First Invader Dynamics in Diffusion-Controlled Absorption

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Abstract.

We investigate the average time for the earliest particle to hit a spherical absorber when a homogeneous gas of freely diffusing particles with density ρ and diffusivity D is prepared in a deterministic state and is initially separated by a minimum distance ℓ from this absorber. In the high-density limit, this first absorption time scales as $\frac{\ell^2}{D}\frac{1}{\ln \rho\ell}$ in one dimension; we also obtain the first absorption time in three dimensions. In one dimension, we determine the probability that the $k^{\rm th}$-closest particle is the first one to hit the absorber. At large k, this probability decays as $k^{1/3}\exp(-Ak^{2/3})$, with $A = 1.93299\ldots$ analytically calculable. As a corollary, the characteristic hitting time T_k for the $k^{\rm th}$-closest particle scales as $k^{4/3}$; this corresponds to superdiffusive but still subballistic motion.

1. Statement of the Problem

Suppose that a gas of independent random walkers is uniformly and deterministically distributed with density ρ at time $t = 0$ in the exterior region that is a distance ℓ beyond a spherical absorber of radius a (Fig. 1). For $t > 0$, the particles diffuse freely and are absorbed when they hit the absorber. This flux, or reaction rate, is fundamental to our understanding of many diffusion-controlled kinetic processes (see e.g., [1–6]). In this work, we are interested in the behavior of this flux at short times. Specifically: (a) What is the average time for the earliest particle in the gas to first hit the absorber? (b) What is the probability that the k^{th}-closest particle hits the absorber first?

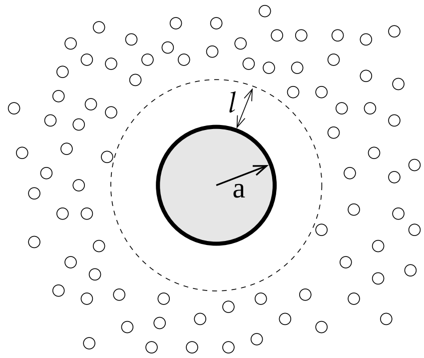


Figure 1. Model geometry in two dimensions. A gas of density ρ occupies the region $r > a + \ell$ exterior to a circular absorber centered at the origin.

These first-hitting properties can be equivalently viewed as the survival probability of a static absorber in the presence of a gas of density ρ of diffusing particles with diffusivity D that kill the absorber upon reaching it. This process, that is known as the "scavenger" or "target" problem has been extensively studied for an initial random (Poisson) distribution of particles [8–15]. In one dimension, the survival probability asymptotically decays as $\exp\big[-C_1\rho(Dt)^{1/2}\big]$, where C_1 is a constant of order 1 that is exactly known. In general spatial dimension d, the corresponding survival probability is $\exp\big[-C_d\,\rho(Dt)^{d/2}\big]$ for $d < 2$ and $\exp(-C_d\,\rho a^{d-2}Dt)$ for $d > 2$ [8–15]. Various aspects of the spatial distribution of the random walkers at the first absorption event have been considered in Ref. [16]. Here we focus both on when the absorber is first hit and on the complementary property of the identity of the random walker that hits the absorber first. In contrast to previous works, we consider a *deterministic* initial condition in which there is a fixed number of particles at each lattice site. We find that for $d = 1$ this initial determinism leads to different asymptotic results for the probability that the absorber has not yet been hit by time t compared to the previously-studied case of a random initial distribution of diffusing particles.

In the next section, we derive the dependence of the average first hitting time on system parameters in one and in three dimensions. We then determine the probability that the k^{th}-closest particle is the first to hit the absorber in one dimension. We also show that this k^{th}-closest particle typically moves faster than diffusively, so that it actually can be the particle that hits the absorber first, but slower than ballistically.

2. First Hitting Time

2.1. One Dimension

In one dimension, the radius of the absorber is irrelevant, and the resulting system (Fig. 2) is characterized by three parameters: the initial distance ℓ between the absorber and the closest particle, the diffusion coefficient D, and the density ρ. From these, we can form two parameter combinations with units of time: ℓ^2/D, the time to diffuse from the closest particle to the absorber, and $1/(D\rho^2)$, the time to diffuse between neighboring particles. The first hitting time may generally be written as

$$T = \frac{\ell^2}{D} F\left(\frac{\ell^2/D}{1/(D\rho^2)}\right) = \frac{\ell^2}{D} f(\rho\ell) . \tag{1}$$

Our goal is to determine the function f.

