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Temporal diffusion

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Abstract. – We consider the general problem of the first-passage distribution of particles whose displacements are subject to time delays. We show that this problem gives rise to a *propagation-dispersion equation* which is obtained as the large-distance (hydrodynamic) limit of the exact microscopic *first-visit equation*. The propagation-dispersion equation should be contrasted with the advection-diffusion equation as the roles of space and time are reversed, hence the name *temporal diffusion*, which is a generic behavior encountered in an important class of systems.

One of the fundamental physical paradigms, applicable to a wide variety of physical processes, is that of spatial diffusion. The textbook example is of a random walker on a one-dimensional lattice (see, *e.g.*, [1]). At each tick of the clock, the walker takes a step either left or right, the direction chosen randomly with equal probabilities, and one asks what is the probability that the walker will be at a given position after a given time. If the walker starts at a known point, the answer is a binomial distribution which, in the continuum limit, becomes a Gaussian. The variance of the Gaussian grows with time, so that the localization of the walker decreases and we say that the walker disperses. If the probability for the walker to step in one direction is greater than that for the opposite direction, then the walker propagates in the direction of higher probability and will eventually visit each site of the lattice in that direction. The typical diffusive behavior is then manifested in the continuum limit as a Gaussian about a most-likely position which moves at a constant velocity. However, there are a number of situations in which it is more natural to ask how long it will take to reach a given point —more precisely for a stochastic process, what is the distribution of times taken to reach that point [2]. Everyday examples involve processes in which the goal is to arrive at a given point as quickly as possible: for example, a marathon (wherein we ask for the distribution of finishing times), certain financial instruments, such as stock options (wherein we ask for the distributions of times needed for an asset to reach a certain value), traffic flow (wherein we ask for the distribution of arrival times at destination), and packet transport over the internet. A more technical example, which inspired the present work, is the behavior of certain

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cellular automata which model the motion of a particle on a substrate of scatterers (in 1 or 2 dimensions) where, for certain types of scatterers, the particle ends up propagating along a particular channel [3–5], and, again, the first-passage time is the physical quantity of interest.

In this letter, we show that this general problem gives rise to a *propagation-dispersion equation*, much like the biased random walker, with the important difference that the roles of space and time are reversed: the distribution of first-passage times is Gaussian in the time variable with a variance that grows with increasing distance from the origin. In analogy with spatial diffusion that occurs in ordinary diffusive phenomena, we call this generic behavior *temporal diffusion*.

Consider a walker on a one-dimensional lattice and let $\hat{f}(t/\delta t; r/\delta r)$ be the probability that it takes $t/\delta t$ time steps to reach the lattice position $r/\delta r$, given that the walker is at the origin at time $t = 0$. Whatever the microscopic dynamics, we assume that we are given, or can work out, the set of probabilities $\{p_j(r)\}_{j=1}^\infty$ that the time between the first visit of the lattice site $r/\delta r$ and the first visit of the next position, $r/\delta r + 1$, is $j\delta t$. Conceptually, these represent the probabilities of various waiting times from the first visit of lattice site $r/\delta r$ until the first visit to $r/\delta r + 1$, *i.e.* the distribution of single-step waiting times. It is then clear that the probability that it takes the walker time t to reach the lattice site $r + \delta r$ is equal to the probability that it takes time t to reach lattice site r and that the waiting time is zero, plus the probability that it takes time $t - \delta t$ and that the waiting time is δt , plus ... so that the master equation is [6]

$$\hat{f}(t/\delta t; r/\delta r + 1) = \sum_{j=0}^{\infty} p_j(r) \hat{f}(t/\delta t - j; r/\delta r). \quad (1)$$

