) holds.

Thus, for \( t \gtrsim 1 \) one has

\[ \nabla(t) = \frac{\sin \pi \gamma}{\pi} t^{\gamma - 1} \mu E(t). \] (22)

A similar equation holds, of course, for the current \( J(t) \) flowing through the system:

\[ J(t) = \frac{\sin \pi \gamma}{\pi} t^{\gamma - 1} \sigma E(t). \] (23)

The current response of a CTRW-system to an external field is local in time and depends explicitly on the time elapsed after the system was prepared. Systems in which the response to an external agent depends explicitly on the delay between preparation time and measurement time are referred to as aging systems. This kind of behavior is found to be pronounced in CTRWs with \( 0 < \gamma < 1 \).\[13, 21\]

To obtain the particle’s position and therefore the polarization of the medium we simply have to integrate Eq.\((22)\) over time. Hence:

\[ \overline{X(t)} = \frac{\sin \pi \gamma}{\pi} \int_0^t t_1^{\gamma - 1} \mu E(t_1) dt_1 \] (24)

or

\[ \overline{P(t)} = \frac{\sin \pi \gamma}{\pi} \int_0^t t_1^{\gamma - 1} \sigma E(t_1) dt_1. \] (25)
In the limit $t \to \infty$ these expressions for $\mathbf{X}(t)$ or $\mathbf{P}(t)$ are Mellin-transforms of the external field, i.e.:

$$\mathbf{P}_\infty = \sigma^* \frac{\sin \pi \gamma}{\pi} \mathcal{M}[\mathbf{E} ; \gamma],$$

where $\mathcal{M}[f; s] = \int_0^\infty f(t)t^{s-1} \, dt$. Thus, the response of the CTRW-system to a time-dependent field decays, and its polarization tends to a constant value. Interestingly, the CTRW-system not only ages, but shows a kind of "Freudistic" response: the polarization at time $t$ is mainly due to the early history of the system, immediately after it was prepared in its initial state.

Let us compare the linear response (polarization vs. external field) of a CTRW-system and of a system described by the FFPE. The current through a system described by the FFPE is given by a fractional derivative,

$$J(t) = \frac{\sigma^*}{\Gamma(\gamma)} \frac{d}{dt} \int_0^t (t - t_2)^{\gamma-1} \mathbf{E}(t_2) \, dt_2$$

and the polarization of the system by a fractional integral

$$\mathbf{P}(t) = \frac{\sigma^*}{\Gamma(\gamma)} \int_0^t (t - t_2)^{\gamma-1} \mathbf{E}(t_2) \, dt_2.$$  

For the constant field $\mathbf{E}(t_1) = \mathbf{E}_0$ both expressions, Eqs. (25) and (28), describe essentially the same time-evolution (if one sets $(\sigma \sin \pi \gamma)/\pi = \sigma^*/\Gamma(\gamma) = \sigma_0$), since Eqs. (25) and (28) are equivalent to each other under the change of variable $t_2 = t - t_1$. This equivalence doesn’t hold anymore for the time-dependent-field. Note that the main difference of the response, Eq. (25) as compared with Eq. (28), is the fact that here the polarization is affected mainly by the latest events, and that the memory of the early history of the system fades away.

### IV. EXAMPLES

As examples we discuss two simple situations of the response of CTRW and of FFPE systems to external fields. We first choose a rectangular pulse switched on at $t = t_w$ and off at $t = t_z$ and then a sinusoidal field switched on at $t = 0$. We consider here a highly symmetric system described by a scalar conductivity $\sigma$, in which the current flows in the direction of the external field.

