A generalized master equation approach to modelling anomalous transport in animal movement

Luca Giuggioli\textsuperscript{1,2}, Francisco J Sevilla\textsuperscript{3,4} and V M Kenkre\textsuperscript{4}

\textsuperscript{1} Bristol Centre for Complexity Sciences, Department of Engineering Mathematics and School of Biological Sciences, University of Bristol, Bristol, UK
\textsuperscript{2} Department of Ecology and Evolutionary Biology, Princeton University, Princeton, NJ, USA
\textsuperscript{3} Instituto de Física, UNAM, Apdo. Postal 20-364, 01000 México DF, Mexico
\textsuperscript{4} Consortium of the Americas for Interdisciplinary Science, University of New Mexico, Albuquerque, NM 87131, USA

E-mail: Luca.Giuggioli@bristol.ac.uk, fjsevilla@fisica.unam.mx and kenkre@unm.edu

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Abstract

We present some models of random walks with internal degrees of freedom that have the potential to find application in the context of animal movement and stochastic search. The formalism we use is based on the generalized master equation which is particularly convenient here because of its inherent coarse-graining procedure whereby a random walker position is averaged over the internal degrees of freedom. We show some instances in which non-local jump probabilities emerge from the coupling of the motion to the internal degrees of freedom, and how the tuning of one parameter can give rise to sub-, super- and normal diffusion at long times. Remarks on the relation between the generalized master equation, continuous time random walks and fractional diffusion equations are also presented.

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1. Introduction

Ecology is a notoriously complex science\textsuperscript{[1]}. The myriad degrees of freedom and the multiple length and temporal scales governing the phenomena make ecological observations inherently integrative. Disentangling the various mechanisms and identifying unequivocally the reasons underlying a given process almost always present a daunting task. Animal movement of foraging animals, and the ensuing stochastic search processes, fall in this category.

The disparate modelling efforts that have attempted to understand how animals move and forage bespeak of the complexity of the problem. Evolutionary time scales are considered, for example, in constructing models of foraging behaviour that maximizes the animal fitness
(or reproductive success) on the basis of its internal energy reserves and the actions of their neighbours (e.g., see [2]). On shorter time scales, food availability and predator presence are considered as the key ingredients for animal foraging behaviour [3]. In regard to spatial dimensions, food patch areas and patch density distribution generate a plethora of length scales that affect animal behaviour [4].

Many of these different aspects of foraging have extensively been studied in the past, but despite the literature including recent studies on optimization of encounter rates via Lévy search strategies in random environment [5, 6], not much work exists at the animal cognitive level. Experimental as well as theoretical studies of how an animal perceives its surroundings, processes the environmental cues, and then moves its body in a certain direction are still in their infancy [6].

In this report we discuss some simple models of animal movements that possess internal degrees of freedom. They are reminiscent of the (energy) state-dependent foraging behaviour on one hand, where the internal states represent the amount of energy reserve [2], and of information processing on the other, where a transition between internal states indicates the completion of a cognitive task (e.g., see [7]).

The modelling that we employ here is based on the generalized master equation (GME) approach inherent in numerous early descriptions of transport and reviewed and emphasized by one of the present authors [8, 9]. Given the large literature on the application of continuous time random walks (CTRW) approach [10] to animal movement [11], as well as more recent applications of the fractional diffusion equation (FDE) to model foraging seabirds [12], we dedicate section 2 to describe the general relation between the three formalisms. Section 3 deals with our general choice of random walk models with internal degrees of freedom, whereas examples of random walkers, whose coupling to the internal degrees of freedom tends to enhance the movement, are treated in section 3.1. Examples of coupling situations that slow down the movement are discussed in section 3.2. Effects of the type of coupling on the mean square displacement (m.s.d.) are discussed in section 3.3, and finally conclusions form section 4.

2. The GME–CTRW–FDE equivalence

The three mathematical objects that are commonly used to represent a random walker that diffuses anomalously, i.e., whose m.s.d. does not grow linearly with time, are the GME, the CTRW and the FDE. These three mathematical objects represent the time evolution of the probability distribution of the spatial position of the walker. The CTRW typically involves an integral equation, is the generalization of Montroll and Weiss [10] to continuous time of the discrete-time random walk [13], wherein the walker is allowed to pause before taking the next step. The GME is an integro-differential equation that has arisen naturally from the use of projection techniques [14] made by Nakajima [15] and Zwanzig [16] in their studies to help understand how macroscopic irreversibility emerges from reversible microscopic dynamics. It has been particularly successful in resolving long debated issues in transport theory [8, 17] and explaining transport experiments in a variety of contexts including in organic materials [18]. The FDE, a differential equation with fractional index, introduced more recently by Schnyder and Wyss [19], has been extended by various authors [20–23] to its most general form with a fractional operator not only in time but also in space (space-time FDE) [24, 25].

In general, these mathematical objects are considered formally equivalent to one another. This indeed was proved in 1973 for the GME–CTRW formalisms [26] in a simple case and in 1974 [17] for the completely general situation including with internal states (or coupled space-time situations). The general equivalence given in [17] appears to have gone unnoticed.
as it has been reported by several authors subsequently \cite{27–29} as a generalization of \cite{26}. See \cite{8} and a recent reference \cite{30} for a discussion\footnote{We have followed an anonymous referee’s suggestion to clarify the chronology but are confident that the later generalizations were all arrived at independently in different physical contexts.}. The FDE was shown to represent a special case of the CTRW in 1995 \cite{31}. From these works it follows that the FDE is also an equivalent subset of the GME. More recently, in the presence of the so-called ageing systems \cite{32}, very interesting results on the relation between the GME and the CTRW have emerged (see \cite{33} and references therein). These however are not of our concern in this paper.

As it appears that the formal equivalence between the GME and the FDE has not been shown in the literature, we explicitly derive here the relation between the spatial and temporal kernel of the FDE with the spatial kernel and the memory of the GME, respectively. We do so by considering the so-called decoupled case of the GME in 1D continuous space, corresponding at the stochastic level to a complete independence of the distribution of jump length from the time correlation between the steps, namely

\[
\frac{\partial P(x,t)}{\partial t} = \int_{0}^{t} ds \, \phi(t-s) \int_{-\infty}^{\infty} dy \, W(x-y) P(y,s),
\]

where the spatial kernel \( W(x) \) and the memory \( \phi(t) \) multiply one another. These simplifications have been made here only for ease of display.