Rather than solving this equation directly, we appeal to a more intuitive picture. Let \hat{t}_l be the time that transpires from the first visit of lattice site l to the first visit of lattice site $l + 1$. The probability distribution for this discrete stochastic variable is precisely the set of probabilities $\{p_j(l\delta r)\}_{j=0}^\infty$ defined above. Next, define $\hat{T}_{l+1} = \sum_{i=0}^l \hat{t}_i$ which is the total time required to reach the lattice site $l + 1$: the probability that \hat{T}_{l+1} takes on the value t is precisely $f(t/\delta t; r/\delta r + 1)$. Since each of the elementary stochastic processes \hat{t}_i is independent, the distribution of \hat{T}_{l+1} in the limit of large l is immediately known, by application of the central limit theorem, to be

$$f(t, r) = \lim_{r/\delta r \gg 1} \frac{1}{\delta t} \hat{f}(t/\delta t; r/\delta r + 1) = \sqrt{\frac{1}{2\pi\sigma^2(r)}} \exp\left[-\frac{(t - \tau(r))^2}{2\sigma^2(r)}\right], \quad (2)$$

where the most likely time is

$$\tau(r) = \sum_{k=1}^{r/\delta r} \langle \hat{t}_{k-1} \rangle = \delta t \sum_{k=1}^{r/\delta r} \sum_{j=0}^{\infty} j p_j((k-1)\delta r), \quad (3)$$

and the width of the distribution is

$$\begin{aligned} \sigma^2(r) &= \sum_{k=1}^{r/\delta r} \left(\langle \hat{t}_{k-1}^2 \rangle - \langle \hat{t}_{k-1} \rangle^2 \right) \\ &= (\delta t)^2 \sum_{k=1}^{r/\delta r} \left[\sum_{j=0}^{\infty} p_j((k-1)\delta r) j^2 - \left(\sum_{j=0}^{\infty} p_j((k-1)\delta r) j \right)^2 \right]. \end{aligned} \quad (4)$$

(We note in passing that the exact solution to eq. (1) is a multinomial distribution, as discussed in detail in [7].) If the probability distribution of single-step waiting times is independent of position, then $\tau(r)$ and $\sigma^2(r)$ reduce, respectively, to

$$\tau(r) = r \frac{\delta t}{\delta r} \sum_{j=0}^{\infty} j p_j, \quad (5)$$

$$\sigma^2(r) = r \frac{(\delta t)^2}{\delta r} \left[\sum_{j=0}^{\infty} j^2 p_j - \left(\sum_{j=0}^{\infty} j p_j \right)^2 \right], \quad (6)$$

which prompts us to define an inverse propagation speed as

$$\frac{1}{c} = \frac{\tau(r)}{r} = \sum_{j=0}^{\infty} j p_j \frac{\delta t}{\delta r}, \quad (7)$$

and a temporal dispersion coefficient as

$$\gamma = \frac{\sigma^2(r)}{r} = \left[\sum_{j=0}^{\infty} j^2 p_j - \left(\sum_{j=0}^{\infty} j p_j \right)^2 \right] \frac{(\delta t)^2}{\delta r}. \quad (8)$$

So the distribution of first-passage times is

$$f(t, r) = \sqrt{\frac{1}{2\pi\gamma r}} \exp \left[-\frac{(t - r/c)^2}{2\gamma r} \right], \quad (9)$$

which is in precise analogy to the spatial distribution of a simple, biased random walker: the most likely first-visit time grows linearly with increasing distance and the width of the distribution grows as the square-root of the distance.

The distributions given in eqs. (2) and (9) are particular solutions for the initial condition that the walker is localized at $r = 0$ and $t = 0$, or $f(t/\delta t; r/\delta r = 0) = \delta(t)$. To complete our description of the first-passage time problem, it is interesting to display the continuum equivalent of the first-passage equation, eq. (1), which would govern the problem for all initial conditions. First, we notice that, since the exact first-passage time equation is linear, the particular solutions given above are the Green's functions for the general problem. Explicitly, if $f(t/\delta t; r/\delta r = 0) = f_0(t)$ then the distribution for finite distances must be

$$f(t, r) = \int_{-\infty}^{\infty} \sqrt{\frac{1}{2\pi\sigma^2(r)}} \exp \left[-\frac{(t - t' - \tau(r))^2}{2\sigma^2(r)} \right] f_0(t') dt', \quad (10)$$

from which one finds the equation of motion, the *propagation-dispersion equation*,