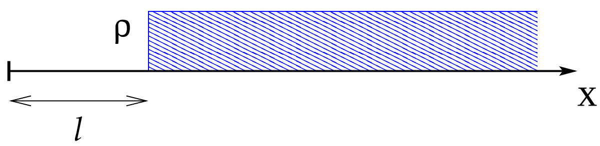


Figure 2. Model geometry in one dimension. A gas of density ρ occupies the region $x > \ell$, with an absorber at the origin.

We begin by considering the gas to consist of a single particle at $x = \ell$. The first-passage probability that this particle to first hit the origin at time t is [17]

$$f(\ell, t) = \frac{\ell}{\sqrt{4\pi D t^3}} \, e^{-\ell^2/4Dt} . \tag{2}$$

While the particle eventually hits the origin because $\int_0^\infty f(\ell,t)\,dt = 1$, the average time to reach the origin, $\int_0^\infty t\, f(\ell,t)\,dt$, is infinite because of the $t^{-3/2}$ tail in the first-passage probability. From (2), the probability that the hitting time for a single particle is longer than t (equivalently the particle survival probability up to time t), is

$$S(\ell, t) = \int_t^\infty f(\ell, t')\,dt' = \mathrm{erf}(\ell/\sqrt{4Dt}) . \tag{3}$$

For a localized group of $\Delta n = \rho\,\Delta x$ particles that are initially in the interval $[x, x+\Delta x]$, the probability that the hitting time is longer that t is $\big[S(x,t)\big]^{\Delta n}$. Consequently, the cumulative probability that the hitting time exceeds t for a gas that occupies the region

$x \geq \ell$ is

$$Q(t) = \prod_{m=0}^{\infty} \left[S(\ell + m\Delta x, t)\right]^{\Delta n} = \exp\left\{\Delta n \sum_{m=0}^{\infty} \ln S(\ell + m\Delta x, t)\right\}$$
$$\simeq \exp\left\{\rho \int_{\ell}^{\infty} \ln\left[\mathrm{erf}(x/\sqrt{4Dt})\right] dx\right\}$$
$$= \exp\left\{\rho\ell\sqrt{\tau} \int_{1/\sqrt{\tau}}^{\infty} \ln\left[\mathrm{erf}(z)\right] dz\right\} \equiv \exp\left[\rho\,\ell\,\Phi(\tau)\right] . \quad (4)$$

Here we define the scaled time $\tau = 4Dt/\ell^2$, the dimensionless variable $z = x/\sqrt{4Dt}$, and

$$\Phi(\tau) \equiv \sqrt{\tau} \int_{1/\sqrt{\tau}}^{\infty} \ln\left[\mathrm{erf}(z)\right] dz \, . \quad (5)$$

The probability that a particle first hits the origin at time t is $q(t) = -\frac{\partial Q}{\partial t}$, so that the average first hitting time is

$$T = \int_0^{\infty} t\; q(t)\, dt = \int_0^{\infty} Q(t)\, dt = \frac{\ell^2}{4D} \int_0^{\infty} d\tau\; \exp\left[\rho\,\ell\,\Phi(\tau)\right] . \quad (6)$$

The dependence of this first hitting time on system parameters may be extracted from the asymptotic behaviors of $\Phi(\tau)$. As shown in Appendix A, these are:

$$\Phi(\tau) = \begin{cases} -E_{\infty}\sqrt{\tau} + \ln\sqrt{\tau} + 1 - \ln\frac{2}{\sqrt{\pi}} + \ldots\,, & \tau \to \infty\,, \\ -\frac{\tau^{3/2}}{2\sqrt{\pi}}\, e^{-1/\tau}\,, & \tau \to 0\,, \end{cases} \quad (7)$$

with $E_{\infty} \equiv -\int_0^{\infty} \ln\left[\mathrm{erf}(z)\right] dz = 1.034415\ldots$ as computed numerically. As a result, the controlling factor in the cumulative distribution has the limiting behaviors:

$$Q(\tau) \simeq \begin{cases} \exp\left(-E_{\infty}\,\rho\ell\,\sqrt{\tau}\right), & \tau \gg 1\,, \\ \exp\left(-\rho\,\ell\,\frac{\tau^{3/2}}{2\sqrt{\pi}}\, e^{-1/\tau}\right), & \tau \ll 1\,. \end{cases} \quad (8)$$