The general 1D space-time decoupled FDE can be written in the form \cite{24}

\[
\frac{D^\beta}{D^\alpha} P(x,t) = P(x,0) \frac{t^{-\alpha}}{\Gamma(1-\beta)} = \frac{D^\alpha}{D^\beta} P(x,t),
\]

where \( D^\alpha \) is the symmetric Riesz–Feller space-fractional derivative operator of order \( 0 < \alpha \leq 2 \) (the case \( \alpha = 1 \) is a special limiting case), \( D^\beta \) is the Riemann–Liouville fractional integral of order \( 0 < \beta \leq 2 \) and \( P(x,0) \) is the initial distribution. In order to determine the explicit equivalence of (1) with (2), one first applies the operator \( D^{-\beta} \) transforming equation (2) into \cite{25} (see appendix A)

\[
P(x,t) - P(x,0) = D^{-\beta} D^{\alpha} P(x,t).
\]

By writing out explicitly equation (3) one obtains

\[
P(x,t) = \mathcal{K}_{\alpha,\beta} \int_{0}^{t} ds \frac{(t-s)^{\beta-1}}{\Gamma(\beta)} \int_{-\infty}^{\infty} dy \frac{\Gamma(1+\alpha) \sin(\pi \alpha/2)}{\pi |x-y|^{1+\alpha}} P(y,s) + P(x,0),
\]

where \( \mathcal{K}_{\alpha,\beta} \) is the generalized diffusion constant, with units \((\text{length})^\beta (\text{time})^{-\alpha}\). Note that differentiation in time converts equation (4) to a form that is more often encountered in the literature (see e.g. \cite{23}). The equivalence can now be shown by solving for the probability function in equations (1) and (4) in the Fourier–Laplace domain and equating the resulting form \cite{26}. In particular one can show that the FDE is an equivalent subset of the GME when \( W(x) = \mathcal{K}_{\alpha,\beta} \Gamma(1+\alpha) \sin(\pi \alpha/2) \pi^{-1} |x|^{1-\alpha} \) and \( \rho(\epsilon) = \rho^{1-\beta} \).

In more general terms if one considers a generalization of the FDE where the temporal kernel is a generic function \( \rho(t) \) instead of being of the form \( t^{\beta-1}/\Gamma(\beta) \) as in equation (4), one can show that

\[
\phi(\epsilon) = \epsilon \rho(\epsilon),
\]

where \( \rho(\epsilon) \) is the Laplace transform of \( \rho(t) \).\footnote{It is interesting to note that, for certain choices of the function \( \rho(t) \) that possesses a Laplace transform, it might not be possible to formally derive the memory \( \phi(t) \) explicitly, if the condition for the existence of the inverse Laplace transform \cite{34}, i.e., \( \lim_{s \to \infty} \epsilon \rho(\epsilon) = 0 \), does not hold. This however is of little importance to their equivalence since the Laplace domain is just a linear transformation of the time domain and thus of equal importance, in as much as the Fourier domain has equal importance as the spatial domain.}
In the simple cases such as when the spatial kernel is Brownian, i.e., in the limit $\alpha \to 2$ when the Riesz–Feller fractional derivative operator becomes a second derivative in space, one can show that the solution of the FDE shows superdiffusive behaviour when $\beta > 1$, corresponding to a memory of the form $\phi(t) = t^{\beta-2}/\Gamma(\beta-1)$, and simple diffusive behaviour when $\beta = 1$, corresponding to $\phi(t) = \delta(t)$. A subdiffusive behaviour, characterized by a memory that changes sign, is obtained instead when $\beta < 1$.

The choice of which of the three mathematical frameworks (GME, CTRW or FDE) one ought to use in a given situation depends very much on the problem at hand. Even if there are no practical criteria that suggest which formalism to use, there are however certain situations that appear to favour one of the three. In the presence of ageing systems, for example, it is suggested [33] that the GME–CTRW equivalence [26] makes sense when observation and preparation times are identical, favouring the CTRW description when systems exhibit ageing. The FDE appears to be convenient when modelling a random walker that moves anomalously within a confining potential [23], while the GME, by its own construction, is particularly suited when the variable evolution is obtained by coarse-graining over the remaining degrees of freedom of the system [35]. We exploit here this natural feature of the GME to discuss some ‘microscopic’ mechanisms that generate anomalous statistics. We do so in the next section by giving some examples where the translational motion of a random walker is coupled with its internal states and gives rise to anomalous diffusion.

3. The random walker movement coupled with its internal states

For general purposes, we study a random walker moving in discrete space, the continuous space description being obtained with the standard limiting procedures. An early study based on equations with internal states was given in 1977 by one of the present authors [33].

Let us consider the following discrete master equation

$$\frac{dP_m(t)}{dt} = \sum_{n,N} \left[ R_{mn}^{MN} P_n(t) - R_{mn}^{NM} P_m(t) \right], \quad (6)$$

that describes a random walker on a 1D lattice of $N$ sites with internal degrees of freedom denoted by the integer $m$. In equation (6), the object $R_{mn}^{MN}$ gives the transfer rates for ‘jumping’ from the lattice site $N$ and internal state $n$ to the lattice site $M$ and internal state $m$. We consider that the lattice is subjected either to periodic boundary conditions or $N$ becomes infinite taking on values from $-\infty$ to $+\infty$, whereas we assume that natural boundaries [35] exist for the internal dynamics, making the index $m$ at least semi-infinite. We take the specific form

$$R_{mn}^{MN} = \gamma_{mn} \delta_{M,N} + F_m^{MN} \delta_{m,n}, \quad (7)$$

with $\delta_{p,q}$ a Kronecker delta, indicating that the transitions among internal states only occur at the same lattice site, while ‘jumps’ among the different sites of the lattice depend on the internal states. With these assumptions, equation (6) can be written as

$$\frac{dP_m(t)}{dt} = \sum_n \left[ \gamma_{mn} P_n(t) - \gamma_{nm} P_m(t) \right] + \sum_N \left[ F_m^{MN} P_N(t) - F_m^{NM} P_M(t) \right]. \quad (8)$$

We are interested in knowing what are the conditions on $F_m^{MN}$ and $\gamma_{mn}$ such that the m.s.d., $\langle M^2 \rangle = \sum_m M^2 P_m(t)$, of the coarse-grained probability $P_M(t) = \sum_m P_m(t)$, does not increase linearly with respect to time. In asking such a question, for simplicity we restrict our analysis to the case when the particles are allowed to jump only to nearest-neighbour sites, i.e., $F_m^{MN} = F_m [\delta_{M,N+1} + \delta_{M,N-1}]$. This choice of rates represents conditions in which the
dynamics of the internal degrees of freedom may affect the movement of the walker, while the walker displacement does not have any feedback on the internal dynamics, as can be seen by summing over \( M \) in equation (8). In the following we refer to \( F_m \) as the coupling or coupling coefficient.

