

Counting statistics: A Feynman-Kac perspective

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By building upon a Feynman-Kac formalism, we assess the distribution of the number of collisions in a given region for a broad class of discrete-time random walks in absorbing and nonabsorbing media. We derive the evolution equation for the generating function of the number of collisions, and we complete our analysis by examining the moments of the distribution and their relation to the walker equilibrium density. Some significant applications are discussed in detail: in particular, we revisit the gambler's ruin problem and generalize to random walks with absorption the arcsine law for the number of collisions on the half-line.

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I. INTRODUCTION

Many physical processes can be described in terms of a random walker evolving in the phase space [1–4], and one is often interested in assessing the portion of time t_V that the system spends in a given region V of the explored space when observed up to time t [5–13]. This is key to understanding the dynamics of radiation transport, gas flows, research strategies, or chemical and biological species migration in living bodies, just to name a few, the time spent in V being proportional to the interaction of the particle with the target medium [14–20].

For Brownian motion, a celebrated approach to characterizing the probability density of the residence time t_V has been provided by Kac (based on Feynman path integrals) in a series of seminal papers, and later extended to Markov continuous-time processes [21–24]. For a review, see, for instance, [25]. The Feynman-Kac formalism basically allows us to write down the evolution equation for the moment generating function of t_V for arbitrary domains, initial conditions, and displacement kernels. This approach has recently attracted a renewed interest [26–33], and it has also been extended to non-Markovian processes [10,34–36]. As a particular case, imposing leakage boundary conditions leads to the formulation of first-passage problems [5,6,37]. However, for those physical systems that are intrinsically discrete, the natural variable is the number of collisions n_V in V when the process is observed up to the n th step, rather than time t_V [33,38–41]. When n_V is large, we can approximate the number of collisions in V by $n_V \propto t_V$ (the so-called diffusion limit), but this simple proportionality breaks down when V is small with respect to the typical step size of the walker and/or the effects of absorption are not negligible, so the diffusion limit is not attained [32,42].

In this paper, we derive a discrete Feynman-Kac equation for the evolution of the probability generating function of n_V for a broad class of stochastic processes in absorbing and nonabsorbing media, and we illustrate this approach by explicitly working out calculations for some significant examples, such as the gambler's ruin problem or the arcsine law. For the arcsine law, in particular, the Feynman-Kac formulas allow us to generalize the well-known Sparre Andersen results to random walks with absorption. Our analysis of the counting statistics is then completed by examining the moments of n_V , which can also be obtained by building upon the Feynman-Kac

formalism, and their asymptotic behavior when n is large. In particular, we show that the asymptotic moments can be expressed as a function of the particle equilibrium distribution, which generalizes analogous results previously derived in terms of survival probabilities [32].

This paper is organized as follows. In Sec. II, we introduce a discrete Feynman-Kac formula for a class of random walkers in absorbing and nonabsorbing media. Then, in Sec. III we discuss some applications where the generating function can be explicitly inverted to give the probability of the number of collisions. In Sec. IV, we extend our analysis to the moments of n_V , and in Sec. V we examine some examples of moment formulas. A short digression on the diffusion limit is given in Sec. VI. Perspectives are finally discussed in Sec. VII.

II. FEYNMAN-KAC EQUATIONS

Consider the random walk of a particle starting from an isotropic point source $S(\mathbf{r}|\mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0)$ located at \mathbf{r}_0 . At each collision, the particle can be either scattered (i.e., change direction) with probability p_s or absorbed with probability $p_a = 1 - p_s$ (in which case the trajectory terminates). We introduce the quantity $T(\mathbf{r}' \rightarrow \mathbf{r})$, namely the probability density of performing a displacement from \mathbf{r}' to \mathbf{r} , between any two collisions [43,44]. For the sake of simplicity, we assume that scattering is isotropic and that displacements are equally distributed.

Suppose that a particle emitted from \mathbf{r}_0 is observed up to entering the n th collision. Our aim is to characterize the distribution $P_n(n_V|\mathbf{r}_0)$, where n_V is the number of collisions in a domain V . We can formally define

$$n_V(n) = \sum_{k=1}^n V(\mathbf{r}_k), \quad (1)$$

where $V(\mathbf{r}_k)$ is the marker function of the region V , which takes the value 1 when the point $\mathbf{r}_k \in V$, and vanishes elsewhere. We adopt here the convention that the source is not counted, i.e., the sum begins at $k = 1$. Clearly, n_V is a stochastic variable depending on the realizations of the underlying process and on the initial condition \mathbf{r}_0 . The behavior of its distribution, $P_n(n_V|\mathbf{r}_0)$, is most easily described in terms of the associated probability generating function,

$$F_n(u|\mathbf{r}_0) = \langle u^{n_V} \rangle_n(\mathbf{r}_0) = \sum_{n_V=0}^{+\infty} P_n(n_V|\mathbf{r}_0) u^{n_V}, \quad (2)$$

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which can be interpreted as the discrete Laplace transform (the transformed variable being u) of the collision number distribution. The derivation of an evolution equation for $F_n(u|\mathbf{r}_0)$ is made simpler if we initially consider trajectories starting with a particle entering its first collision at \mathbf{r}_1 . Random flights are semi-Markovian (i.e., Markovian at collision points), which allows splitting the trajectory into a first jump, from \mathbf{r}_1 to $\mathbf{r}_1 + \Delta$ (the displacement Δ obeying the jump length density T), and then a path from $\mathbf{r}_1 + \Delta$ to \mathbf{r}_n , conditioned to the fact that the particle is not absorbed at \mathbf{r}_1 . If the collision is an absorption, the trajectory ends and there will be no further events contributing to n_V . Hence,

$$\tilde{F}_{n+1}(u|\mathbf{r}_1) = \langle p_s u^{V(\mathbf{r}_1)+V(\mathbf{r}_1+\Delta)+\dots+V(\mathbf{r}_{n+1})} + p_a u^{V(\mathbf{r}_1)} \rangle, \quad (3)$$

where the term $u^{V(\mathbf{r}_1)}$ is not stochastic and can be singled out. The tilde is used to recall that we are considering trajectories starting with a single particle entering the first collision at \mathbf{r}_1 . By observing that $\langle u^{V(\mathbf{r}_1+\Delta)+\dots+V(\mathbf{r}_{n+1})} \rangle = \tilde{F}_n(u|\mathbf{r}_1 + \Delta)$, we have then the following equation for the generating function:

$$\tilde{F}_{n+1}(u|\mathbf{r}_1) = u^{V(\mathbf{r}_1)} [p_s \langle \tilde{F}_n(u|\mathbf{r}_1 + \Delta) \rangle + p_a], \quad (4)$$

where expectation is taken with respect to the random displacement Δ . We make use then of the discrete Dynkin's formula, which relates any sufficiently well behaved function f of a stochastic process with the adjoint kernel $T^*(\mathbf{r}' \rightarrow \mathbf{r})$ associated to $T(\mathbf{r}' \rightarrow \mathbf{r})$ [45], namely

$$\langle f(\mathbf{r}_1 + \Delta) \rangle = \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) f(\mathbf{r}') d\mathbf{r}'. \quad (5)$$