For CTRW Eq. (25) gives

$$J(t) = \begin{cases} 0 & t < t_w \\ \sigma_0 E_t^{\gamma-1} & t_w \leq t \leq t_z \\ 0 & t > t_z \end{cases}$$

which is a causal response concentrated on the time interval in which the field acts. On the other hand, from Eq. (27) it follows for FFPE that

$$J(t) = \begin{cases} 0 & t < t_w \\ \sigma_0 E(t - t_w)^{\gamma-1} & t_w \leq t \leq t_z \\ \sigma_0 E \left[ (t - t_w)^{\gamma-1} - (t - t_z)^{\gamma-1} \right] & t > t_z \end{cases}$$

Equations (29) and (30) coincide only if one takes $t_w = 0$, $t_z \to \infty$. This limit parallels the findings of Ref. [7]. In general, however, they are different. Eq. (29) describes a response concentrated on the time-interval of the field-action, $t_w \leq t \leq t_z$: no afteraction effects are seen. The current never changes sign and has finite jumps at $t = t_w$ and $t = t_z$. On the other hand, Eq. (30) shows considerable afteraction: the current does not vanish for $t > t_z$. The current diverges at $t = t_w$ and $t = t_z$ and changes its sign from positive to negative at $t = t_z$. Furthermore, the overall response described by Eq. (30) is invariant under time translation, i.e. it depends only on the differences $t - t_w$ and $t - t_z$, which is not the case for CTRW, Eq. (29).

**FIG. 1.** Shown is the current $J(t)$ in response to two rectangular field pulses of unit amplitude acting during the intervals $1 < t < 2$ and $4 < t < 5$. The thick solid line represents the CTRW-response, while the dashed line represents the response of a system described FFPE, see text for details.

Fig.1 shows the systems’ response to the two pulses of unit length and unit amplitude following at times $t_1 = 1$ and $t_2 = 4$ as follows from Eq. (25) and Eq. (27). The parameters are $\sigma_0 = 1$ and $\gamma = 1/2$. The response to the first pulse follows exactly Eqs. (29) and (30), hence the differences between CTRW and FFPE can be seen clearly. The comparison of the response of the two systems to a second pulse is also very instructive. For systems described by the FFPE the response to the first and to the second pulses do not differ (note that the superposition principle holds and that the responses are additive). On the other hand, in the case of a CTRW-system the second pulse causes a much weaker reaction than the first one. The susceptibility of the system (the conductivity) decays with time.

Let us now turn to the response of the system to a sinusoidal force switched on at $t = 0$, $E(t) = E_0 \sin(\omega t) \theta(t)$. **
The current through the quasiequilibrium (FFPE) system is described by the corresponding fractional derivative, $J(t) \propto d^{1/2}E(t) \propto \sigma_0 E_0 t^{-1/2} \sin(\omega t + \pi/4) - \sqrt{2} \text{Gres}(\sqrt{\omega t})$, whereas

$$P(t) \propto d^{-1/2}E(t) \propto \sigma_0 E_0 t^{-1/2} \sin(\omega t - \pi/4) + \sqrt{2} \text{Fres}(\sqrt{\omega t})$$

whereas

where $S(x)$ is the Fresnel integral. Note that since $\lim_{x \to \infty} S(x) = 1/2$, as time grows the polarization tends to a constant value $P_{\infty} \propto E_0/\sqrt{\omega}$ as time grows. The behavior of $J(t)$ and $P(t)$, Eqs. (33) and (34) is shown in the lower panel of Fig. 2 for the same values of parameters as before.

V. CONCLUSIONS

We have considered the linear response of systems governed by CTRW and by FFPE dynamics to time-dependent external fields. The form of the response for cases described by CTRW displays a "Freudistic" memory and no afteraction after switching off the field. This differs considerably from the response shown by systems obeying FFPE.

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For a CTRW system under the same sinusoidal external field the current through the system decays as

$$J(t) \propto \sigma_0 E_0 t^{-1/2} E(t) \propto \sigma_0 E_0 t^{-1/2} \sin \omega t,$$

while the polarization follows:

$$P(t) = \int_0^t J(t)dt \propto \sigma_0 E_0 \int_0^t t^{-1/2} \sin \omega t dt$$

$$= \sigma_0 E_0 \sqrt{\frac{2\pi}{\omega}} S(\sqrt{\omega t}),$$

where $S(x)$ is the Fresnel integral. Note that since $\lim_{x \to \infty} S(x) = 1/2$, as time grows the polarization tends to a constant value $P_{\infty} \propto E_0/\sqrt{\omega}$ as time grows. The behavior of $J(t)$ and $P(t)$, Eqs. (33) and (34) is shown in the lower panel of Fig. 2 for the same values of parameters as before.

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