By multiplying equation (8) by \( M^2 \) and summing over \( m \) and \( M \), it is easy to see that independently of \( \gamma_{mn} \), we obtain

\[
\frac{d(M^2)}{dr} = 2 \sum_m F_m P_m.
\]

indicating that without coupling to the internal states of the walker, i.e., for an \( F_m \) that does not depend explicitly on \( m \), the movement can only be diffusive. Since any coupling of the form \( F_m = C + F Z(m) \), with \( Z(m) \) being a generic non-singular function of \( m \), may mask the anomalous time dependence emerging from the internally coupled motion, we consider in our study situations where the constant rate \( C \) is negligible compared to the magnitude of the rate \( F \).

In the following subsections we show the effects of specific coupling and/or internal rates on the movement of the walker at the macroscopic level. We do so by determining the space-time kernel of the GME for the coarse-grained probability distribution. We also investigate under what conditions equation (9) is anomalous at long times, which can be achieved for example with transitory internal dynamics, that is to say, when no stationary distribution exists for \( P_m(t) = \sum_m P_m^M(t) \). One may obtain transitory states for example when the internal transition rates are time dependent or when the time-independent rates do not satisfy the detailed balance. We analyse in the following three examples of this transitory dynamics. The former situation is studied in section 3.1, while the latter is described in section 3.2. For Brownian dispersion on the internal states (transitory dynamics), how the type of coupling affects the long-time dependence of the m.s.d. is the subject of section 3.3.

### 3.1. Linearly dependent coupling with decay process transfer rates

The simplest assumption on the dependence of \( F_m \) on \( m \) is \( F_m = F m \). This is a particular case of \( F_m = C + F m \), used in the study of vibrational relaxation on intermolecular excitation transfer [36, 37] with internal dynamics defined over a semi-infinite set of states \((m \geq 0)\).

For the internal dynamics a very common situation occurs when the rates \( \gamma_{mn} \) describe linear one-step processes [35], i.e., \( \gamma_{mn} = \gamma_n^+ \delta_{m-1,n} + \gamma_n^- \delta_{m+1,n} \), where \( \gamma_n^\pm \) are linear functions of \( n \). This is the case, for example, in the theory of relaxation of Montroll and Shuler [38] or their generalization by Seshadri and Kenkre [37] where \( \gamma_n^+ = kn \) and \( \gamma_n^- = k(n + H - 1) e^{-\tilde{\omega}} \), which arise from the harmonic-oscillator selection rules, wherein \( \tilde{\omega} = \Delta/k_B T \) is the Boltzmann factor (with \( \Delta \) being the oscillator energy, \( k_B \) the Boltzmann constant and \( T \) the temperature), \( k \) is the characteristic rate, and \( H \) is the degeneracy of the oscillator [36]. Another example is the decay processes, where the transitions are directed to lower states only \((\gamma_n^- = 0)\) and given by \( \gamma_n^+ = \gamma n \). In such a case the dynamics of the internal states, obtained by summing equation (8) over \( M \), is governed by

\[
\frac{dP_m(t)}{dr} = \gamma[(m + 1)P_{m+1}(t) - mP_m(t)],
\]

with \( P_m(0) = \delta_{m,r} \), wherein \( r > 1 \) represents the internal level occupied at time \( t = 0 \). The case \( r = 0 \) is not considered here: it corresponds to an initial condition such that the internal dynamics has already reached its steady state.

By following the general procedure derived by two of the present co-authors in [39] and detailed here in appendix B, it is possible to show that a coupled space-time GME memory
emerges. One obtains in fact that the macroscopic probability distribution of the walker is
governed by
\[ \frac{dP^M(t)}{dt} = 2F \int_0^t ds \sum_N \partial_\phi(M - N, t - s)[P^{N+1}(s) + P^{N-1}(s) - 2P^N(s)]. \tag{11} \]

With the definition \( h_1(k) = 4F \sin^2(\pi k/N) \) and \( h_2(k) = \gamma + h_1(k) \) one can write the space-
time-coupled GME kernel in the Fourier–Laplace domain
\[ \tilde{\partial}_\phi(k, \epsilon) = \frac{1}{2h_1(k)} \left\{ \frac{1}{\gamma} \sum_{j=0}^r \frac{(-1)^j}{\Gamma(2r + 1)} \left( \frac{\gamma}{h_2(k)} \right)^j \right. \\
\left. \times \frac{\Gamma(2r + \epsilon/h_2(k))}{\Gamma(j + 1 + 2r + \epsilon/h_2(k))} \right\}^{-1} - \epsilon \right\}. \tag{12} \]

\( \tilde{\partial}_\phi(k, \epsilon) \) is independent of \( k \) only when \( r = 1 \). For all other situations it does depend on \( k \).
This is an interesting finding since it implies that, at the macroscopic scale, effective transfer
rates to non-nearest-neighbour sites are generated by the internal dynamics, even if they were
not imposed at the outset. Examples of effective non-local transfer rates generated by the
dynamics of a system can be found in [40, 41] in the context of exciton transport in molecular
crystals. These non-local space effects are due to the coupling \( F_m \) linear in \( m \), that makes it
easier for the walker to move longer distances the higher the value \( m \). The higher the
internal excitation the faster the walker moves to the neighbouring sites, leading to jumps that
effectively connect sites further away when the description is coarse grained over the internal
degrees of freedom.