Intuitively, the adjoint kernel T^* displaces the walker backward in time. We therefore obtain the discrete Feynman-Kac equation

$$\tilde{F}_{n+1}(u|\mathbf{r}_1) = u^{V(\mathbf{r}_1)} \left[p_s \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) \tilde{F}_n(u|\mathbf{r}') d\mathbf{r}' + p_a \right], \quad (6)$$

with the initial condition $\tilde{F}_1(u|\mathbf{r}_1) = u^{V(\mathbf{r}_1)}$. Finally, by observing that the first collision coordinates \mathbf{r}_1 obey the probability density $T(\mathbf{r}_0 \rightarrow \mathbf{r}_1)$, it follows that

$$F_n(u|\mathbf{r}_0) = \int \tilde{F}_n(u|\mathbf{r}_1) T(\mathbf{r}_0 \rightarrow \mathbf{r}_1) d\mathbf{r}_1. \quad (7)$$

Knowledge of $F_n(u|\mathbf{r}_0)$ allows us to explicitly determine $P_n(n_V|\mathbf{r}_0)$. Indeed, by construction the probability generating function $F_n(u|\mathbf{r}_0)$ is a polynomial in the variable u , the coefficient of each power u^k being $P_n(n_V = k|\mathbf{r}_0)$. In particular, the probability that the particles never touch (or come back to, if the source $\mathbf{r}_0 \in V$) the domain V is obtained by evaluating $F_n(u|\mathbf{r}_0)$ at $u = 0$, i.e., $P_n(0|\mathbf{r}_0) = F_n(0|\mathbf{r}_0)$.

III. COLLISION NUMBER DISTRIBUTION: EXAMPLES OF CALCULATIONS

Direct calculations based on the discrete Feynman-Kac formulas, Eqs. (6) and (7), are in some cases amenable to exact results concerning $P_n(n_V|\mathbf{r}_0)$, at least for simple geometries

and displacement kernels. In this section, we shall discuss some relevant examples.

A. The gambler's ruin

Consider a gambler whose initial amount of money is $x_0 \geq 0$. At each (discrete) time step, the gambler either wins or loses a fair bet, and his capital increases or decreases, respectively, by some fixed quantity s with equal probability. One might be interested to know the probability that the gambler is not ruined (i.e., that his capital has not reached zero, yet) at the n th bet, starting from the initial capital x_0 . This well-known problem [46] can be easily recast in the Feynman-Kac formalism by setting a particle in motion on a straight line, starting from x_0 , with scattering probability $p_s = 1$ and a discrete displacement kernel $T(x' \rightarrow x) = \delta(x - x' - s)/2 + \delta(x - x' + s)/2$. Setting $s = 1$ amounts to expressing the capital x_0 in multiple units of the bet, and entails no loss of generality. The counting condition is imposed by assuming a Kronecker delta $V(x) = \delta_{x,0}$ in Eq. (6): since the walker cannot cross $x = 0$ without touching it, solving the resulting equation for the quantity $F_n(0|x_0)$ gives, therefore, the required probability that the gambler is not ruined at the n th bet. We integrate now Eq. (6) and use Eq. (7): we start from the initial condition $\tilde{F}_1(u|x_1) = u^{V(x_1)} = u^{\delta_{x_1,0}}$. Then, by observing that by symmetry T and T^* have the same functional form, and performing the integrals Eq. (7) over the δ functions, we obtain $F_1(u|x_0) = (u^{\delta_{x_0+1,0}} + u^{\delta_{x_0-1,0}})/2$. By injecting thus $\tilde{F}_1(u|x_1)$ in Eq. (6) and integrating again over the δ functions, we get $\tilde{F}_2(u|x_1) = u^{\delta_{x_1,0}}(u^{\delta_{x_1-1,0}} + u^{\delta_{x_1+1,0}})/2$. Finally, by integrating (7) we get $F_2(u|x_0) = (u^{\delta_{x_0-1,0}}u^{\delta_{x_0-2,0}} + u^{\delta_{x_0+1,0}}u^{\delta_{x_0,0}} + u^{\delta_{x_0-1,0}}u^{\delta_{x_0,0}} + u^{\delta_{x_0+1,0}}u^{\delta_{x_0+2,0}})/4$. Proceeding by recursion and identifying the coefficient of the zeroth-order term in the polynomial yields then the first terms in the series,

$$\begin{aligned} P_n(0|1) &= \left\{ \frac{1}{2}, \frac{2}{4}, \frac{3}{8}, \frac{6}{16}, \frac{10}{32}, \frac{20}{64}, \frac{35}{128}, \frac{70}{256}, \dots \right\}, \\ P_n(0|2) &= \left\{ \frac{2}{2}, \frac{3}{4}, \frac{6}{8}, \frac{10}{16}, \frac{20}{32}, \frac{35}{64}, \frac{70}{128}, \frac{126}{256}, \dots \right\}, \\ P_n(0|3) &= \left\{ \frac{2}{2}, \frac{4}{4}, \frac{7}{8}, \frac{14}{16}, \frac{25}{32}, \frac{50}{64}, \frac{91}{128}, \frac{182}{256}, \dots \right\}, \\ P_n(0|4) &= \left\{ \frac{2}{2}, \frac{4}{4}, \frac{8}{8}, \frac{15}{16}, \frac{30}{32}, \frac{56}{64}, \frac{112}{128}, \frac{210}{256}, \dots \right\} \end{aligned} \quad (8)$$

for $x_0 = 1, 2, 3, \dots$, respectively.¹ After some rather lengthy algebra, by induction one can finally recognize the formula

$$P_n(0|x_0) = \sum_{k=0}^{\lfloor (n+x_0-1)/2 \rfloor} \left[\binom{n}{k} - \binom{n}{k-x_0} \right] 2^{-n}, \quad (9)$$

$\lfloor \cdot \rfloor$ denoting the integer part. The quantity $P_n(0|x_0)$ is displayed in Fig. 1 as a function of n for a few values of x_0 . The larger the initial capital x_0 , the longer $P_n(0|x_0) \simeq 1$ before decreasing. At large n , taking the limit of Eq. (9) leads to the scaling $P_n(0|x_0) \simeq \sqrt{2/\pi} x_0 n^{-1/2}$, in agreement with the findings in

¹The quantity $u^{\delta_{x,0}}$ evaluated at $u = 0$ is equal to 1 when $x = 0$, and vanishes otherwise.

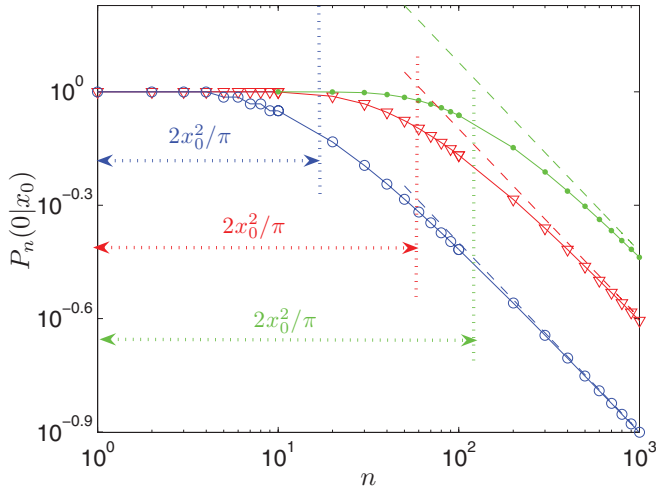


FIG. 1. (Color online) The probability $P_n(0|x_0)$ that the gambler is not ruined at the n th bet, given an initial capital x_0 . Bets are modeled by discrete random increments of fixed size $s = \pm 1$. Blue circles: $x_0 = 5$; red triangles: $x_0 = 10$; green dots: $x_0 = 15$. Lines have been added to guide the eye. Dashed lines correspond to the asymptotic result $P_n(0|x_0) \simeq \sqrt{2/\pi x_0} n^{-1/2}$. The interval $2x_0^2/\pi$ is also shown for each x_0 .