$$\frac{\partial}{\partial r} f(t, r) + \frac{1}{c(r)} \frac{\partial}{\partial t} f(t, r) = \frac{1}{2} \gamma(r) \frac{\partial^2}{\partial t^2} f(t, r) \quad (11)$$

with

$$\frac{1}{c(r)} = \frac{\partial}{\partial r} \tau(r), \quad (12)$$

$$\gamma(r) = \frac{\partial}{\partial r} \sigma^2(r). \quad (13)$$

Equation (11) can also be derived directly from eq. (1) by means of a multi-scale expansion (see [7]). Finally, we note that the derivation given here applies as well to the case in which the waiting times are continuous stochastic processes with the result that eq. (2) is again obtained.

As a first example, consider a biased random walker in one dimension. At each tick of the clock, the walker moves to the right with probability p and to the left with probability $q = 1 - p$. If the walker is at some particular lattice site, say l , then the probability that it moves to $l + 1$ with the next step is p , the probability that it takes three steps to move to $l + 1$ is $p(pq)$ since the probability of moving left, to $l - 1$, and back is pq and in general, the probability that it takes $2m + 1$ steps to reach $l + 1$ is evidently of the form $p_{2m+1} = a_m(pq)^m p$, where a_m is a combinatorial factor independent of p , since a delay of $2m$ ticks, starting and ending at lattice site l , requires some combination of m steps to the left and m steps to the right. (Obviously, the probability to reach $l + 1$ in an even number of steps is zero.) If $p > q$, we expect that the walker must eventually reach the next lattice site to the right so that $\sum_{m=0}^{\infty} a_m(pq)^m p = 1$. Introducing $y = p(1 - p)$, one has $p = \frac{1}{2}(1 \pm \sqrt{1 - 4y})$ with the positive sign appropriate for $p > 1/2$ and the negative sign otherwise; the normalization condition can then be written as (for $p > 1/2$)

$$\sum_{m=0}^{\infty} a_m y^{m+1} = \frac{1}{2}(1 - \sqrt{1 - 4y}), \tag{14}$$

and expansion of the right-hand side gives $a_m = \frac{(2m)!}{(m+1)!m!}$. Then, having the single-step waiting-time probabilities, and noting that

$$\sum_{m=0}^{\infty} \binom{2m+1}{m} p^{m+1} q^m = (p - q)^{-1}, \tag{15}$$

the first and second moments of the waiting times can be evaluated to give

$$\frac{1}{c} = \frac{\delta t}{\delta r} \frac{1}{(p - q)}, \tag{16}$$

$$\gamma = \frac{(\delta t)^2}{\delta r} \frac{4pq}{(p - q)^3}, \tag{17}$$

and the distribution of first-passage times is given by (9). The continuous limit, in which both δr and δt go to zero, gives finite results for both the propagation speed and the dispersion coefficient only if we simultaneously require that $p - q$ go to zero (just as in the usual discussion of the spatial-diffusion of the biased random walker [1]). Writing $\delta r \rightarrow \epsilon \delta r_0$, $\delta t \rightarrow \epsilon^\alpha \delta t_0$ and $p - q \rightarrow k \epsilon^\beta$, we find that

$$\frac{1}{c} \longrightarrow \frac{\delta t_0}{k \delta r_0} \epsilon^{\alpha - \beta - 1}, \tag{18}$$

$$\gamma \longrightarrow \frac{(1 - k^2 \epsilon^{2\beta})(\delta t_0)^2}{k^3 \delta r_0} \epsilon^{2\alpha - 1 - 3\beta}, \tag{19}$$

which are finite provided that $\alpha = 2$ and $\beta = 1$. This scaling is identical to that used to obtain the spatially diffusive limit of the biased random walker: the propagation speeds are identical, but the dispersion coefficients are quite different, because in spatial diffusion the diffusion coefficient is independent of the scaling of the probabilities ($D \rightarrow (\delta r_0)^2 / \delta t_0$). The

temporal dispersion coefficient is $\gamma = D/c^3$, which is also what one obtains by performing a change of variables ($r \rightarrow ct, t \rightarrow r/c$) in the advection-diffusion equation.