It is worth emphasizing that the long-time behavior of $Q(\tau)$ is given by $\exp\left(-C\rho\ell\,\sqrt{\tau}\right)$ in the case of *randomly* (Poisson) distributed particles at $t = 0$, with $C = 1/\sqrt{\pi} = 0.564189\ldots$ [8–15]; our result is qualitatively similar, except that the coefficient in the exponential is $E_{\infty} = 1.034415\ldots$. The distribution $Q(\tau)$ also has an extraordinarily sharp double exponential cutoff for short times. This makes it extremely unlikely that the first particle hits the absorber much earlier than the diffusion time, as reflected in the behavior of the average hitting time given below.

Let us now focus on the average first hitting time in the interesting high-density limit of $\rho\ell \gg 1$, for which

$$T \simeq \frac{\ell^2}{4D} \int_0^{\infty} d\tau\; \exp\left(-\rho\,\ell\,\frac{\tau^{3/2}}{2\sqrt{\pi}}\, e^{-1/\tau}\right), \qquad \rho\ell \gg 1\,. \quad (9a)$$

A non-vanishing contribution to the integral arises only where the argument of the exponential is less than one. Ignoring subdominant factors, this condition is satisfied when $\tau < (\ln \rho\ell)^{-1}$. In this regime, we approximate the entire exponential factor by 1 and integrate over the region $\tau < (\ln \rho\ell)^{-1}$ to give

$$T \sim \frac{\ell^2}{4D}\,\frac{1}{\ln \rho\ell}\,, \qquad\qquad \ln(\rho\ell) \gg 1\,. \tag{9b}$$

By accounting for the subdominant factor $\tau^{3/2}/(2\sqrt{\pi})$ in the exponential in (9a), a better estimate of the point where the integrand is non-negligible is $\rho\,\ell\,\tau^{3/2}\,e^{-1/\tau}/2\sqrt{\pi} = 1$. This gives the more accurate asymptotic

$$T = \frac{\ell^2}{4D\ln\left(\frac{\rho\ell}{2\sqrt{\pi}}\right)}\left[1+\frac{3\ln\ln\left(\frac{\rho\ell}{2\sqrt{\pi}}\right)}{2\ln\left(\frac{\rho\ell}{2\sqrt{\pi}}\right)}+\ldots\right]\,, \qquad\qquad \rho\ell \gg 1\,. \tag{9c}$$

In this high-density limit, the average first hitting time T is finite, even though the average first hitting time for any individual particle is infinite. The first hitting time is of the order of the average time for the closest particle to diffuse to the absorber that is modified by a logarithmic factor. Because of the logarithmic density dependence, a huge increase in the density leads to only a modest decrease in T. This weak dependence shows that most particles, especially distant ones, play a negligible role in the first hitting event, as expected intuitively.

In the opposite limit of $\rho\ell \ll 1$, we use the large-τ behavior of $\Phi(\tau)$ in (7) to give

$$T \simeq \frac{\ell^2}{4D}\int_0^\infty d\tau\, \exp\left(-\rho\,\ell\, E_\infty\sqrt{\tau}+\rho\ell\ln\sqrt{\tau}+\ldots\right)\,, \qquad\qquad \rho\ell \ll 1\,. \tag{9d}$$

Now the contribution to the integral is non-negligible when $\rho\ell\sqrt{\tau} \sim 1$ or $\tau_* \sim (\rho\ell)^{-2}$. This allows us to neglect the logarithmic term in the exponent and leads to the estimate

$$T \simeq \frac{1}{2E_\infty^2 D\rho^2} = \frac{0.46728\ldots}{D\rho^2}\,, \qquad\qquad \rho\ell \ll 1\,. \tag{9e}$$

This limit corresponds to the situation of no initial separation between the gas and the absorber, namely, $\ell = 0$.