Ref. [47]. This means that asymptotically the gambler is almost sure not to be ruined, yet, up to $n \simeq 2x_0^2/\pi$ bets. Note that Eq. (9) is the survival probability of the gambler: the first-passage probability $W_n(0|x_0)$, i.e., the probability that the gambler is ruined exactly at the n th bet, can be obtained from $W_n(x_0) = P_{n-1}(0|x_0) - P_n(0|x_0)$. As a particular case, for $0 < x_0 \leq n$ and $n + x_0$ even, we recover the result in Ref. [46], namely

$$W_n(x_0) = \frac{x_0}{2^n n} \binom{n}{\frac{n+x_0}{2}}. \quad (10)$$

Finally, observe that when $x_0 = 0$,

$$P_n(0|0) = \left\{ 1, \frac{1}{2}, \frac{2}{4}, \frac{3}{8}, \frac{6}{16}, \frac{10}{32}, \frac{20}{64}, \frac{35}{128}, \dots \right\} \quad (11)$$

for $n \geq 1$. This is easily recognized as being the series

$$P_n(0|0) = \binom{n-1}{\lfloor \frac{n-1}{2} \rfloor} 2^{1-n}, \quad (12)$$

which is, however, unphysical, since the gambler should not be allowed to bet when lacking an initial amount of money.

B. The arcsine law with discrete jumps

Consider a walker on a straight line, starting from x_0 . We are interested in assessing the distribution $P_n(n_V|x_0)$ of the number of collisions n_V that the walker performs at the right of the starting point when observed up to the n th collision. This amounts to choosing $V(x) = H(x - x_0)$, H being the Heaviside step function, in Eq. (6). To fix the ideas, without loss of generality we set $x_0 = 0$, and we initially assume that $p_s = 1$, i.e., the walker cannot be absorbed along the trajectory. This is a well known and long-studied problem for both Markovian and non-Markovian processes [10,13,46,48–51]: for Brownian motion, the average residence time in V is simply $\langle t_V \rangle_t = t/2$, whereas

t_V itself is known to obey the so-called Lévy's arcsine law $P_t(t_V) = 1/\sqrt{t_V(t-t_V)}\pi$, whose U shape basically implies that the particle will most often spend its time being always either on the positive or negative side of the axis [46,47,52]. This counterintuitive result has been shown to asymptotically hold also for discrete-time random walks without absorption, for which one has $P_n(n_V|0) \simeq 1/\sqrt{n_V(n-n_V)}\pi$ when n and n_V are large (see, for instance, [47]).

The Feynman-Kac approach allows us to explicitly derive $P_n(n_V|0)$. Again, assume a displacement kernel with discrete jumps $T(x' \rightarrow x) = \delta(x - x' - s)/2 + \delta(x - x' + s)/2$, with $s = 1$. Then, by integrating Eq. (6) and subsequently using Eq. (7), we compute the coefficients of the polynomial, which can be organized in an infinite triangle, whose first terms read

n	$n_V = 0$	1	2	3	4	5	6	7
0	1							
1	$\frac{1}{2}$	$\frac{1}{2}$						
2	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{2}{4}$					
3	$\frac{2}{8}$	$\frac{1}{8}$	$\frac{2}{8}$	$\frac{3}{8}$				
4	$\frac{3}{16}$	$\frac{2}{16}$	$\frac{2}{16}$	$\frac{3}{16}$	$\frac{6}{16}$			
5	$\frac{6}{32}$	$\frac{3}{32}$	$\frac{4}{32}$	$\frac{3}{32}$	$\frac{6}{32}$	$\frac{10}{32}$		
6	$\frac{10}{64}$	$\frac{6}{64}$	$\frac{6}{64}$	$\frac{6}{64}$	$\frac{6}{64}$	$\frac{10}{64}$	$\frac{20}{64}$	
7	$\frac{20}{128}$	$\frac{10}{128}$	$\frac{12}{128}$	$\frac{9}{128}$	$\frac{12}{128}$	$\frac{10}{128}$	$\frac{20}{128}$	$\frac{35}{128}$

Observe that this result is independent of s . To identify the elements $P_n(n_V|0)$, we initially inspect the column $n_V = 1$ of the triangle, and we recognize the underlying series as being given by terms of the kind $\binom{n-2}{\lfloor \frac{n-2}{2} \rfloor} 2^{-n}$. Then we realize that columns with $n_V \geq 2$ are related to the first column by a shift in the index n . The column $n_V = 0$ can be obtained from normalization. Proceeding by induction, the elements in the triangle can be finally recast in the compact formula

$$P_n(n_V|0) = \binom{n-n_V-1}{\lfloor \frac{n-n_V-1}{2} \rfloor} \binom{n_V}{\lfloor \frac{n_V}{2} \rfloor} 2^{-n}. \quad (13)$$

Note that our result is slightly different from Ref. [46], where collisions are counted in pairs. When both n and n_V are large, we obtain the limit curve $P_n(n_V|0) \simeq 1/\sqrt{n_V(n-n_V)}\pi$.

When the scattering probability can vary in $0 \leq p_s \leq 1$, the triangle can be generated as above, and the first few terms read

n	$n_V = 0$	1	2	3	4
0	1				
1	$\frac{1}{2}$	$\frac{1}{2}$			
2	$\frac{2-p_s}{4}$	$\frac{2-p_s}{4}$	$\frac{2p_s}{4}$		
3	$\frac{4-2p_s}{8}$	$\frac{4-2p_s-p_s^2}{8}$	$\frac{2p_s(2-p_s)}{8}$	$\frac{3p_s^2}{8}$	
4	$\frac{8-4p_s-p_s^3}{16}$	$\frac{8-4p_s-2p_s^2}{16}$	$\frac{2p_s(4-2p_s-p_s^2)}{16}$	$\frac{3p_s^2(2-p_s)}{16}$	$\frac{6p_s^3}{16}$

Now, the identification of the polynomial coefficients $P_n(n_V|0)$ becomes more involved, because each coefficient is itself a polynomial with respect to p_s . The strategy in the

identification is the same as above. By induction, the column for $n_V = 1$ can be identified as being

$$P_n(1|0) = \frac{1 - p_s + \sqrt{1 - p_s^2}}{4} + \left(\frac{p_s}{2}\right)^{4+2y} \binom{2+2y}{1+y} \times \frac{{}_2F_1\left(1, \frac{3}{2} + y, 3 + y, p_s^2\right)}{2(2+y)} \quad (14)$$

for $n \geq 2$, with $y = \lceil (n-3)/2 \rceil$, and $P_1(1|0) = 1/2$. Once $P_n(1|0)$ is known, by inspection one realizes that the other columns $P_n(n_V|0)$ are related by

$$P_n(n_V|0) = \left(\frac{p_s}{2}\right)^{n_V-1} \binom{n_V}{\lceil \frac{n_V}{2} \rceil} P_{n-n_V+1}(1|0) \quad (15)$$

for $n_V \geq 2$. The probability $P_n(0|0)$ is finally obtained from normalization, and reads

$$P_n(0|0) = \frac{p_s - 1 + \sqrt{1 - p_s^2}}{2p_s} + \left(\frac{p_s}{2}\right)^{2+2z} \binom{2z}{z} \times \frac{{}_2F_1\left(\frac{1}{2} + z, 1, 2 + z, p_s^2\right)}{p_s(1+z)}, \quad (16)$$

with $z = \lceil n/2 \rceil$. These results generalize Eq. (13), and are illustrated in Fig. 2, where we compare $P_n(n_V|0)$ as a function of n_V for $n = 10$ and different values of p_s . When $p_s = 1$, the distribution approaches a U shape, as expected. As soon as $p_s < 1$, the shape changes considerably, and in particular $P_n(n_V|0)$ becomes strongly peaked at $n_V = 0$ as the effects of absorption overcome scattering. The presence of a second peak at $n_V = n$ is visible when $p_s \simeq 1$ and progressively disappears as p_s decreases: when p_s is small, $P_n(n_V|0)$ has an exponential