Decay processes such as the one just described or the one considered by Montroll and
Shuler [38] possess a steady-state distribution. As argued before, the m.s.d. at long times
will always be diffusive. However, if the decay process has rates that fade out with time, the
dynamics of the internal states is transitory and the system does not obey the detailed balance.
This might represent the fact that the internal system is kept out of equilibrium as occurs in
the case of energy transfer rates in a conjugated polymer guest–host system [42]. A simple
modification of equation (10) with time-dependent rates can be achieved by converting \( \gamma \) to
\( \gamma/(t + \tau) \) where \( \tau \) represents a characteristic time scale. Evaluation of the m.s.d. then gives
(see appendix B)
\[ \langle M^2(t) \rangle = 2F \tau \frac{r}{1 - \gamma} \left[ \left( \frac{t}{\tau} + 1 \right)^{1 - \gamma} - 1 \right]. \tag{13} \]

for any \( \gamma \neq 1 \), while \( M^2(t) \sim \ln(t) \) when \( \gamma = 1 \). If the decay rates are too strong (\( \gamma > 1 \)),
the only internal state that remains populated is the ground state and thus the coupling to the
walker steps is lost for our choice \( F_m = Fm \). However for weak decay rates (\( \gamma < 1 \)),
the internal excitation decays slowly enough to influence the movement of the walker. The
generated macroscopic memory is a complicated coupled space-time kernel where effective
jumps to distant sites are possible however slowed down by the fact that the internal excitation
is decaying. The subdiffusion in the form of equation (13) is the result of the walker effectively
jumping at random to distant sites and, at the same time, the tendency of not moving due to
the internal dynamics that is relaxing to the ground state.

For completeness we would like to point out that, in place of equation (10) with time-
dependent rates, by considering transition rates \( \gamma_{mn}^{\pm} \) with \( m \geq 1 \) such that \( \gamma_m = \gamma/(t + \tau) \) and

\[ \langle M^2(t) \rangle = 2F \tau \frac{r}{1 - \gamma} \left[ \left( \frac{t}{\tau} + 1 \right)^{1 - \gamma} - 1 \right]. \tag{13} \]
Unless the level \( \gamma^* \), the internal dynamics is governed by

\[
\frac{dP_m(t)}{dt} = \frac{\gamma}{t + \tau}[(m - 1)P_{m-1}(t) - mP_m(t)].
\]  

(14)

With initial conditions such that \( P_m(0) = \delta_{m,0} \) it is possible to show (see appendix B) that

\[
\langle M^2(t) \rangle = 2Ft^\gamma r \left[ \frac{t}{\tau + 1} \right]^{1+\gamma},
\]

(15)

giving a superdiffusive dependence for any positive \( \gamma \).

3.2. Coupling to a single level with internal long range transfer rate

Subdiffusive movement at long times can also be generated without introducing time-dependence between the internal states. We consider for this purpose a walker that moves only if its internal state is in the ground level \( m = 0 \). We thus have that \( F_m = F\delta_{m,0} \). This converts equation (9) to

\[
\frac{d\langle M^2 \rangle}{dt} = 2FP_0(t).
\]

(16)

Unless the level \( P_0(t) \) remains constant over time, anomalous dispersion will always be manifest in this model. If the internal states are transitory, then \( \langle M^2 \rangle \) is not diffusive at long times. Here we build one such example by considering the spectrum of internal states to be semi-infinite and with an internal dynamics that does not satisfy the detailed balance. The internal rates of our system are chosen such that \( \gamma_m = \sigma_0 \delta_{0,0} + \rho_0 \delta_{m,0} \) with \( \sigma_0 = \rho_0 = 0 \) indicating that transitions occur from the ‘ground’ state to any of the remaining levels \( m \) with rate \( \sigma_m \) and from any level \( n > 0 \) to the ‘ground’ state with rate \( \rho_n \). As a first example we choose an \( n \)-dependence such that \( \rho_n = \sigma_n = fn^{-\alpha} \) with \( \alpha > 1 \). This power law \( n \)-decay of \( \sigma_n \) allows the higher internal levels to be populated, depleting the ground state and thus slowing down the movement. However, this effective deceleration does not bring the walker to a halt because all the decay transitions are to the ground state, which is the internal state when the walker steps to the nearest-neighbour sites.

If we write the system of equations that govern the dynamics for the internal degrees of freedom we have

\[
\frac{\partial P_0(t)}{\partial t} = \sum_{n=1}^{+\infty} \rho_n P_n(t) - \sum_{n=1}^{+\infty} \sigma_n P_0(t),
\]

\[
\frac{\partial P_n(t)}{\partial t} = -\rho_n P_n(t) + \sigma_n P_0(t).
\]

(17)

Solving for \( P_0(t) \) can be achieved by converting equation (17) to the Laplace domain giving \( \tilde{P}_0(\epsilon) = \left[ \epsilon + \sum_{m=1}^{+\infty} \sigma_m/(\epsilon + \rho_m) \right]^{-1} \) for the initial condition \( P_n(0) = \delta_{m,0} \). Equivalently, one may write the evolution for the macroscopic probability \( P_M(t) \) in the GME form

\[
\frac{dP^M(t)}{dt} = F \int_0^t ds \phi(t - s)[P^{M+1}(s) + P^{M-1}(s) - 2P^M(s)],
\]

(18)

with the memory

\[
\tilde{\phi}(\epsilon) = \left( 1 + \sum_{m=1}^{+\infty} \frac{\sigma_m}{\epsilon + \rho_m} \right)^{-1}.
\]

(19)

From equation (19) our choice for the rates \( \sigma_m \) and \( \rho_m \) becomes clear now. Given the relation

\[
\frac{d\langle M^2(t) \rangle}{dt} = \int_0^t dt' \int_0^t dt'' \phi(t''),
\]

in order to have a subdiffusive \( t^{1-\beta} \) m.s.d. at long times
with $0 < \beta < 1$, it is necessary to satisfy two conditions: (i) $\int_0^\infty \rho(t) \, dt = \delta(0) = 0$ which can be achieved if the series $\sum_{m=1}^\infty \sigma_m/\rho_m$ diverges and (ii) $\phi(t) \sim t^{-\beta}$ at long times. If $\rho_0 = \sigma_0$, the first requirement is satisfied, whereas for the second requirement it is necessary to study the dependence of $\phi(t)$ for small $\epsilon$. This can be done by studying the Mellin transform of the series $\sum_{m=1}^\infty \sigma_m/(\epsilon + \rho_m)$ (see appendix C), showing that for $\alpha > 1$, the memory $\phi(t) \sim t^{-\frac{\alpha}{\beta}}$ at long times thus leading to subdiffusive m.s.d. with $\beta = \alpha^{-1}$.