2.2. Three Dimensions

In two dimensions and above, the radius a of the absorber must be non-zero so that the probability to hit it is non-zero. In three dimensions, the probability that a diffusing particle initially at radius $r > a$ eventually hits the absorber is [4, 17]

$$h(r) = \frac{a}{r}\,. \tag{10}$$

While it is not certain that a single diffusing particle will eventually hit the absorber, one of the particles from an infinite gas will. To show this fact, consider a gas of density

ρ that uniformly fills the exterior space. The probability that no particles with radii in the range r and $r + \Delta r$ will reach the absorber is

$$\left(1 - \frac{a}{r}\right)^{4\pi\rho r^2 \Delta r}.$$

The probability P that no gas particles reach the absorber is

$$P = \prod_{m=0}^{\infty} \left(1 - \frac{a}{a + m\Delta r}\right)^{4\pi\rho r^2 \Delta r}. \tag{11}$$

In the continuum limit

$$\ln P = \int_a^{\infty} 4\pi r^2 \ln\left(1 - \frac{a}{r}\right) dr\,,$$

which diverges to $-\infty$ at the upper integration limit; thus it is impossible for all particles to miss the absorber. This fact is actually obvious because this system evolves to a steady state with a constant average diffusive flux to the absorber [1–6].

We now take advantage of two simplifications to reduce the three-dimensional diffusion problem to one dimension. First, the flux to the surface of a spherical absorber can be calculated by replacing the true initial condition, a delta-function at the initial particle location (r_0, θ_0, ϕ_0), by a normalized spherically-symmetric initial condition of radius r_0. Then we can use the classic device of reducing a spherically-symmetric three-dimensional diffusion problem to one dimension [2, 17]. For the concentration $\rho(r,t)$ in three dimensions that depends only on the radial coordinate, the quantity $u(r,t) = r\rho(r,t)$ obeys the one-dimensional diffusion equation. That is, if ρ solves

$$\frac{\partial \rho}{\partial t} = D\nabla^2_{3d}\rho, \tag{12a}$$

where ∇^2_{3d} is the radial Laplacian operator in three dimensions, then $u = r\rho$ satisfies

$$\frac{\partial u}{\partial t} = D\nabla^2_{1d} u. \tag{12b}$$

For a single particle that is initially at $r = r_0$, the effective spherically-symmetric concentration can be written as a sum of a Gaussian and an anti-Gaussian, with the latter accounting for the absorbing boundary condition at $r = a$. From this expression, the first-passage probability to the surface of the absorber is given by [2, 17]

$$f(r_0, t) = \frac{a(r_0 - a)}{r_0\sqrt{4\pi D t^3}}\; e^{-(r_0-a)^2/4Dt}\,, \tag{13}$$

and the corresponding survival probability up to time t is

$$S(r_0, t) = 1 - \frac{a}{r_0}\mathrm{erfc}\left(\frac{r_0 - a}{\sqrt{4Dt}}\right)\,, \tag{14}$$

where $\mathrm{erfc}\, z = 1 - \mathrm{erf}\, z$. Notice that $S(r_0, t \to \infty) = 1 - a/r_0$, consistent with Eq. (10).

For a gas of uniform density ρ that lies beyond a minimal radius ℓ, with $\ell > a$, the number of particles within the range r and $r+\Delta r$ is $\Delta n = 4\rho\pi r^2\Delta r$. The expression for $Q(t)$ that is the analog of Eq. (4) is

$$Q(t) = \prod_{m=0}^{\infty}\left[S(\ell+m\Delta r,t)\right]^{\Delta n} \simeq \exp\left\{4\pi\rho\int_{a+\ell}^{\infty} r^2 \ln\left[1-\frac{a}{r}\,\mathrm{erfc}\left(\frac{r-a}{\sqrt{4Dt}}\right)\right]dr\right\}$$
$$\equiv \exp\left[\rho\,\ell\,\Phi_{3\mathrm{d}}(\tau)\right]\,, \tag{15}$$

where we now define

$$\Phi_{3\mathrm{d}}(\tau) = 4\pi\sqrt{\tau}\int_{\frac{\ell}{(a+\ell)\sqrt{\tau}}}^{\infty}(\sqrt{\tau}\,\ell z+a)^2\ln\left(1-\frac{a}{\sqrt{\tau}\,\ell z+a}\,\mathrm{erfc}\,z\right)dz\,, \tag{16}$$

with $\tau = 4Dt/\ell^2$ the scaled time and z the dimensionless variable $z=(r-a)/\sqrt{4Dt}$. In the limit of $\tau\to\infty$ we can set the lower integration limit to zero and neglect the term a in the expressions $\sqrt{\tau}\,\ell z+a$ in the integrand. Since the argument of the logarithm is very close to 1, we obtain

$$\Phi_{3\mathrm{d}}(\tau) \simeq -4\pi\tau a\ell\int_0^{\infty} z\,\mathrm{erfc}\,z\,dz \simeq -\pi\tau a\ell = -\frac{4\pi aDt}{\ell}. \tag{17}$$

Then Eq. (15) yields, as expected, the long-time asymptotic $Q(t)\simeq\exp(-4\pi\rho aDt)$, independent of ℓ.