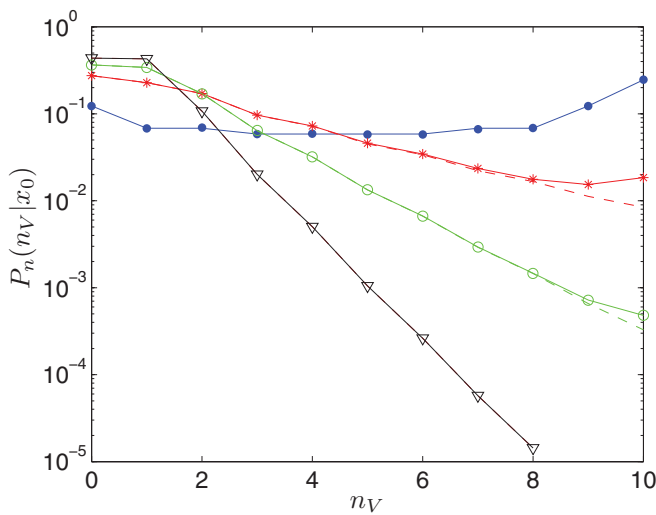


FIG. 2. (Color online) The arcsine law $P_n(n_V|x_0)$ with discrete jump lengths, as a function of n_V . The starting point is $x_0 = 0$, and $n = 10$. Blue dots: $p_s = 1$; red stars: $p_s = 3/4$; green circles: $p_s = 1/2$; black triangles: $p_s = 1/4$. Lines have been added to guide the eye. Dashed curves are the asymptotic Eq. (17) for the corresponding value of p_s .

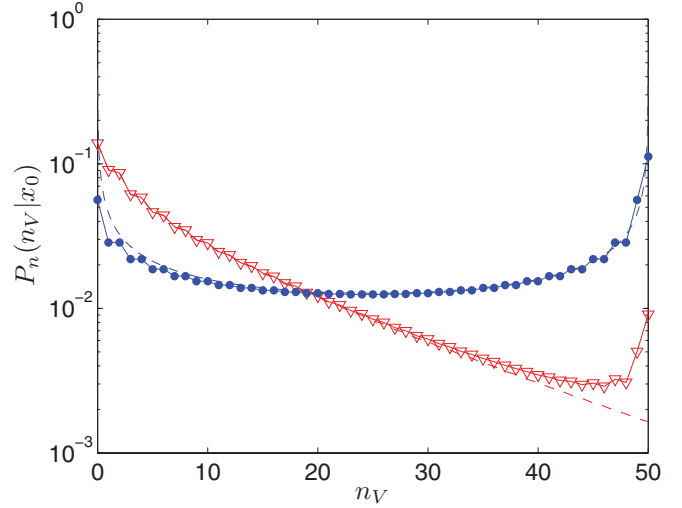


FIG. 3. (Color online) The arcsine law $P_n(n_V|x_0)$ with discrete jump lengths, as a function of n_V . The starting point is $x_0 = 0$, and $n = 50$. Blue dots: $p_s = 1$; dashed line: the asymptotic distribution $1/\sqrt{n_V(n-n_V)}\pi$. Red triangles: $p_s = 0.95$; dashed asymptotic Eq. (17).

tail. When n is large, $P_n(n_V|0)$ approaches the asymptotic curve

$$P_\infty(n_V|0) = \left(\frac{p_s}{2}\right)^{n_V-1} \binom{n_V}{\lceil \frac{n_V}{2} \rceil} \frac{1 - p_s + \sqrt{1 - p_s^2}}{4} \quad (17)$$

for $n_V \geq 1$, and $P_\infty(0|0) = (p_s - 1 + \sqrt{1 - p_s^2})/2p_s$. Remark that when $p_s = 1$, this means that the U shape for large n collapses on the two extremes at $n_V = 0$ and $n_V = n$. Equation (17) is an excellent approximation of $P_n(n_V|0)$ when the scattering probability is not too close to $p_s \simeq 1$: as expected, the discrepancy between the exact and asymptotic probability is most evident when $n_V \simeq n$, as shown in Fig. 2. Figure 3 displays $P_n(n_V|0)$ as a function of n_V for $n = 50$ in order to emphasize the effects of p_s : when $p_s = 1$, the probability $P_n(n_V|0)$ is almost superposed to the asymptotic curve $P_n(n_V|0) \simeq 1/\sqrt{n_V(n-n_V)}\pi$, whereas a deviation in the scattering probability as small as $p_s = 0.95$ is sufficient to radically change the shape of the collision number distribution. Finally, observe that when n_V is also large, which implies $p_a \ll 1$, Eq. (17) behaves as

$$P_\infty(n_V|0) \simeq \sqrt{\frac{1 - p_s}{\pi n_V}} e^{-(1-p_s)n_V}. \quad (18)$$

C. The arcsine law with continuous jumps

When the displacement kernel $T(x' \rightarrow x)$ is continuous and symmetric, $p_s = 1$, and $x_0 = 0$, the distribution of the number of collisions n_V falling in $x \geq x_0$ is universal, in that it does not depend on the specific functional form of $T(x' \rightarrow x)$ (see [47] and references therein). This strong and surprising result stems from a Sparre Andersen theorem [53], whose proof is highly nontrivial (and does not apply to discrete jumps) [47]. This leaves the choice on the form of kernel $T(x' \rightarrow x)$, as far as it satisfies the hypotheses of the theorem. For the sake

of simplicity, we have assumed an exponential distribution of jump lengths, i.e., $T(x' \rightarrow x) = s \exp(-s|x - x'|)/2$, with $s = 1$. Starting from Eqs. (6) and (7), we can generate the infinite triangle.

n	$n_V = 0$	1	2	3	4	5	6	7
0	1							
1	$\frac{1}{2}$	$\frac{1}{2}$						
2	$\frac{3}{8}$	$\frac{2}{8}$	$\frac{3}{8}$					
3	$\frac{3}{16}$	$\frac{5}{16}$	$\frac{5}{16}$	$\frac{3}{16}$				
4	$\frac{35}{128}$	$\frac{20}{128}$	$\frac{18}{128}$	$\frac{20}{128}$	$\frac{35}{128}$			
5	$\frac{63}{256}$	$\frac{35}{256}$	$\frac{30}{256}$	$\frac{30}{256}$	$\frac{35}{256}$	$\frac{63}{256}$		
6	$\frac{231}{1024}$	$\frac{126}{1024}$	$\frac{105}{1024}$	$\frac{100}{1024}$	$\frac{105}{1024}$	$\frac{126}{1024}$	$\frac{231}{1024}$	
7	$\frac{429}{2048}$	$\frac{231}{2048}$	$\frac{189}{2048}$	$\frac{175}{2048}$	$\frac{175}{2048}$	$\frac{189}{2048}$	$\frac{231}{2048}$	$\frac{429}{2048}$