For our choice of rates the inverse Laplace transform of equation (19) is not known analytically. However, it is instructive to show one example where the memory can be calculated analytically. This happens to be the case $\alpha = 1/2$ with $\sigma_m/\rho_m = 2$. One can show that this leads to $1 + \sum_{m=1}^\infty \sigma_m(1 + \rho_m)^{-1} = \pi \sqrt{\tau/\epsilon} \coth(\pi \sqrt{\tau/\epsilon})$, giving a memory (see appendix C)

$$\phi(t) = \delta(t) - \frac{32}{\pi^2} \sum_{n=0}^\infty \frac{e^{-4(n+1)^2 \pi^2 t}}{(2n+1)^2}. \tag{20}$$

The Dirac delta function in the memory is indicative of diffusive behaviour, which however persists only at very short times being replaced by subdiffusion at longer times. It is evident that the memory is positive only at $t = 0$, while it remains negative for $t > 0$, satisfying the necessary requirement for its integral over all times to be zero. The macroscopic m.s.d. corresponding to equation (20) can be evaluated to be exactly

$$\langle M^2 \rangle(t) = \frac{4}{\pi^2} \sum_{n=0}^\infty \left[ 1 - e^{-4(n+1)^2 \pi^2 t} \right], \tag{21}$$

which grows linearly only at short times ($\langle M^2 \rangle(t) \sim 2Ft$). The $t$-dependence at long times for equations (20) and (21) can be calculated through Mellin transform methods (see appendix C), giving, respectively, $\phi(t) \sim -f^{-1/2}(\pi t)^{-3/2}$ and $\langle M^2 \rangle(t) \sim \left(8F/\pi^{3/2}\right)\sqrt{t}/f$.

Slight variations in the choice of the rates such that decay rates to the ground level $\rho_n = fn^{-1}$ and $\sigma_n = fn^{b-1}$ create a memory of the form $\phi(t) = \left(1 + f \sum_{m=1}^\infty m^{b-1}/(f + me)^{-1}\right)^{-1}$ that can be shown to possess those two properties mentioned above when $0 < b < 1$, giving a subdiffusive m.s.d. $\langle M^2 \rangle(t) \sim t^{1-b}$.

### 3.3. Non-diffusive behaviour dependence on the coupling to the internal states

The examples studied in sections 3.1 and 3.2 can be looked upon as two very different types of coupling to the internal dynamics. In the former subsection the coupling does not decay as a function of $m$, but it increases proportionally to $m$ with $F_m = Fm$. In the latter subsection, on the other hand, the coupling is represented through a sharp decreasing function with $F_m = \delta_{m,0}$. These two cases are just two examples of a variety of possible coupling mechanisms to the internal degrees of freedom. We explore below a model that allows us to study the effects on the anomalous diffusion properties of the walker as the coupling mechanism changes.

The number of internal states is semi-infinite ($m \geq 0$) as in the previous cases but with internal dynamics that are considered Brownian:

$$\frac{dP_m(t)}{dt} = \gamma (P_{m+1}(t) + P_{m-1}(t) - 2P_m(t)), \tag{22}$$

supplied with the boundary conditions $P_{-1} = P_0 [43]$, that is to say, a reflecting boundary at site $m = 0$. The coupling $F_m$ is chosen to decrease as a function of $m$ covering both short- and long-range decays, but it can also increase with $m$. The power function allows one to have these features with the use of only one numerical parameter, that we call $\eta (-\infty < \eta < +\infty)$. Accordingly we have chosen $F_m = Fm^{-\eta}(1 - \delta_{m,0})$, where the presence of Kronecker’s delta
is just to avoid rates that become singular when \( m = 0 \). Solution of equation (22) with the reflecting boundary conditions is given by [43, 44] \( P_m(t) = e^{-2\gamma t} [I_m(2\gamma t) + I_{m+1}(2\gamma t)] \) for our choice of initial condition \( P_m(0) = \delta_{m,0} \).

Following equation (9) the derivative of the m.s.d. is obtained by calculating \( \lambda_m(t) = 2F \sum_{m=1}^{\infty} m^{-\eta} P_m(t) \), whose general expression in the Laplace domain is determined to be

\[
\tilde{\lambda}_m(\epsilon) = \frac{F}{4\gamma} \frac{1 + \Omega(\epsilon)}{\sqrt{\epsilon} \left( \frac{\epsilon}{4\gamma} + 1 \right)} \text{Li}_\eta(\Omega(\epsilon)),
\]

where \( \text{Li}_\eta(z) = \sum_{k=1}^{\infty} z^k / k^\eta \) is the polylogarithmic function [45] and \( \Omega(\epsilon) = \left[ \frac{\epsilon}{4\gamma} + 1 - \sqrt{\frac{\epsilon}{4\gamma}} \right]^2 \). The tuning of the parameter \( \eta \) now allows the possibility of changing the long-time dependence of \( \tilde{\lambda}_m(t) \). Any \( \eta < 0 \) would give superdiffusive behaviour, any \( \eta > 0 \) would make the m.s.d. subdiffusive, and with the long-time diffusive case corresponding to \( \lambda_m(t) = 2F \{ 25(t) + 4\gamma(1 - P_0(t)) \} \).