In the short-time $\tau\to 0$ limit, we can neglect the factors $\sqrt{\tau}\ell z$ in the integrand, so that the integration reduces to

$$\int_A^{\infty}\ln\,\mathrm{erf}\,z\,dz, \qquad \text{where}\quad A=\frac{\ell}{(a+\ell)\sqrt{\tau}}\,.$$

Because τ is small, $A\gg 1$, and we can use the large-z expansion $\ln\,\mathrm{erf}\,z\simeq -e^{-z^2}/(\sqrt{\pi}z)$. Since the integrand decays rapidly with z, we write $z=A+\epsilon$ so that $e^{-z^2}\simeq e^{-A^2-2A\epsilon}$, put $z\simeq A$ in the denominator of the integrand and then perform the integral in ϵ. The final result for $\Phi_{3\mathrm{d}}(\tau)$ as $\tau\to 0$ is

$$\Phi_{3\mathrm{d}}(\tau)\simeq -\frac{2\sqrt{\pi}a^2\tau^{3/2}(a+\ell)^2}{\ell^2}\,e^{-\frac{\ell^2}{(a+\ell)^2\tau}}. \tag{18}$$

Using this result in Eq. (15) we obtain, in physical variables,

$$Q\simeq\exp\left[-\frac{16\sqrt{\pi}\rho\,a^2(a+\ell)^2(Dt)^{3/2}}{\ell^5}\,e^{-\frac{\ell^4}{4(a+\ell)^2Dt}}\right] \tag{19}$$

To compute T in the regime when the gas density if large, and the dimensionless time τ is small, we apply the same reasoning as in the evaluation of the corresponding integral (9a) in one dimension and now find, to lowest order

$$T\sim\frac{\ell^4}{4D(a+\ell)^2}\,\frac{1}{\ln\frac{\rho a^2\ell^2}{a+\ell}}\,, \qquad \ln\frac{\rho a^2\ell^2}{a+\ell}\gg 1\,, \qquad d=3\,. \tag{20}$$

In the opposite limit of very low density (corresponding to large τ), the average first hitting time is

$$T \simeq \frac{\ell^2}{4D} \int_0^\infty \exp\left(-\pi\rho a\ell^2\tau\right)\, d\tau = \frac{1}{4\pi\rho a D}. \tag{21}$$

The initial separation does not play a role in this limit.

3. Which Particle Hits First?

We now determine the probability G_k that the $k^{\rm th}$-closest particle is the one that first hits the absorber (Fig. 3). We focus on the one-dimensional system in which freely diffusing particles $1, 2, 3, \ldots$ are at $x_1(t), x_2(t), x_3(t), \ldots$, with the initial condition of one particle at each lattice cite: $x_k(t{=}0) = kh$, with $k \in \mathbb{I}$ and h is the lattice spacing.

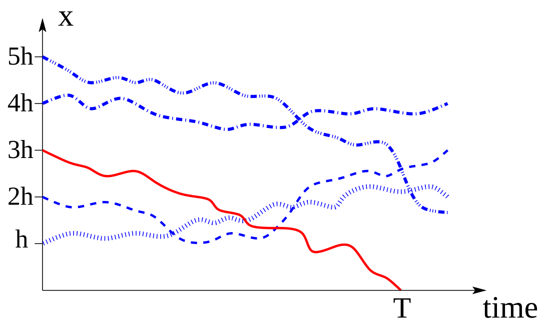


Figure 3. Illustration of hitting in one dimension. Particles are initially at $x = h, 2h, 3h, \ldots$. The first particle (here particle 3) hits the absorber at time T.

As a preliminary, consider two particles, labeled 1 and 2, that are initially at $x = h$ and $x = 2h$. The probability that particle 1 hits the origin first may be written as

$$G_1 = \int_0^\infty dt\, f(h,t) \int_t^\infty dt'\, f(2h,t') = \int_0^\infty dt\, f(h,t)\ \mathrm{erf}(2h/\sqrt{4Dt})\,, \tag{22}$$

where $f(h,t)$ is the first-passage probability to the origin at time t for a particle starting at $x = h$ (Eq. (2)). Equation (22) states that particle 2 must hit the origin after particle 1. Defining $z = h/\sqrt{4Dt}$ reduces the above integral to

$$G_1 = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-z^2}\, \mathrm{erf}(2z)\, dz = \frac{2}{\pi}\tan^{-1} 2 = 0.704833\ldots \tag{23}$$

If instead, the two particles are at ℓ and $\ell+h$, corresponding to the finite gap ℓ between the absorber and the gas, then $G_1 = \frac{2}{\pi}\tan^{-1}\frac{\ell+h}{\ell}$, which approaches the limiting value of $\frac{1}{2}$ as $\ell \to \infty$.