It is easy to verify that the triangle indeed does not depend on s , and that other functional forms of $T(x' \rightarrow x)$ would lead to the same coefficients for the polynomials $P_n(n_V|0)$. This holds true also for Lévy flights, where $T(x' \rightarrow x)$ is a Lévy stable law and jump lengths are unbounded [47]. We start from the column $n_V = 1$, observe the relation with the subsequent columns $n_V \geq 2$, and finally derive the case $n_V = 0$ from normalization. Proceeding therefore by induction, we recognize that the elements of the triangle obey

$$P_n(n_V|0) = \binom{2n - 2n_V}{n - n_V} \binom{2n_V}{n_V} 2^{-2n}. \quad (19)$$

We recover here the celebrated results of the collision number distribution for discrete-time walks with symmetric continuous jumps in the absence of absorption [46,47]. When both n and n_V are large, it is possible to show that Eq. (19) converges to the U shape $1/\sqrt{n_V(n - n_V)}\pi$.

When the scattering probability is allowed to vary in $0 \leq p_s \leq 1$, it turns out that the polynomial coefficients $P_n(n_V|0)$ are the same for several different continuous symmetric kernels $T(x' \rightarrow x)$ (Lévy flights included), and we are therefore led to conjecture that the universality result for the case $p_s = 1$ carries over to random walks with absorption. This allows us to generalize the Sparre Andersen theorem for the collision number distribution on the half-line to a broader class of Markovian discrete-time processes. The first few terms in the triangle [which, for practical purposes, we have generated by resorting to $T(x' \rightarrow x) = s \exp(-s|x - x'|)/2$, with $s = 1$] read

n	$n_V = 0$	1	2	3	4	5
0	1					
1	$\frac{1}{2}$	$\frac{1}{2}$				
2	$\frac{4 - p_s}{8}$	$\frac{4 - 2p_s}{8}$	$\frac{3p_s}{8}$			
3	$\frac{8 - 2p_s - p_s^2}{16}$	$\frac{8 - 4p_s - p_s^2}{16}$	$\frac{3p_s(2 - p_s)}{16}$	$\frac{5p_s^2}{16}$		
4	$\frac{64 - 16p_s - 8p_s^2 - 5p_s^3}{128}$	$\frac{64 - 32p_s - 8p_s^2 - 4p_s^3}{128}$	$\frac{6p_s(8 - 4p_s - p_s^2)}{128}$	$\frac{20p_s^2(2 - p_s)}{128}$	$\frac{35p_s^3}{128}$	
5	$\frac{128 - 32p_s - 16p_s^2 - 10p_s^3 - 7p_s^4}{256}$	$\frac{128 - 64p_s - 16p_s^2 - 8p_s^3 - 5p_s^4}{256}$	$\frac{6p_s(16 - 8p_s - 2p_s^2 - p_s^3)}{256}$	$\frac{10p_s^2(8 - 4p_s - p_s^2)}{256}$	$\frac{35p_s^3(2 - p_s)}{256}$	$\frac{63p_s^4}{256}$

As above, identification of the terms $P_n(n_V|0)$ becomes more involved, because each coefficient is itself a polynomial with respect to p_s . By induction, the column for $n_V = 1$ can be identified as being

$$P_n(1|0) = \frac{\sqrt{1 - p_s}}{2} + \left(\frac{p_s}{4}\right)^n \binom{2n - 2}{n - 1} \times \frac{{}_2F_1\left(-\frac{1}{2} + n, 1, 1 + n, p_s\right)}{n} \quad (20)$$

for $n \geq 1$. Once $P_n(1|0)$ is known, the subsequent columns $P_n(n_V|0)$ are observed to obey

$$P_n(n_V|0) = \left(\frac{p_s}{4}\right)^{n_V - 1} \binom{2n_V - 1}{n_V} P_{n - n_V + 1}(1|0) \quad (21)$$

for $n_V \geq 2$. The probability $P_n(0|0)$ is finally obtained from normalization, and reads

$$P_n(0|0) = \frac{p_s - 1 + \sqrt{1 - p_s}}{p_s} + \left(\frac{p_s}{4}\right)^n \binom{2n}{n} \times \frac{{}_2F_1\left(\frac{1}{2} + n, 1, 2 + n, p_s\right)}{2(1 + n)}. \quad (22)$$

These results are illustrated in Fig. 4, where we compare $P_n(n_V|0)$ as a function of n_V for $n = 10$ and different values of p_s . The findings for continuous jumps closely resemble those for discrete displacements. When $p_s = 1$, the distribution approaches a U shape, as expected. As soon as $p_s < 1$, the shape again changes abruptly, and in particular $P_n(n_V|0)$ becomes strongly peaked at $n_V = 0$ when absorption dominates scattering. When p_s is small, $P_n(n_V|0)$ decreases exponentially at large n_V . When n is large, $P_n(n_V|0)$ approaches the asymptotic curve

$$P_\infty(n_V|0) = \left(\frac{p_s}{4}\right)^{n_V - 1} \binom{2n_V - 1}{n_V} \frac{\sqrt{1 - p_s}}{2} \quad (23)$$

for $n_V \geq 1$, and $P_\infty(0|0) = (p_s - 1 + \sqrt{1 - p_s})/p_s$. Again, Eq. (23) is an excellent approximation of $P_n(n_V|0)$ when the scattering probability is not too close to $p_s \simeq 1$, as shown in Fig. 4. Figure 5 displays $P_n(n_V|0)$ as a function of n_V for $n = 50$ in order to emphasize the effects of p_s : when $p_s = 1$, the probability $P_n(n_V|0)$ is almost superposed to the asymptotic curve $P_n(n_V|0) \simeq 1/\sqrt{n_V(n - n_V)}\pi$, whereas a deviation in the scattering probability as small as $p_s = 0.95$ is sufficient to radically change the shape of the collision number distribution. Finally, observe that when n_V is also large, which implies $p_a \ll 1$, Eq. (23) yields the same scaling as Eq. (18). All analytical calculations discussed here have been

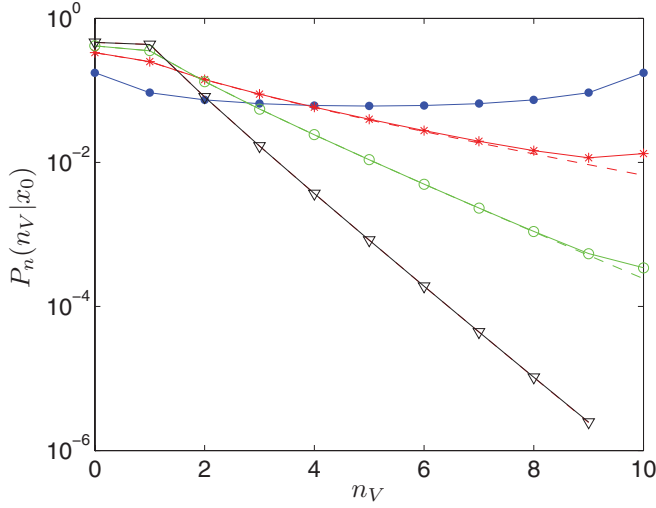


FIG. 4. (Color online) The arcsine law $P_n(n_V|x_0)$ with exponential jump lengths, as a function of n_V . The starting point is $x_0 = 0$, and $n = 10$. Blue dots: $p_s = 1$; red stars: $p_s = 3/4$; green circles: $p_s = 1/2$; black triangles: $p_s = 1/4$. Lines have been added to guide the eye. Dashed curves are the asymptotic Eq. (23) for the corresponding value of p_s .

verified by comparison with Monte Carlo simulations with 10^6 particles.

