The span of one-dimensional multiparticle Brownian motion

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A closed-form expression is obtained for the time evolution of the territory covered by \( N \) independently diffusing particles starting from the origin in one-dimension, with and without bias. For the latter case, the transcendental-approximation derived is essentially exact for any number of particles. © 1996 American Institute of Physics. [S0021-9606(96)50208-0]

INTRODUCTION

The number of distinct sites visited by a random walker is considered one of the basic properties in lattice random walks. In one-dimension, the “number of sites” is equivalent to the “span” of a diffusion process namely, to the farthest point from the origin visited by time \( t \). In the continuous limit, the average span is closely related to the first moment in extrema statistics.

In recent years there has been growing interest in generalizing the one particle result to \( N \) independent particles. Specifically, the asymptotic large \( N \) and large \( r \) behavior has been considered using often involved mathematics. In the absence of bias, it is clear that the number of sites visited on the line is asymptotically \( \sqrt{t \ln N} \). However, only one work claims to obtain the correct prefactor for this term, and none have obtained a correction term or compared with the exact integral. In the presence of bias (e.g., an external field) the mathematical analysis becomes considerably more complex. While in principle this is just a problem in integration, in practice the most compact and accurate route for its evaluation remains obscure.

The present work focuses on the continuous limit, in which we obtain accurate approximations for the average \( N \)-particle span in one-dimension with and without bias. Using the most pedestrian approach, based on the observation that the \( N \)-particle survival probability tends asymptotically to a step-function, we derive a transcendental equation whose solution coincides asymptotically with the exact integral. For free-diffusion (bias-less case), matching this \( N \)-particle solution with that of a single-particle yields an approximation which is uniformly valid for any number of particles.

I. GENERAL

Consider \( N \) independent random walkers on the line, all initially located at the origin. With time, the particles diffuse away (diffusion coefficient \( D \)). The maximal distance that any of the particles has achieved from the origin in the \( +x \) direction by time \( t \) is the (one-sided) span, \( S_N(t) \), of the \( N \)-particle random walk. Denote by \( \Gamma_N(t|r) \) the probability that no particle reaches a distance \( r \) from the origin by time \( t \). Thus \( 1 - \Gamma_N(t|r) \) is the probability that at least one walker has reached \( x=r \) by time \( t \). In the continuous limit, the probability density for reaching a distance between \( r \) and \( r+dr \) is \( -d(1-\Gamma_N)/dr=d\Gamma_N/dr \), which is therefore the probability density for the \( N \)-particle span.

We are interested in estimating the mean distance (average span) covered by the diffusing particles in the \( +x \) direction. Averaging \( r \) with respect to \( d\Gamma_N/dr \) gives

\[
\langle S_N(t) \rangle = \int_0^\infty (d\Gamma_N(t|r)/dr)rdr = \int_0^\infty [1-\Gamma_N(t|r)]dr.
\]

The second equality follows from integration by parts, using \( 1-\Gamma_N(r) \rightarrow 0 \) for \( r \rightarrow \infty \). It could also be deduced directly, since a fraction \( 1-\Gamma_N \) of the population contributes an additional increment \( dr \) to the span. It is amusing to note that Eq. (1) is completely analogous to the definition of the mean lifetime, \( \tau \), which is given by

\[
\tau = -\int_0^\infty (d\Gamma_N(t|r)/dt)tdt = \int_0^\infty \Gamma_N(t|r)dt.
\]

This follows because the probability density of the lifetime is \( d\Gamma_N/dt \).