The long-time dependence of \( \lambda_m(t) \) can be inferred from the behaviour of \( \tilde{\lambda}_m(\epsilon) \) at small values of \( \epsilon \) with \( \Omega(\epsilon) \to 1 \) as \( \epsilon \to 0 \). If \( \eta > 1 \) the polylogarithm equals the Riemann zeta function \( \text{Li}_\eta(\Omega(0)) = \zeta(\eta) \) and \( \tilde{\lambda}_{m+1}(\epsilon) \sim \epsilon^{-1/2} \), implying that \( \tilde{\lambda}_{m+1}(t) \sim t^{-1/2} \) and \( \langle M^2 \rangle(t) \sim t^{1/2} \) for \( t \to +\infty \). The internal Brownian dynamics has the effect of evenly populating all the internal states \( m \). Values of \( \eta > 1 \) mean rates of coupling to higher levels \( m \) that decays proportionally to \( m^{-\eta} \). As time evolves higher internal states get occupied, making the walker move less favourably, effectively slowing it down. The \( I \)-Bessel function dynamics with its long-time decay of the probability \( P_m(t) \) determines the long-time behaviour of the m.s.d.

A coupling to the internal states that decays faster than power laws does not change this picture and the walker moves subdiffusively with a \( t^{1/2} \) in its m.s.d. long-time dependence. One can show that even in the extreme limit when \( F_m \) is different from zero only at one site, as for example in section 3.2, the movement dynamics is not slowed down further and the walker subdiffuses with an exponent 1/2.

For values \( 0 < \eta < 1 \), \( \text{Li}_\eta(\Omega(0)) \) diverges and the subdiffusive dynamics at long times depends on the value \( \eta \). \( \text{Li}_\eta(\Omega(\epsilon)) = -\ln[1 - \Omega(\epsilon)] \) and the dominant term in \( \tilde{\lambda}_1(\epsilon) \) for \( \epsilon \to 0 \) is \( \ln(\sqrt{\epsilon})/\sqrt{\epsilon} \) giving \( a = \ln(t)/\sqrt{t} \) and \( \langle M^2 \rangle(t) \sim -\sqrt{t} \ln(t) \) long-time dependence. For \( 0 < \eta < 1 \), \( \text{Li}_\eta(\Omega(\epsilon)) \sim \Gamma(1 - \eta)(1 - \Omega(\epsilon))^{\eta-1} \) and \( \tilde{\lambda}_m(\epsilon) \sim \epsilon^{\eta/2 - 1} \) as \( \epsilon \) approaches 0. With the parameter \( 0 < \eta < 1 \) now one can tune the m.s.d. as \( \langle M^2 \rangle(t) \sim t^{1-\eta/2} \) for \( t \to +\infty \).

Similar calculations for the superdiffusive cases show that \( \langle M^2 \rangle(t) \sim t^{1-\eta/2} \) at long times pointing to a sub-ballistic \((-2 < \eta < 0)\) and a super-ballistic \((\eta < -2)\) m.s.d.. For the special cases when \( \eta \) is equal to some negative integers, the polylogarithm reduces to the ratio of polynomials of \( \Omega(\epsilon) \) [46] and in some cases the infinite sum in \( \tilde{\lambda}_\eta(t) \) can be computed. One such case is obtained when \( \eta = -1 \)

\[
\lambda_{-1}(t) = F \left[ 2\gamma t P_0(t) + e^{-2\gamma t} I_0(2\gamma t) - 1 \right],
\]

which is linear at short times and then becomes \( t^{1/2} \) at long times, producing an initial ballistic movement followed by long-time sub-ballistic \( t^{3/2} \) m.s.d.

4. Conclusions

The organizers of the wonderful collection of highly instructive random search articles that forms this volume indicated to us that it would be useful to contribute to the volume a few of our
ideas about general aspects of random walk formalisms used in stochastic search and related descriptions. Accordingly we have reported here some simple models of random walkers with internal degrees of freedom within the GME formalism. Additionally we have derived the relation between the GME and the FDE which appears (to be probably known to many but) perhaps missing in explicit form from the literature. We have exploited the fact that the GME is particularly convenient when the system observed at the ‘macroscopic’ level involves a coarse-graining over the ‘microscopic’ degrees of freedom, constructing non-local memories by coupling the movement steps of a random walker to its internal states. For the models selected, we have been able to write the kernels explicitly in the Fourier–Laplace domain showing for example how non-local transfer rates in one case may emerge from the coupling to the internal dynamics. For the case where there is coupling only through one internal level, we have been able to indicate the necessary conditions under which subdiffusion is present at long times. Subdiffusive stochastic search, in contrast to the more popular superdiffusive one, might become a convenient strategy when there is partial information about the environment, as recently reported in two species of Mediterranean seabirds during their foraging trips in the presence of fishing activities [12]. We have also constructed a random walk model where the interaction with its internal degrees of freedom is controlled by just one parameter in such a way that anomalous diffusion at long times can be tuned from sub-, to normal- and super-diffusion.

The specific choice of the internal dynamics and the coupling strengths have been inspired from realistic examples and observations but dictated also by considerations of the ease with which the ensuing calculations have allowed us to understand the emergent dynamics. Our interest, however, is always to stimulate further studies on the subject and actually to look for experimental systems that might be represented, even if only approximately, by our rudimentary models.

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Appendix A. The derivation of the GME–FDE relation

Here we describe some essential details of section 2. We start by pointing out that in equation (2) for the purpose of comparing the FDE to the GME, which only requires an initial $P(x, 0)$, we have omitted the initial term containing $dP(x, 0)/dr$. This initial term only appears when $\beta > 1$, i.e., when the temporal kernel is of the superdiffusive type. In such cases we thus assume that $dP(x, 0)/dr = 0$.

In dimensionless form the operator $D^\beta$ corresponds to [24]

$$
\frac{d^k}{dt^k} g(t) = \begin{cases} 
\frac{d^k}{dr^k} \left[ \frac{1}{\Gamma(k - \beta)} \int_0^t ds (r - s)^{k-\beta-1} g(s) \right], & k - 1 < \beta < k, \\
\frac{d^k}{dt^k} g(t), & \beta = k,
\end{cases}
$$

(A.1)
wherein \( k = 1 \) or 2 and \( g(t) \) is a generic continuous function of time. Application of the Riemann–Liouville operator of fractional integration

\[
\dot{D}^{-\beta} g(t) = \frac{1}{\Gamma(\beta)} \int_0^t ds (t-s)^{\beta-1} g(s) \tag{A.2}
\]
to equation (2) leads to equation (3). In transforming (2) into (3) one exploits the fact that

\[
\dot{D}^{-\beta} \frac{t^{-\beta}}{\Gamma(1-\beta)} = 1, \tag{A.3}
\]
and that

\[
\dot{D}^{-\beta}(D^\beta) P(x, t) = P(x, t) - \sum_{j=0}^{k-1} \left[ \dot{D}^{\beta-j} P(x, t) \right]_{t=0} \frac{t^{\beta-j}}{\Gamma(1+\beta-j)}, \tag{A.4}
\]
with the last term to the right in equation (A.4) being zero [22, 25] because

\[
\lim_{t \to 0} [\Gamma(j-\beta)]^{-1} \int_0^t (t-s)^{\beta-j-1} P(x, s) = 0. \tag{A.5}
\]

### Appendix B. Calculation of the space-time-coupled memory function \( \mathcal{D}_0(M, t) \)

In this section we present how equation (11) is obtained with the explicit form of the memory (coupled in time and space) given in (12).