IV. MOMENTS FORMULAS

A complementary tool for characterizing the distribution $P_n(n_V|\mathbf{r}_0)$ is provided by the analysis of its moments. Toward this end, it is convenient to introduce the function $\tilde{G}_n(u|\mathbf{r}_1) = \tilde{F}_n(1/u|\mathbf{r}_1)$. By construction, $\tilde{G}_n(u|\mathbf{r}_1)$ is the (rising) factorial

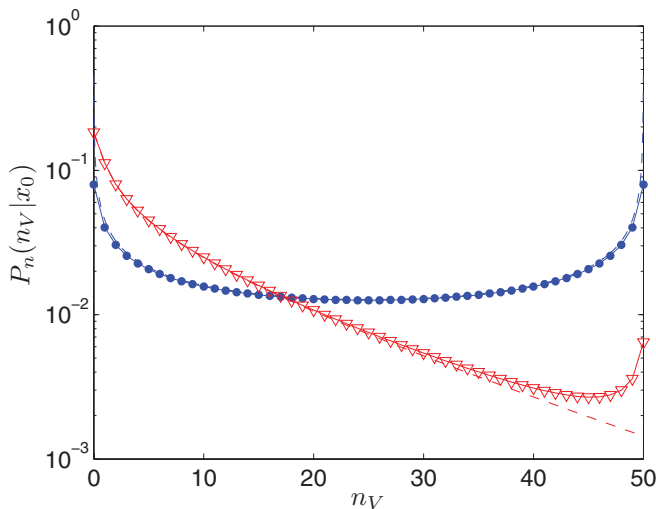


FIG. 5. (Color online) The arcsine law $P_n(n_V|x_0)$ with exponential jump lengths, as a function of n_V . The starting point is $x_0 = 0$, and $n = 50$. Blue dots: $p_s = 1$; dashed line: the asymptotic distribution $1/\sqrt{n_V(n-n_V)}\pi$. Red triangles: $p_s = 0.95$; dashed line: asymptotic Eq. (23).

moment generating function for trajectories entering their first collision at \mathbf{r}_1 , which implies

$$\langle \tilde{n}_V^{(m)} \rangle_n(\mathbf{r}_1) = (-1)^m \frac{\partial^m}{\partial u^m} \tilde{G}_n(u|\mathbf{r}_1)|_{u=1}, \quad (24)$$

$x^{(k)} = x(x+1)\cdots(x+k-1)$ being the rising factorial [54]. The tilde is used to recall that the moments refer to trajectories starting from the first collision at \mathbf{r}_1 . Combining Eqs. (6) and (24) yields the recursion property

$$\begin{aligned} \langle \tilde{n}_V^{(m)} \rangle_{n+1}(\mathbf{r}_1) - p_s \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) \langle \tilde{n}_V^{(m)} \rangle_n(\mathbf{r}') d\mathbf{r}' \\ = mV(\mathbf{r}_1) \langle \tilde{n}_V^{(m-1)} \rangle_{n+1}(\mathbf{r}_1) \end{aligned} \quad (25)$$

for $m \geq 1$, with the conditions $\langle \tilde{n}_V^{(0)} \rangle_n(\mathbf{r}_1) = 1$ and $\langle \tilde{n}_V^{(m)} \rangle_1(\mathbf{r}_1) = m!V(\mathbf{r}_1)$. Finally, the factorial moments $\langle n_V^{(m)} \rangle_n(\mathbf{r}_0)$ for particles emitted at \mathbf{r}_0 are obtained from

$$\langle n_V^{(m)} \rangle_n(\mathbf{r}_0) = \int \langle \tilde{n}_V^{(m)} \rangle_n(\mathbf{r}_1) T(\mathbf{r}_0 \rightarrow \mathbf{r}_1) d\mathbf{r}_1. \quad (26)$$

When trajectories are observed up to $n \rightarrow +\infty$, we can set $\langle n_V^{(m)} \rangle = \lim_{n \rightarrow +\infty} \langle n_V^{(m)} \rangle_n$, and from Eq. (25) we find

$$\begin{aligned} \langle \tilde{n}_V^{(m)} \rangle(\mathbf{r}_1) - p_s \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) \langle \tilde{n}_V^{(m)} \rangle(\mathbf{r}') d\mathbf{r}' \\ = mV(\mathbf{r}_1) \langle \tilde{n}_V^{(m-1)} \rangle(\mathbf{r}_1) \end{aligned} \quad (27)$$

for $m \geq 1$, provided that $\langle \tilde{n}_V^{(m)} \rangle(\mathbf{r}_1)$ is finite. It turns out that the asymptotic moments $\langle \tilde{n}_V^{(m)} \rangle(\mathbf{r}_1)$ are related to the equilibrium distribution of the particles [32,39,40]. To see this, we introduce the incident propagator $\Psi_n(\mathbf{r}|\mathbf{r}_0)$, i.e., the probability density of finding a particle emitted at \mathbf{r}_0 entering the n th collision ($n \geq 1$) at \mathbf{r} . We have

$$\Psi_{n+1}(\mathbf{r}|\mathbf{r}_0) = p_s \int T(\mathbf{r}' \rightarrow \mathbf{r}) \Psi_n(\mathbf{r}'|\mathbf{r}_0) d\mathbf{r}', \quad (28)$$

with $\Psi_1(\mathbf{r}|\mathbf{r}_0) = T(\mathbf{r}_0 \rightarrow \mathbf{r})$. We introduce then the incident collision density

$$\Psi(\mathbf{r}|\mathbf{r}_0) = \lim_{N \rightarrow \infty} \sum_{n=1}^N \Psi_n(\mathbf{r}|\mathbf{r}_0), \quad (29)$$

which can be interpreted as the particle equilibrium distribution [32,33,43,44]. Now, by making use of the formal Neumann series [43], from Eq. (28) it follows that the collision density satisfies the stationary integral transport equation

$$\Psi(\mathbf{r}|\mathbf{r}_0) = p_s \int T(\mathbf{r}' \rightarrow \mathbf{r}) \Psi(\mathbf{r}'|\mathbf{r}_0) d\mathbf{r}' + T(\mathbf{r}_0 \rightarrow \mathbf{r}). \quad (30)$$

The transport equation (30) can be understood as follows: at equilibrium, the stationary particle density entering a collision at \mathbf{r} for a source emitting at \mathbf{r}_0 is given by the sum of all contributions entering a collision at \mathbf{r}' , being scattered and then transported to \mathbf{r} , plus the contribution of the particles emitted from the source and never collided up to entering \mathbf{r} . Now, by resorting to the relation between T and its adjoint T^* in Eq. (A4), and observing that at equilibrium (for isotropic source and scattering)

$$\int T(\mathbf{r}_0 \rightarrow \mathbf{r}') \Psi(\mathbf{r}|\mathbf{r}') d\mathbf{r}' = \int \Psi(\mathbf{r}'|\mathbf{r}_0) T(\mathbf{r}' \rightarrow \mathbf{r}) d\mathbf{r}', \quad (31)$$