An alternative solution that involves minimal computation is to make a correspondence (see Fig. 4) between the two particles diffusing on the half line to the diffusion of a single effective particle in two dimensions that obeys suitable boundary conditions [17, 19]. The effective particle has initial coordinates $(x_1 = h, x_2 = 2h)$ and

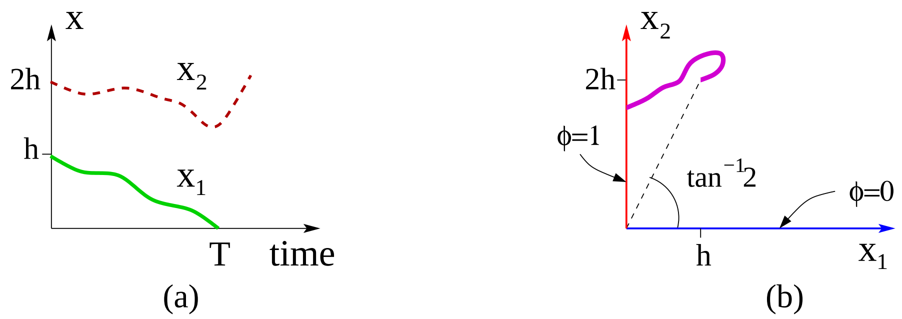


Figure 4. Correspondence between (a) two particles diffusing on the positive half line and (b) an effective particle, with coordinates x_1 and x_2, diffusing in the positive quadrant in two dimensions.

is constrained to remain within the positive quadrant $x_1, x_2 > 0$. The probability G_1 is equivalent to the effective particle first hitting the line $x_1 = 0$, while x_2 always remains positive. This hitting probability equals the electrostatic potential at $(h, 2h)$ when the line $x_1 = 0$ is held at potential $\phi = 1$ (corresponding to particle 1 first hitting the origin) and the line $x_2 = 0$ is held at potential $\phi = 0$ (corresponding to particle 2 first hitting the origin) [4, 17]. For this geometry, the electrostatic potential at a point (r, θ) inside the quadrant is $\phi(\theta) = \frac{2\theta}{\pi}$. Because the point $(h, 2h)$ corresponds to polar angle $\tan^{-1} 2$, the probability that particle 1 first hits the boundary is just $\frac{2}{\pi}\tan^{-1} 2$, as already given in (23).

To generalize to an infinite number of particles that are initially placed deterministically at the lattice sites is conceptually straightforward. Following the same steps that led to Eq. (4), the analog of Eq. (22) for an infinite gas is

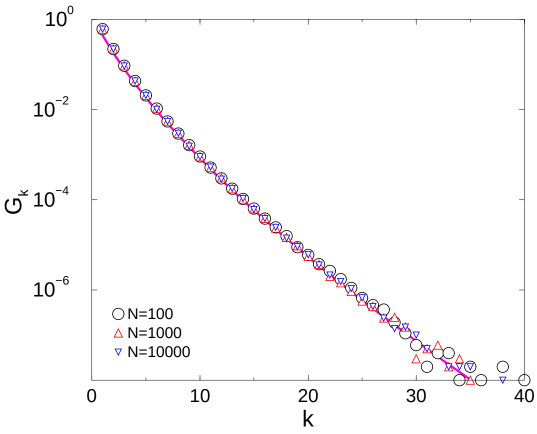
$$
\begin{aligned}
G_1 &= \int_0^\infty dt\, \frac{h}{\sqrt{4\pi D t^3}}\; e^{-h^2/4Dt} \prod_{n=2}^{\infty} \operatorname{erf}(na/\sqrt{4Dt}) \\
&= \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{d\tau}{\tau^{3/2}}\; e^{-1/\tau}\; \exp\left\{\sqrt{\tau}\int_{2/\sqrt{\tau}}^{\infty} dz\, \ln\left[\operatorname{erf}(z)\right]\right\}.
\end{aligned} \tag{24}
$$