For the biased random walker in the continuum limit, the exact first-passage time distribution is known [1, 8] to be

$$f(t; r) = \frac{r}{\sqrt{2\pi D} t^{3/2}} \exp \left[-\frac{(r - ct)^2}{2Dt} \right]. \quad (20)$$

The difference between this expression and our result is due to the fact that the latter is an approximation which is only valid for large r . In this regime, the exact result only gives a non-zero probability for $(r - ct)^2/2Dt = \mathcal{O}(1)$ which implies $ct = r + \mathcal{O}(\sqrt{2Dr/c}) = r(1 + \mathcal{O}(\sqrt{2D/cr}))$. So, for large r we can use this approximation to write the exact distribution as

$$f(t; r) = \frac{c^{3/2}}{\sqrt{2\pi D} r^{1/2}} \exp \left[-\frac{(r - ct)^2}{2Dr/c} \right] (1 + \mathcal{O}(\sqrt{2D/cr})), \quad (21)$$

which, with $D/c^3 = \gamma$, agrees with the large-distance result (9). We emphasize that eq. (20) is exact in the continuum limit, *i.e.* for vanishing δr and δt , whereas the only restrictions on the general result, (9), are that r is large and that the first two moments of the elementary waiting time distribution, $\tau(r)$ and $\gamma(r)$, exist. The latter condition precludes the limit of the symmetric random walker, $c \rightarrow 0$, for which $\tau = r/c$ diverges (see eq. (7)).

A more complex example is provided by a walker moving on a lattice with scatterers inducing time delays at some (or all) lattice sites, a model which may serve as a paradigm for various processes such as signal propagation in computer networks [9], traffic flows [10], and evolutionary dynamics [3]. Of particular interest are models in which the properties of the scatterers also change with each scattering process. As a simple example, consider a particle moving on a one-dimensional lattice which has scatterers at each lattice site. The scatterers can be in one of two states characterized by their “spin” which can take on the values “up” and “down”. When a particle moves to a lattice site with spin-up, nothing happens to it whereas at a spin-down site, its velocity is reversed. In both cases, the spin of the lattice site is reversed. This model was solved in [5], where it was shown that, for any initial distribution of spins (including the random distribution), the particle always ends up propagating in one direction or the other at a constant (average) rate. More surprisingly, the same result is obtained on a 2D triangular lattice with an analogous dynamics (spin-up (-down) rotates the velocity by $+(-)2\pi/3$) [5] and on the square lattice (when all scatterers are initially in the same state and rotate the velocity of the particle by $\pm\pi/2$ depending on the state). The latter model is known in the literature as “Langton’s ant” [3]. As discussed in [6], the distribution of first-passage times *along the direction of propagation* in all of these examples can be cast in the general form

$$\widehat{f}(t/\delta t; (r + \rho)/\delta r) = \sum_{j=0}^{\infty} \tilde{p}_j \widehat{f}((t - \tau_j)/\delta t; r/\delta r), \quad (22)$$

where ρ represents the elementary space increment along the propagation strip and $\tau_j = (1 + a_j)b\delta t$ (a and b are lattice-dependent integer constants [6]). Equation (22) can be mapped onto the form given in eq. (1) by setting $p_{(1+a_j)b} = \tilde{p}_j$ and all other p_j ’s = 0. All of these models will therefore, in the limit of large spatial separations, be described by the propagation-dispersion equation and the distribution of first-passage times will be Gaussian.

In fig. 1 we give an illustration of temporal diffusive behavior in an inhomogeneous system, where we compare the theoretical large-distance solution with simulation data. The time