Eq. (27) can be inverted (see Appendix), and gives

$$\begin{aligned} \langle \tilde{n}_V^{(m)} \rangle(\mathbf{r}_1) &= m p_s \int_V \Psi(\mathbf{r}'|\mathbf{r}_1) \langle \tilde{n}_V^{(m-1)} \rangle(\mathbf{r}') d\mathbf{r}' \\ &\quad + m V(\mathbf{r}_1) \langle \tilde{n}_V^{(m-1)} \rangle(\mathbf{r}_1) \end{aligned} \quad (32)$$

for $m \geq 1$, where Ψ is the solution of Eq. (30). Thus, by using Eqs. (26) and (31), from Eq. (32) it follows that

$$\langle n_V^{(m)} \rangle(\mathbf{r}_0) = m \int_V \Psi(\mathbf{r}'|\mathbf{r}_0) \langle \tilde{n}_V^{(m-1)} \rangle(\mathbf{r}') d\mathbf{r}'. \quad (33)$$

Hence, by induction we finally get the desired relation between the factorial moments and the equilibrium distribution, namely

$$\langle n_V^{(m)} \rangle(\mathbf{r}_0) = \sum_{k=1}^m L_{m,k} p_s^{k-1} C_k(\mathbf{r}_0), \quad (34)$$

where

$$C_k(\mathbf{r}_0) = k! \int_V \cdots \int_V \prod_{i=1}^k d\mathbf{r}_i \Psi(\mathbf{r}_i|\mathbf{r}_{i-1}) \quad (35)$$

are k -fold convolution (Kac) integrals over the equilibrium distribution $\Psi(\mathbf{r}|\mathbf{r}_0)$, and the coefficients $L_{m,k} = \binom{m}{k} (m-1)! / (k-1)!$ are the Lah numbers [54]. Observe that a result analogous to Eq. (34) has been derived in Ref. [32] building upon survival probabilities.

V. FIRST AND SECOND MOMENT OF COLLISION NUMBER: EXAMPLES OF CALCULATIONS

To illustrate the approach proposed in the preceding section, we compute here the average collision number $\langle n_V^{(1)} \rangle_n(x_0)$ and the second factorial moment $\langle n_V^{(2)} \rangle_n(x_0)$ in a bounded domain V in one dimension. We choose an exponential displacement kernel $T(x' \rightarrow x) = s \exp(-s|x-x'|)/2$, with $s=1$, which is often adopted as a simplified random-walk model (the so-called exponential flights) to describe gas dynamics, radiation propagation, or biological species migration [55–60]. In this respect, the average $\langle n_V^{(1)} \rangle_n(x_0)$ is a measure of the passage of the particles through the region V (the deposited energy, for instance), whereas the second moment $\langle n_V^{(2)} \rangle_n(x_0)$ is proportional to the incertitude on the average [32,33].

The calculations stemming from Eqs. (25) and (26) are rather cumbersome, so it is preferable to visually represent our results instead of writing down the explicit formulas. In Fig. 6, we display the behavior of the moments $\langle n_V^{(1)} \rangle_n(x_0)$ and $\langle n_V^{(2)} \rangle_n(x_0)$ for the volume V being the interval $[-R, R]$, with $R=1$. When $p_s=1$, the moments diverge as n increases, since exponential flights in one dimension are recurrent random walks, and revisit their starting point infinitely many times. In particular, we observe that for large n , the average grows as $n^{1/2}$, and the second moment as n^1 , which is coherent with the results in Ref. [35] for Brownian motion. When $p_s < 1$, they converge instead to an asymptotic value, which can be computed based on Eq. (34) by observing that the collision density for this example is

$$\Psi(x|x_0) = \frac{e^{-\sqrt{1-p_s}|x-x_0|}}{2\sqrt{1-p_s}}, \quad (36)$$

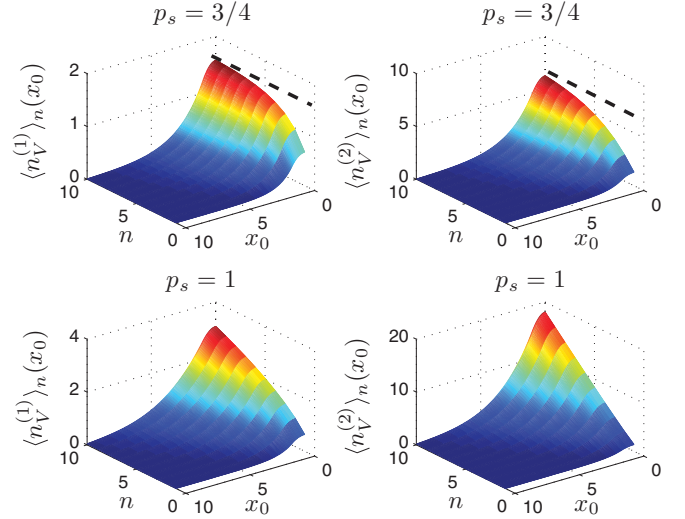


FIG. 6. (Color online) One-dimensional exponential flights in $V = [-1, 1]$. Upper half: First (left) and second factorial moment (right) of n_V as a function of n and x_0 , with $p_s = 3/4$. The asymptotic values for $x_0 = 0$ are shown as dashed lines for reference. Lower half: First (left) and second factorial moment (right) of n_V in the same domain, when $p_s = 1$.

as discussed in Ref. [32]. Moreover, Fig. 6 shows that the moments decrease as the distance of the source x_0 from the region V increases, as expected. As we have chosen here a symmetric interval, we have $\langle n_V^{(m)} \rangle_n(x_0) = \langle n_V^{(m)} \rangle_n(-x_0)$, so we can plot the moments only for positive values of x_0 . All results presented in this section have been verified by comparison with Monte Carlo simulations with 10^6 particles. Other kinds of boundary conditions (leakage, for instance, which implies that particles are lost upon crossing the frontier of V [32,33]) have also been successfully tested, but will not be presented here.

VI. DIFFUSION LIMIT

To conclude our analysis, in this section we comment on the scaling limit of the discrete Feynman-Kac equation, which is achieved when n_V is large, and at the same time the typical jump length ϵ is vanishingly small. We set $t_V = n_V dt$ and $t = n dt$, where dt is some small time scale, related to ϵ by the usual diffusion scaling $\epsilon^2 = 2D dt$, the constant D playing the role of a diffusion coefficient. When T is not symmetric, so that displacements have mean μ , we further require $\mu = v dt$, where the constant v is a velocity. By properly taking the limit of large n_V and vanishing dt , t_V converges to the residence time in V . The quantity n_V can only be large if the absorption probability p_a is small, and it is natural to set $p_a = \lambda_a dt$, the quantity λ_a being an absorption rate per unit of dt . Observe that when both ϵ and μ are small for any displacement kernel, we have the Taylor expansion

$$\int T(\mathbf{r}' \rightarrow \mathbf{r}) f(\mathbf{r}') d\mathbf{r}' \simeq f(\mathbf{r}) - \mu \partial_{\mathbf{r}} f(\mathbf{r}) + \frac{1}{2} \epsilon^2 \partial_{\mathbf{r}}^2 f(\mathbf{r}), \quad (37)$$

where the first-order derivative vanishes if the kernel is symmetric. A similar expansion holds for the kernel T^* ,

namely

$$\int T^*(\mathbf{r}' \rightarrow \mathbf{r}_0) f(\mathbf{r}') d\mathbf{r}' \simeq f(\mathbf{r}_0) + \mu \partial_{\mathbf{r}_0} f(\mathbf{r}_0) + \frac{1}{2} \epsilon^2 \partial_{\mathbf{r}_0}^2 f(\mathbf{r}_0). \quad (38)$$