For \( N \)-independent particles the calculation simplifies considerably, since

\[
\Gamma_N(t|r) = \Gamma(t|r),
\]

where \( \Gamma = \Gamma_1 \) is the single-particle survival probability. It represents the probability of a particle, having started a distance \( r \) from the origin at \( t=0 \) to survive absorption at the origin up to time \( t \). Suppose one knows the probability density, \( p(x,t|r) \), which solves the appropriate diffusion equation subject to an absorbing boundary at the origin,

\[
p(0,t) = 0,
\]

and an initial delta-function condition

\[
p(x,0|r) = \delta(x-r), \quad r > 0.
\]

The probability of surviving absorption is then

\[
\Gamma(t|r) = \int_0^\infty p(x,t|r)dx.
\]

In simple cases analytic expressions for \( p(x,t|r) \) are available, so that the derivation becomes an exercise in integration. In the present communication we concentrate on the Smoluchowski equation for diffusion in a linear potential.

\[
\frac{\partial p(x,t|r)}{\partial t} = D \frac{\partial}{\partial x} \exp(-\mu x) \frac{\partial}{\partial x} \exp(\mu x)p(x,t|r),
\]
where \(\mu\) is a measure of the bias. For \(r>0\), \(\mu>0\) biases the diffusion process towards the origin, decreasing the survival probability.

The strategy of the derivation is simple and straightforward. \(\Gamma(t|r)\), calculated from Eq. (6), increases monotonically with \(r\): from 0 at \(r=0\) to 1 at infinity. For any function with this property, the \(N\)'th power approaches a step function
\[
\Gamma^N(t|r) \rightarrow \begin{cases} 0, & r<r^* \\ 1, & r>r^* \end{cases}
\]
as \(N\rightarrow\infty\). Since \(\Gamma(t|r)\) tends to unity only at infinity, \(r^*\) tends to infinity with increasing \(N\) (and \(t\)). In the limit of large \(N\), Eq. (1) reduces to
\[
\langle S_N(t) \rangle = r^*(N,t).
\]
As the derivative of a step-function, the probability density for the span of \(N\) independent particles approaches a delta-function
\[
d\Gamma_N/dr \rightarrow \delta(r-\langle S_N(t) \rangle),
\]
as \(N\rightarrow\infty\). This was suggested (without proof) in Ref. 10. The location, \(r^*\), of the step is estimated by the point of maximal slope
\[
0 = \left. \frac{d^2 \Gamma_N(t|r)}{dr^2} \right|_{r=r^*},
\]
namely, we demand that at \(r=r^*
\]
\[
\Gamma(t|r) = \left. \frac{d^2 \Gamma_N(t|r)}{dr^2} + (N-1) \left. \frac{d \Gamma(t|r)}{dr} \right| \right)^2 = 0,
\]
Evidently, the above criterion is only applicable for \(N>1\), since \(\text{erf}(x)\) has no inflection point at a finite value of \(x\).

In the limit of large \(N\), \(\langle S_N(t) \rangle\) is easily calculated from Eqs. (9) and (12) given \(\Gamma=\Gamma_1\). We demonstrate this procedure below. Matching this solution with the analytic result for \(N=1\), generates a useful approximation over the whole range of \(N\).

II. FREE DIFFUSION

Consider first the free diffusion case, \(\mu=0\). The solution of Eq. (7) with the boundary and initial conditions of Eqs. (4) and (5), respectively, are given by
\[
p(x,t|r) = (4\pi Dt)^{1/2} \exp\left[-(x-r)^2/4Dt\right]
\exp\left[-(x+r)^2/4Dt\right].
\]
The integral in Eq. (6) is then
\[
\Gamma(t|r) = \text{erf}(\zeta),
\]
where \text{erf} is the error function and we define
\[
\zeta = r\sqrt{4Dt}.
\]
In the case \(N=1\) the integral over \(r\) in Eq. (1) is analytical, giving
\[
\langle S_1(t) \rangle = (4Dt)^{1/2} \int_0^\infty \text{erfc}(\zeta) d\zeta = (4Dt\pi)^{1/2}.\]

For \(N \gg 1\) we invoke the approximation in Eq. (9).

From the condition (12) on the second derivative of \(\Gamma_N\), we obtain the following transcendental equation
\[
(N-1)e^{-\zeta^2} = \sqrt{\pi} \zeta \text{ erf}(\zeta^*).
\]
For large \(N\), \(\zeta^*\) will be large and one could replace \(N-1\) by \(N\) and \(\text{erf}(\zeta^*)\) by 1. Thus Eq. (17) reduces to
\[
Ne^{-\zeta^2} = \sqrt{\pi} \zeta^*.
\]
This approximation is actually valid up to the second term in the asymptotic expansion \(\text{erf}(x) \sim 1-\exp(-x^2)/x\sqrt{\pi}\), as can be verified by inserting it into Eq. (17).