We can extend (24) to the probability G_k that the $k^{\rm th}$ particle hits the origin first:

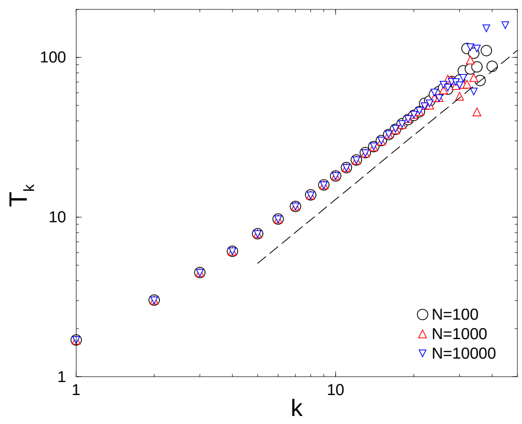
$$
\begin{aligned}
G_k &= \int_0^\infty dt\, \frac{kh}{\sqrt{4\pi D t^3}}\; e^{-(kh)^2/4Dt} \prod_{n=1}^{k-1} \operatorname{erf}(nh/\sqrt{4Dt}) \times \prod_{n=k+1}^{\infty} \operatorname{erf}(nh/\sqrt{4Dt}) \\
&= \int_0^\infty dt\, \frac{kh}{\sqrt{4\pi D t^3}}\; \frac{e^{-(kh)^2/4Dt}}{\operatorname{erf}(kh/\sqrt{4Dt})} \left[\prod_{n=1}^{\infty} \operatorname{erf}(nh/\sqrt{4Dt})\right].
\end{aligned} \tag{25}
$$

We evaluate asymptotic behavior of this integral for $k \gg 1$ by first identifying the asymptotic behavior of the integrand and then applying the Laplace method (Appendix B). The result is:

$$
G_k \simeq \frac{2\pi^{3/4}\, k^{1/3}}{\sqrt{3}\,(E_\infty/2)^{1/6}}\; e^{-3(E_\infty/2)^{2/3}\, k^{2/3}}, \qquad\qquad k \gg 1. \tag{26}
$$



(a)



(b)

Figure 5. (a) Probability that the $k^{\rm th}$ particle is the first one to hit the origin when initially N particles are located at lattice sites for $N = 10, 10^2, 10^3, 10^4$. The curve is our asymptotic estimate (26). (b) The average time for the $k^{\rm th}$-closest particle to hit the origin for those realizations where this $k^{\rm th}$ particle is also the first one to hit the origin. The dashed line corresponds to the power-law behavior $t_k \sim k^{4/3}$. The data are based on 10^8 realizations.

As shown in Fig. 5(a), this prediction is in excellent agreement with numerical simulation data. Surprisingly, this agreement arises even for relatively small k. In our simulations, the system contains N particles, with one particle at each lattice site $h, 2h, \dots Nh$. In an update event, one of the N particles is chosen at random and moved by $\pm h$, and the time is incremented by $\frac{1}{N}$. This update is repeated until one of the particles first hits the origin, where the identity of this first invader and the hitting time are recorded.

A natural complement to the question of which particle first hits the origin, is the characteristic time T_k that is needed for the $k^{\rm th}$-closest particle to hit the origin, given that this particle is the first one to hit. From the Laplace evaluation of the integral in Eq. (25), the maximum of the integral arises when $t \propto \frac{h^2}{D} k^{4/3}$. This behavior suggests that T_k also scales as $k^{4/3}$. While we are unable to obtain appreciable data for $k \gtrsim 40$ because of the extreme improbability of a particle more distant than 40 being the first one to hit the origin, our numerical results are consistent with $T_k \sim \frac{h^2}{D}\, k^{4/3}$ (Fig. 5(b)). This is faster than diffusion, but slower than ballistic motion. Faster than diffusive motion is to be expected; if a distant particle is going to be the first invader, it needs to do so quickly or else another particle that is initially closer to the origin will be the first invader. However, we do not have an intuitive explanation for the anomalous k dependence of this first invader time $T_k \sim \frac{h^2}{D}\, k^{4/3}$.

4. Concluding Remarks

While the diffusive flux to an absorber is a classic and well-understood quantity, we have uncovered new microscopic features of this flux. We focused specifically on the properties of the first particle to reach the absorber. For a gas that is initially separated from the absorber by a distance ℓ, the earliest hitting time is of the order of the diffusion time, but modified by a logarithmic function of the gas density. This weak dependence means that it requires an extremely high density of the gas to reduce the first hitting time much below the diffusion time.