It is expedient to introduce the quantity $Q_t(u|\mathbf{r}_0) = F_t(e^{-u}|\mathbf{r}_0)$, which is the moment generating function of $t_V = n_V dt$, i.e.,

$$\langle t_V^m \rangle_t(\mathbf{r}_0) = (-1)^m \frac{\partial^m}{\partial u^m} Q_t(u|\mathbf{r}_0)|_{u=0}, \quad (39)$$

when trajectories are observed up to $t = ndt$. Under the previous hypotheses, combining Eqs. (6) and (7) yields

$$Q_{t+dt}(u|\mathbf{r}_0) - Q_t(u|\mathbf{r}_0) \simeq \mathcal{L}_{\mathbf{r}_0}^* Q_t(u|\mathbf{r}_0) dt - uV(\mathbf{r}_0) Q_t(u|\mathbf{r}_0) dt + \lambda_a dt, \quad (40)$$

where we have neglected all terms vanishing faster than dt , and $\mathcal{L}_{\mathbf{r}_0}^* = D \partial_{\mathbf{r}_0}^2 + v \partial_{\mathbf{r}_0} - \lambda_a$. Taking the limit $dt \rightarrow 0$, we recognize then the Feynman-Kac equation for a Brownian motion with diffusion coefficient D , drift v , and absorption rate λ_a , namely

$$\frac{\partial Q_t(u|\mathbf{r}_0)}{\partial t} = \mathcal{L}_{\mathbf{r}_0}^* Q_t(u|\mathbf{r}_0) - uV(\mathbf{r}_0) Q_t(u|\mathbf{r}_0) + \lambda_a. \quad (41)$$

In other words, in the diffusion limit the statistical properties of the hit number in V behave as those of the residence time of a Brownian motion, as is quite naturally expected on physical grounds [27,28,33]. Finally, from Eq. (39) stems the recursion property for the moments

$$\frac{\partial \langle t_V^m \rangle_t(\mathbf{r}_0)}{\partial t} = \mathcal{L}_{\mathbf{r}_0}^* \langle t_V^m \rangle_t(\mathbf{r}_0) + mV(\mathbf{r}_0) \langle t_V^{m-1} \rangle_t(\mathbf{r}_0), \quad (42)$$

in agreement with the results in Refs. [29,30] for Brownian motion.

VII. CONCLUSIONS

In this paper, we have examined the behavior of the distribution $P_n(n_V|\mathbf{r}_0)$ of the number of collisions n_V in a region V for a broad class of stochastic processes in absorbing and nonabsorbing media. Key to our analysis has been a discrete version of the Feynman-Kac formalism. We have shown that this approach is amenable to explicit formulas for $P_n(n_V|\mathbf{r}_0)$, at least for simple geometries and displacement kernels. The moments of the distribution have also been detailed, and their asymptotic behavior for large n has been related to the walker equilibrium distribution. Finally, the diffusion limit and the convergence to the Feynman-Kac formulas for Brownian motion have been discussed.

We conclude by observing that a generalization of the present work to more realistic transport kernels, including anisotropic source and scattering, would be possible, for instance by resorting to the formalism proposed in Ref. [61]. Moreover, while in this paper we have focused on counting statistics, and therefore chosen $V(\mathbf{r})$ to be the marker function of a given domain in phase space, the Feynman-Kac formalism can be adapted with minor changes to describing the statistics of other kinds of functionals, such as, for instance, hitting probabilities [5,35,62].

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APPENDIX: THE STATIONARY MOMENT EQUATION

We want to solve an integral equation

$$f(\mathbf{r}_1) - p_s \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) f(\mathbf{r}') d\mathbf{r}' = g(\mathbf{r}_1) \quad (A1)$$

for the function $f(\mathbf{r}_1)$, where $g(\mathbf{r}_1)$ is known. We propose a solution in the form

$$f(\mathbf{r}_1) = p_s \int g(\mathbf{r}') \Psi(\mathbf{r}'|\mathbf{r}_1) d\mathbf{r}' + g(\mathbf{r}_1) \quad (A2)$$

and ask which is the equation satisfied by the integral kernel $\Psi(\mathbf{r}'|\mathbf{r}_1)$. By injecting Eq. (A2) into Eq. (A1), one obtains

$$\begin{aligned} & \int g(\mathbf{r}') \Psi(\mathbf{r}'|\mathbf{r}_1) d\mathbf{r}' \\ &= p_s \int \int \Psi(\mathbf{r}''|\mathbf{r}') T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) g(\mathbf{r}'') d\mathbf{r}' d\mathbf{r}'' \\ &+ \int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) g(\mathbf{r}') d\mathbf{r}'. \end{aligned} \quad (A3)$$

Recall that the adjoint and direct displacement kernels are related to each other by the scalar products

$$\begin{aligned} & \int g(\mathbf{r}) \int T(\mathbf{r}' \rightarrow \mathbf{r}) f(\mathbf{r}') d\mathbf{r}' d\mathbf{r} \\ &= \int f(\mathbf{r}) \int T^*(\mathbf{r}' \rightarrow \mathbf{r}) g(\mathbf{r}') d\mathbf{r}' d\mathbf{r} \end{aligned} \quad (A4)$$

for any test functions f and g [43]. From the definition of the scalar product in Eq. (A4), it follows that the second term on the right-hand side of Eq. (A3) is given by

$$\int T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) g(\mathbf{r}') d\mathbf{r}' = \int T(\mathbf{r}_1 \rightarrow \mathbf{r}') g(\mathbf{r}') d\mathbf{r}'. \quad (A5)$$

From Eqs. (A4) and (31), the first term on the right-hand side of Eq. (A3) becomes

$$\begin{aligned} & \int \int \Psi(\mathbf{r}''|\mathbf{r}') T^*(\mathbf{r}' \rightarrow \mathbf{r}_1) g(\mathbf{r}'') d\mathbf{r}' d\mathbf{r}'' \\ &= \int \int \Psi(\mathbf{r}'|\mathbf{r}_1) T(\mathbf{r}' \rightarrow \mathbf{r}'') g(\mathbf{r}'') d\mathbf{r}' d\mathbf{r}''. \end{aligned} \quad (A6)$$

Therefore, $\Psi(\mathbf{r}'|\mathbf{r}_1)$ obeys

$$\begin{aligned} & \int g(\mathbf{r}') \Psi(\mathbf{r}'|\mathbf{r}_1) d\mathbf{r}' \\ &= p_s \int \int \Psi(\mathbf{r}'|\mathbf{r}_1) T(\mathbf{r}' \rightarrow \mathbf{r}'') g(\mathbf{r}'') d\mathbf{r}' d\mathbf{r}'' \\ &+ \int T(\mathbf{r}_1 \rightarrow \mathbf{r}') g(\mathbf{r}') d\mathbf{r}', \end{aligned} \quad (A7)$$

which for the arbitrariness of $g(\mathbf{r}')$ finally implies Eq. (30), i.e., the required kernel Ψ satisfies the integral transport equation.

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