It is a general property of the master equation (8) that, after summing over all internal states and taking the discrete Fourier transform, the coarse-grained probability distribution \( P^k(t) = \sum_m e^{2\pi i m k/N} P_m(t) \) satisfies the equation

\[
\frac{dP^k(t)}{dr} = 2 \left[ \cos \left( \frac{2\pi k}{N} \right) - 1 \right] \sum_m F_m P_m^k(t). \tag{B.1}
\]

Under the assumptions made in section 3, an exact analytical solution for \( \hat{G}^k(z, t) = \sum_{m=0}^{\infty} e^{2\pi i M k/N} P_m(t) \) can be found. For the decay process with time-independent transfer rates and \( F_m = F_m \), \( \hat{G}^k(z, t) \) is explicitly given by

\[
\hat{G}^k(z, t) = \left\{ \frac{z}{\sqrt{\gamma + 4F \sin^2 \frac{\pi k}{N}}} \left[ 1 - e^{-(\gamma + 4F \sin^2 \frac{\pi k}{N}) t} \right] \right\}^r. \tag{B.2}
\]

This expression is obtained by solving the first-order partial differential equation corresponding to equation (8) in the \( k-z \) domain.

For \( F_m = F_m \), the quantity \( F \sum_m m P_m^k(t) \) in (B.1) can be computed from (B.2) as \( \sum_m m P_m^k(t) = z \hat{G}^k(z, t) \big|_{z=1} \), the result can be rewritten in terms of \( P^k(t) = \hat{G}^k(z, t) \big|_{z=1} \), giving the expression

\[
\frac{dP^k(t)}{dr} = 2F \hat{D}_x(k, t) \left[ \cos \left( \frac{2\pi k}{N} \right) - 1 \right] P^k(t), \tag{B.3}
\]

which leads, after inverting the discrete Fourier transform, to a spatially nonlocal master equation with time-dependent ‘jumping’ rate \( \mathcal{D}_x(M, t) \) given by

\[
\hat{D}_x(k, t) = r \left[ 1 + \frac{\alpha}{\alpha + 4F \sin^2 \frac{\pi k}{N}} \left[ e^{(\alpha + 4F \sin^2 \frac{\pi k}{N}) t} - 1 \right] \right]^{-1}. \tag{B.4}
\]

It is precisely this spatial non-locality (see [39]) that allows us to write the equivalent generalized master equation (11) for \( P^M(t) \), characterized by a memory function which is nonlocal in space and time, denoted with \( \mathcal{D}_0(M, t) \).
Explicitly, \( \mathcal{D}_\gamma(M, t) \) is given in the Fourier–Laplace domain through the relation
\[
\mathcal{D}_\gamma(k, \epsilon) = \frac{1}{8F \sin^2 \frac{\pi k}{N}} \left[ \frac{1}{L \left[ e^{-4F \sin^2 \frac{\pi k}{N} t} \mathcal{D}_\gamma(k, \epsilon) \right]} - \epsilon \right].
\] (B.5)

In our particular case we are able to calculate explicitly the integral \( \int_0^\infty \text{d}x \mathcal{D}_\gamma(k, x) \) as well as the Laplace transform indicated in (B.5). After evaluating the integral using expression (B.4), the function to be transformed has the time dependence
\[
e^{-\gamma(F+4F \sin^2 \frac{\pi k}{N})t} \left[ \frac{\gamma \left( e^{4F \sin^2 \frac{\pi k}{N} t} - 1 \right)}{\gamma + 4F \sin^2 \frac{\pi k}{N}} + 1 \right].
\] (B.6)

The Laplace transform can be performed by expanding the factor in square parentheses and then using the result \( L \{ (e^{at} - 1)^\gamma \} = \frac{(-1)^\gamma \Gamma(\gamma+1)}{\Gamma(\gamma+1+a)} t^{\gamma+a} \). The final result is given by
\[
\frac{1}{\gamma} \sum_{j=0}^r \frac{(-1)^j \Gamma(r+1) \Gamma(j+1)}{\Gamma(r-j+1) \Gamma(r+1) \Gamma(j+1)} \left( \frac{\gamma}{\gamma + 4F \sin^2 \frac{\pi k}{N}} \right)^{j+1},
\] (B.7)

after substitution of this in (B.5) we get precisely expression (12).

We now show the explicit time dependence of the m.s.d. when the decay rates fade out with time as \( 1/t \). To do so, we first find the probability distribution for the internal states \( P_m(t) \) by solving the equation
\[
\frac{dP_m(t)}{dt} = \frac{\gamma}{t+\tau} [(m+1)P_{m+1}(t) - mP_m(t)].
\] (B.8)

This can be achieved by using the transformation \( G(z, t) = \sum_{m=0}^\infty z^m P_m(t) \), then, by multiplying the last equation by \( z^m \) and summing over all internal states we find that \( G(z, t) \) satisfies the equation
\[
\frac{\partial G(z, t)}{\partial t} = \frac{\gamma}{t+\tau} (1 - z) \frac{\partial G(z, t)}{\partial z}.
\] (B.9)

This equation may be solved with the method of characteristics [48] giving
\[
G(z, t) = \left[ 1 + (z-1) \left( \frac{t}{\tau} + 1 \right) \right]^{-\gamma},
\] (B.10)

where the initial condition \( P_m(0) = \delta_{m,0} \) has been used. We can directly compute \( \sum_{m=0}^\infty m P_m(t) \) by noting that \( \langle m(t) \rangle = \sum_{m=0}^\infty z^m P_m(t) \), which leads to \( \langle m(t) \rangle = \frac{r}{\gamma} \left( \frac{t}{\tau} + 1 \right)^{-\gamma}. \)

Finally, when we substitute the last expression into (9), with \( F_m = Fm \), we obtain
\[
\langle M^2(t) \rangle = 2F \tau \ln \left( \frac{t+\tau}{\tau} \right)
\] (B.11)

for \( \gamma = 1 \) and equation (13) for \( \gamma \neq 1 \). In the long-time limit we have sub-diffusion when \( 0 < \gamma < 1 \) and logarithmic growth for \( \gamma = 1 \).