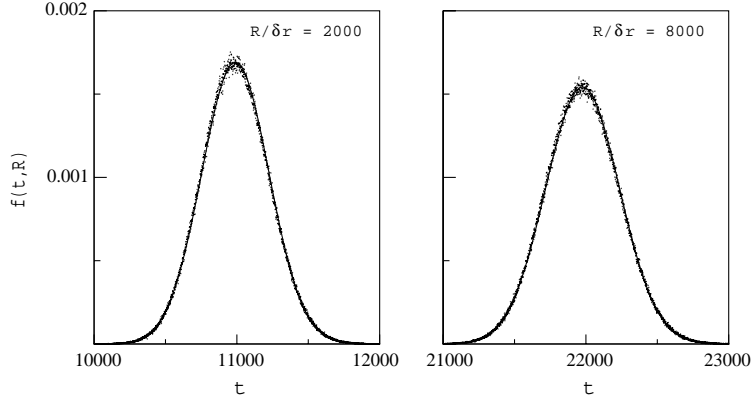


Fig. 1 – Temporal-dispersion curve: $f(t, R)$ at $R/\delta r = 2000$ and 8000 (in lattice units). Simulation data (dots) are obtained from the first-visit equation (22) with $\tilde{p}_{j=k} = p(1 - p)^{k-1}$, where $p \equiv p(r) = 0.1 + 10^{-4}r/\delta r$. The theoretical curve (solid line) is the Gaussian solution of the propagation-dispersion equation (11) with $\tau(R)/\delta t = Rc^{-1}(R)(\delta t)^{-1} = \sum_{r=1}^{r=R} p^{-1}(r) = 10989$ and 21977 , and half-width $[2R\gamma(R)]^{1/2}(\delta t)^{-1} = [\sum_{r=1}^{r=R} (1 - p(r))p^{-2}(r)]^{1/2} = 334$ and 366 , at $R/\delta r = 2000$ and 8000 , respectively.

delay probability is taken to be $\tilde{p}_{j=k} = p(1 - p)^{k-1}$, where p is linearly space dependent: $p \equiv p(r) = p(0) + \chi r/\delta r$. The dots are the simulation data obtained by solving numerically the microscopic equation (22) and the solid line is the solution of the propagation-dispersion equation (11). Notice that for space-independent probabilities, the width of the Gaussian in (9) increases like \sqrt{r} , *i.e.* in the example given in fig. 1 the width at $8000\delta r$ should be twice that at $2000\delta r$. Here we observe essentially no change in the respective widths, a consequence of the spatial dependence of the waiting-time probabilities.

Recently, Buminovich and Khlabytova [11] have studied models in which the scatterers only change state after multiple scattering events. In this case, the distribution of elementary waiting times becomes dependent on the lattice position, and the propagation speed and dispersion coefficient acquire a spatial dependence. Thus, while the distributions of first-passage times are still Gaussian, they are not “diffusive” in the usual sense since the inverse propagation speed and dispersion coefficient are not constants (eqs. (11)-(13) and ref. [7]).

A more practical example is found in a recent report [12] which describes an experiment where small beads are dropped into a container filled with larger beads. The small beads, driven by gravity, percolate through the array of larger beads, and their propagation is carefully measured. Intuitively, one would imagine that the various deflections of the small bead as it collides with the larger ones would induce time delays in its downward propagation, in which case the distribution of arrival times would be given by eq. (9). This is indeed confirmed by the experimental results which exhibit the signature of a temporal-dispersion process (see fig. 9 in ref. [12]).

In summary, we have demonstrated that the distribution of first-visit times of a particle propagating with stochastic time delays on a one-dimensional lattice, or the one-dimensional version of a multidimensional process, satisfies a temporal propagation-dispersion equation in the limit of large separations. This generic behavior is analogous to the generic diffusive behavior which describes the spatial distribution of the same process as a function of time. For a simple biased random walker, the propagation speed is the same in the temporal and spatial descriptions, while the temporal- and spatial-dispersion coefficients differ. The temporal-

dispersion description is relevant to a class of one- and two-dimensional cellular automata in which mobile particles and fixed scatterers interact with one another. Experiments in granular media also show behavior described by temporal dispersivity. We have restricted our discussion to the case where the variance of the elementary time delay processes exists. There is an interesting class of similar processes which are described by power law distributions, *e.g.* $p_j \sim j^{-(1+\nu)}$, in which case, for $0 < \nu \leq 1$, the distribution appearing in the central limit theorem is no longer Gaussian (see, *e.g.*, [13] and the appendix in [14]). This and the related problem of absorbing barriers [15] will be treated in a forthcoming publication.

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