While Eq. (18) was not meant to be valid for \(N=1\), it is approximately obeyed even in this limit. Indeed, for \(N=1\) the right-hand side (r.h.s.) is \(\sqrt{\pi} \zeta^*=1\), as may be verified from the exact solution, Eqs. (15) and (16). Under these conditions, the l.h.s. gives exp\((-1/\pi)=0.73\), which is not that different from unity. We make use of this property to generalize our derivation to arbitrary \(N\).

When \(N\) is small, \(\zeta^*\) may not be sufficiently large for the approximation \(\text{erf}(\zeta^*)=1\) to hold. Let us then define a parameter \(\alpha\) by
\[
\alpha = \pi [\text{erf}(\zeta^*)]^2.
\]
Since \(0<\text{erf}(x)<1\), we expect \(0<\alpha<\pi\). With this notation, Eq. (17) becomes
\[
Ne^{-\zeta^2} = \sqrt{\alpha} \zeta^*.
\]
Since for large \(N\) (hence large \(\zeta^*\)) the solution of Eq. (20) becomes independent of \(\alpha\), one has the freedom of choosing \(\alpha\) so it satisfies this equation also for \(N=1\). Inserting \(\zeta^*=1/\sqrt{\pi}\) into Eq. (20) gives
\[
\alpha = \pi \exp(-2/\pi) = 1.66,
\]
which, as we shall see, is an excellent approximation.

The transcendental equation (20) may be further simplified to yield an explicit expression for \(\zeta^*\). To a first approximation, \(\zeta^* \approx \ln N\) in both limits of \(N \rightarrow 1\) and \(N \rightarrow \infty\). This means that the r.h.s. of Eq. (20) is of order unity. Indeed, if \(N=1\) then \(\sqrt{\alpha} \zeta^* = \sqrt{\alpha} \ln N \approx 0.73\), while say, for \(N=10^6\), \(\sqrt{\alpha} \ln N = 4.8\) which is unity as compared with \(N\). Substituting \(\zeta^* = \ln N\) in the r.h.s. of Eq. (20) gives
\[
\zeta^* = \sqrt{\ln N - \ln \alpha \ln N}.
\]
Using Eqs. (9) and (15), the final result for the mean \(N\)-particle span is \(\langle S_N(t) \rangle = \sqrt{4Dt} = \zeta^*\).

Figure 1 compares the above approximation with the exact numerical integration of Eq. (1). It is seen that the transcendental equation (20) with \(\alpha\) from Eq. (21) is essentially exact for any number of particles, while the additional approximation in Eq. (22) is just slightly worse. It is amusing to note that an \(\alpha'\) calculated from Eq. (19) rather than from
The average span, \(\langle S_N \rangle\), of \(N\) independently diffusing particles on the line with and without a biasing field. The particles start from the same point and their span is calculated for the down-field direction for \(N=3-10^7\). The two bold curves represent a numerical evaluation of the exact integral, Eq. (1), for \(\mu=0\) (top) and \(\mu\sqrt{Dt}=5\) (\(\mu=0.5\), \(D=1\), \(t=100\), bottom). For larger values of \(\mu\sqrt{Dt}\) this result no longer changes. The remaining data are from the approximations discussed in the text.

In comparison with Eq. (22), previous work has only derived the \(\sqrt{ \ln N}\) dependence without a prefactor or a correction term, which does not allow comparison with the exact result in Fig. 1. More recently, a prefactor has been obtained\(^9\) e.g., \(\xi^*=\sqrt{2}/\pi \ln N/e=0.92\ln N\). This result is quite reasonable for an approximation not involving a correction term. It intersects the exact curve with a slightly too small a slope, 0.92. The prefactor 1.0 in Eq. (22) is observably better than 0.92, but then the correction term is required for obtaining quantitative agreement.