A similar procedure is followed to derive equations (14) and (15). By using the generating function method it is straightforward to obtain from equation (14) the following first-order partial differential equation
\[
\frac{\partial G(z, t)}{\partial t} = \frac{\gamma}{t+\tau} (z-1) \frac{\partial G(z, t)}{\partial z}.
\] (B.12)

This last equation is then solved with the method of characteristics giving
\[
G(z, t) = \left[ 1 + \left( \frac{1}{z} - 1 \right) \left( \frac{t}{\tau} + 1 \right)^{\gamma} \right]^{-\gamma},
\] (B.13)

using the initial condition \( P_m(0) = \delta_{m,r} \). From this we obtain \( \langle m(t) \rangle = r \left( \frac{t}{\tau} + 1 \right)^{\gamma} \), from which equation (15) follows.
The procedure to invert the Laplace transform is as follows. Given that
\[ \frac{1}{\sqrt{\pi \varepsilon / f}} \tanh \left( \frac{\pi}{\sqrt{\varepsilon / f}} \right), \]
the procedure to invert the Laplace transform is as follows. Given that
\[ \mathcal{L}^{-1} \left\{ \frac{\tanh(\pi \sqrt{\varepsilon})}{\sqrt{\varepsilon}} \right\}(t) = \frac{2}{\pi} \sum_{n=0}^{\infty} e^{-\frac{\pi \sqrt{\varepsilon} t}{\sqrt{n + 1}}}, \]
where \( \mathcal{L}^{-1} \) stands for the inverse Laplace transform, we exploit the relation
\[ \mathcal{L}^{-1} \left\{ g \left( \frac{1}{\varepsilon} \right) \right\}(t) = \int_{0}^{\infty} da f(a) \left[ \delta(t) - \sqrt{\frac{u}{t}} J_{1} \left( 2 \sqrt{au} \right) \right], \]
wherein \( \mathcal{L}^{-1} \{ f(t) \}(\varepsilon) = g(\varepsilon) \), \( \delta(y) \) is a delta function and \( J_{1}(y) \) is a Bessel function of the first kind. The integration in \( u \) can also be done and gives the expression (20). Short-time
dependence of equation (20) and the related equation (21) for the m.s.d. can be easily calculated to be \( \phi(t) \sim \delta(t) - \pi^2/3 + (2\pi^4/15) f^2 t \) for the former and \( (M^2)(t) \sim 2F t - \pi^2 F f^2 t^2/3 \) for the latter. The long-time dependence in both cases can be determined if one knows the behaviour of the coefficients of the series for large \( n \). That can be obtained once again by studying the Mellin transform of the two series in equations (20) and (21), which results in, respectively,

\[
\sum_{n=1}^{+\infty} n^{b-1} e^{-\frac{fn}{f+1}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \Gamma(s)(4^{-s} - 4^{-2})\zeta(4-2s)(ft)^{-s}, \tag{C.6}
\]

with a strip of analyticity \( c > 3/2 \) and

\[
\sum_{n=0}^{+\infty} [1 - e^{-\frac{fn}{f+1}}] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \Gamma(s)(1 - 4^{-s})\zeta(-2s)(ft)^{-s}, \tag{C.7}
\]

with a strip of analyticity \( -1/2 < c < 0 \). The poles in the case of the integrand in equation (C.6) are located at \( s = 3/2 \) due to the Riemann zeta function and at \( s = 0, -1, -2, \ldots \) due to the Gamma function. Similarly there is a pole at \( s = -1/2 \) due to the zeta function in equation (C.7) together with the poles of the Gamma function at \( s = 0 \) and all negative integers. Since we are interested in the long-time dependence we deform the contour to the left of the strip of analyticity in both cases and we look at the contribution coming from the first residue. For the series in equations (C.6) and (C.7) we obtain a \( t^{-3/2} \) and a \( t^{1/2} \) dependence, respectively. We thus have that \( \phi(t) \sim -f^{-1/2}(\pi t)^{-3/2} \) and \( (M^2)(t) \sim (8F/\pi^{3/2})\sqrt{ft} \).

The second example of decay rates considers \( \delta_n = f n^{-1} \) and excitation rates \( \gamma_n = fn^{b-2} \) where \( 0 < b < 1 \). This case is representative of situations where the decay rates from level \( n \) to the ground level are larger than the corresponding excitation from the ground level. We now have a series of the form

\[
\sum_{n=1}^{+\infty} n^{b-1} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \frac{\pi \zeta(s)}{\sin[\pi(s+b)]}(f/e)^{s+b-1}, \tag{C.8}
\]

with \( 1 < c < 2 - b \). The poles are at \( s = 1 \) and at integer values of \( s + b \). The dependence for small \( \epsilon \) can be deduced by deforming the contour to the left of the strip of analyticity. From calculation similar to the previous cases and also detailed in [47] for the specific choice (C.8), it can be shown that \( \sum_{n=1}^{+\infty} n^{b-1} (1 + n\epsilon/f)^{-1} \sim \pi f^b e^{-b}/\sin(\pi b) \). The memory in this case is

\[
\widehat{\phi}(\epsilon) \sim e^{b} + \pi f^b / \sin(\pi b), \tag{C.9}
\]

for \( \epsilon \to 0 \), which implies \( \phi(t) \sim t^{-1+b} \) for \( t \to +\infty \) and \( \widehat{\phi}(0) = 0 \), i.e., a subdiffusive process at long times.

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