### III. BIASED DIFFUSION

With a proper redefinition of \(\xi\), similar approximations are obtained for biased diffusion, \(\mu>0\). Begin by generalizing Eq. (13) as\(^11\)

\[
p(x,t|r) = \frac{1}{\sqrt{4\piDt}} e^{-\mu(x-r+\mu D t/2)^2/2} [e^{-(x-r)^2/4Dt} - e^{-(x+r)^2/4Dt}].
\]

The integral in Eq. (6) is then

\[
\Gamma(t|r) = \frac{1}{2} [\text{erfc}(-\xi_-) - e^{\mu r} \text{erfc}(\xi_+)],
\]

where \(\text{erfc}\) is the complementary error function and we define

\[
\xi_{\pm} = r/\sqrt{4Dt} \pm \mu \sqrt{Dt}/2.
\]

The integral in Eq. (21), namely, \(\alpha' = \pi \text{erf}^2(1/\sqrt{\pi}) = 1.0\), produces a very good agreement between the approximation in Eq. (22) and the exact numerical integral.

In the limit \(\mu = 0\) one has \(\xi_- = \xi_+ = \xi\), Eq. (15). Then, since \(\text{erfc}(-x) = 1 + \text{erfc}(x)\), Eq. (24) reduces to Eq. (14).

For \(N=1\) the integral in Eq. (1) is again analytical,\(^13\) so the one-sided span becomes

\[
\langle S_1(t) \rangle - \mu Dt = \sqrt{\frac{1}{\pi} \frac{D t}{4}} e^{-\mu^2 D t/4} - \frac{1}{2} \mu Dt \text{erfc}(\mu \sqrt{Dt/4}) + \mu^{-1} \text{erfc}(\mu \sqrt{Dt/4}).
\]  

(26a)

The term \(\mu Dt\) on the l.h.s. describes the drift due to the applied linear potential (constant force). Hence the r.h.s. may be interpreted as the effect of the random motion itself. The difference, \(\langle S_1(t) \rangle - \mu Dt\), increases from zero initially as \(\sqrt{4Dt/\pi}\), but saturates at \(1/\mu\) as \(t \to \infty\). This may be seen in Fig. 2. Thus for an infinitely strong field \(\langle S_1 \rangle \to \mu Dt\), as expected. For a strong but finite field, the asymptotic expansion of the error-function with respect to \(\mu \sqrt{Dt}\) gives

\[
\frac{\langle S_1(t) \rangle - \mu Dt}{\sqrt{4Dt}} \sim \frac{1}{2 \mu \sqrt{Dt}} \left(1 - \frac{2}{\mu \pi D t} e^{-\mu^2 D t/4}\right).
\]  

(26b)

because the first two terms on the r.h.s. of Eq. (26a) cancel identically. Thus, in the strong-field limit \((\mu \sqrt{Dt})\), the function \(\xi^*\) plotted in Fig. 1 depends on the single dimensionless variable \(\mu \sqrt{Dt}\) and becomes independent of it as \(\mu \sqrt{Dt} \to \infty\). One might expect this property to carry over to arbitrary \(N\), except that the limiting value of \(\xi^*\) becomes larger than zero. In the opposite limit, \(\mu \to 0\), a Taylor-expansion of the last term on the r.h.s. of Eq. (26a) around \(\mu = 0\) gives

\[
\frac{1}{2} \int_0^\infty e^{\mu r} \text{erfc}(\xi_+) dr = \mu^{-1} \text{erfc}(\mu \sqrt{Dt/4}) \approx \sqrt{Dt/\pi}.
\]  

(27)
So that together with the $\mu \to 0$ limit of the first term on the r.h.s. one regenerates Eq. (16).

For large $N$ and $\mu \sqrt{D t}$, the contribution from $\xi_+$ becomes negligible, so that one may keep only the $\xi_-$ term in Eq. (24). Thus, $\Gamma$ and its derivatives simplify to

$$\Gamma(t) \approx \text{erf}c(-\xi_-)/2,$$

$$d\Gamma(t)/dr \approx \frac{1}{\sqrt{4\pi Dt}} e^{-\xi_-^2},$$

$$d^2\Gamma(t)/dr^2 \approx -\frac{1}{4\pi Dt} 2\sqrt{\pi} \xi_- e^{-\xi_-^2}. \quad (28)$$

These are used in the step-function approximation of Eqs. (8) and (9). Inserting into Eq. (12), one obtains a transcendental equation for $\xi^*$, the location of the step

$$(N-1) e^{-\xi^* N^2} = \sqrt{\pi} \xi^* \text{erf}c(-\xi^*). \quad (29)$$

analogous (but not identical) to Eq. (17). In particular, note that $\text{erf}c(-x) = 1 + \text{erf}(x)$.

Continuing similarly to the field-free case, Eq. (19), one might define a parameter, $\alpha$, by

$$\alpha = \pi [\text{erf}c(-\xi^*)]^2. \quad (30)$$

Then Eq. (29) reduces to Eq. (20) with $\xi^*$ replaced by $\xi_*$. However, it is not altogether clear how to set $\alpha$ so that Eq. (20) with $N=1$ coincides with Eq. (26a).

Successive approximations in Eq. (20) give, as before

$$\xi^* = [\langle S_N(t) \rangle - \mu D t\sqrt{4Dt} \approx \ln N - \ln \alpha \ln N]. \quad (31)$$

which represents our final approximation for the one-dimensional span for diffusion with bias. The r.h.s. is expected to be independent of $\mu$ and $t$ in the limit $\mu \sqrt{D t} \to \infty$, when $\alpha$ should be just a constant. An amusing route to estimate this parameter begins with our observation that in the field-free case $\alpha^* = 1.0$, calculated from Eq. (19) with $\xi^*(N=1) = 1/\sqrt{\pi}$, is the appropriate value to use in Eq. (22). By analogy, we take the large-field limit in Eq. (26a), $\xi^* \to 0$, and insert it into Eq. (30) to yield

$$\alpha^* = \pi \text{erf}c(0) = \pi. \quad (32)$$

Figure 1 shows the large-field limit ($\mu \sqrt{D t} > 5$) for $\xi^*$ in the many-particle case (lower bold curve). The circles, calculated from approximation (31) with $\alpha = 4$ agree quantitatively with the exact result. Thus $\alpha^* = \pi$ (triangles, Fig. 1) is a good estimate for $\alpha$.

IV. CONCLUSION

In this work we have obtained useful approximations for the average span of biased and unbiased $N$-particle diffusion in one-dimension using a unified yet pedestrian approach. Physically, one wishes to determine how the mean distance covered by $N$ independent particles increases with time, $t$, and $N$ and whether it depends on the bias, $\mu$. Mathematically, what is required is a useful means for an accurate evaluation of the corresponding integral in terms of the above parameters.

Our approach is to assume that the integrand approaches a step-function for large $N$. This leads to a transcendental equation for the span. Fortunately, this equation contains a scaling factor, $\alpha$, whose precise numerical value has little effect on its large $N$ solution. Readjusting $\alpha$ to produce the exact single-particle solution in the bias-free case results in the transcendental equation being essentially exact over the whole range of $t$ and $N$. Using successive approximations, one obtains an explicit expression for the span, including a correction term to the leading $\sqrt{\ln N}$ behavior.

The case of bias (linear potential) proceeds by the same route. While it is possible to derive an analytic expression for the single-particle span, it is not clear how to implement it in determining the parameter $\alpha$ in the transcendental equation. However, we are able to give an approximate estimate for its use in the ensuing successive-approximation relation in the large-field limit. As Fig. 1 shows $\langle S_N \rangle - \mu D t$ is smaller in this limit, when $\mu \sqrt{D t} \to \infty$, than when $\mu = 0$, but the difference between the two limits diminishes as $N \to \infty$.

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