As is obvious, it is the closest particle that is the most likely to first reach the absorber. Nevertheless, the probability that a more distant particle is the first one to reach the absorber is not negligible. We computed, in one dimension, the exact probability G_k that the $k^{\rm th}$-closest particle to the absorber will be the one to first reach it. Both analytically and from simulations, we found that the controlling factor in this probability decays at large k as the stretched exponential function $G_k \sim \exp(-Ak^{2/3})$, with A exactly calculable and whose numerical value is $1.93299\ldots$. Correspondingly, the characteristic time T_k for the $k^{\rm th}$ particle to hit the origin scales as $k^{4/3}$. This is much less than the diffusion time, which scales as k^2, but much larger than the ballistic time, which scales as k. As one might anticipate, a distant particle must hit the origin quickly if it is going to be the first one to reach the origin.

In our discussion of the hitting probability G_k of the $k^{\rm th}$-closest particle, we have assumed the deterministic initial condition of a fixed number of particles at each lattice site. If the particles are initially placed with a Poisson distribution of separations, G_k still behaves asymptotically as $G_k \sim \exp(-Bk^{2/3})$, but with B distinct from the above constant $A = 1.93299\ldots\ldots$, and with a different k-dependence in the pre-exponential factor [20].

Finally, it is worth mentioning that the first hitting probability for an N-particle system is, in principle, computable from a corresponding electrostatic formulation. The diffusion of the N particles on the half line is equivalent to the diffusion of a single effective particle in the positive $2^{\rm N}$-tant in N-dimensional space [17,19]. The probability that particle 1 first hits the origin equals the potential at the initial point $(h, 2h, 3h, \ldots)$, with the plane $x_1 = 0$ held at potential $\phi = 1$ and all other planes $x_i = 0$ held at zero potential. While this problem is simple to state, it does not seem to have a simple solution.

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Appendix A. Asymptotics of Φ

When $\tau \gg 1$, we may set the lower integration limit to zero in (5) to give the leading long-time behavior $\Phi(\tau) \to -E_\infty\sqrt{\tau}$, with $E_\infty = -\int_0^\infty \ln\left[\mathrm{erf}(z)\right] dz = 1.034415\ldots$. At the next level of approximation we define $\varepsilon \equiv 1/\sqrt{\tau}$ and write

$$\int_\varepsilon^\infty \ln\left[\mathrm{erf}(z)\right] dz = \int_0^\infty \ln\left[\mathrm{erf}(z)\right] dz - \int_0^\varepsilon \ln\left[\mathrm{erf}(z)\right] dz. \tag{A.1}$$

For $z \ll 1$, we expand the error function in the last term as $\mathrm{erf}(z) = 2z/\sqrt{\pi} + \ldots$ so that

$$\int_0^{\varepsilon} \ln\big[\mathrm{erf}(z)\big]\, dz = -\varepsilon\Big[\ln\varepsilon - 1 + \ln\Big(\frac{2}{\sqrt{\pi}}\Big) + \ldots\Big]\,,$$

which leads to the first line in Eq. (7).

In the opposite limit of $\tau \ll 1$, we substitute the large-argument expansion of the error function

$$\mathrm{erf}(z) = 1 - \frac{e^{-z^2}}{\sqrt{\pi}\, z} + \ldots\,,$$

in the integral for Φ to give

$$\Phi(\tau) \simeq -\sqrt{\tau}\int_{1/\sqrt{\tau}}^{\infty} \frac{1}{\sqrt{\pi}\, z}\, e^{-z^2} dz\,.$$

We estimate this integral by writing $z = \frac{1}{\sqrt{\tau}} + \epsilon$ and expanding for small ϵ to give

$$\Phi(\tau) \simeq -\sqrt{\tau}\int_0^{\infty} \sqrt{\frac{\tau}{\pi}}\, \exp\left(-\frac{1}{\tau} - \frac{2\epsilon}{\sqrt{\tau}}\right) d\epsilon. \tag{A.2}$$

Evaluating this integral leads to the second line in Eq. (7).

Appendix B. Asymptotic Estimate of G_k

Starting with the second line of Eq. (25) (in which the product has been rewritten as the exponential of the sum)

$$G_k = \int_0^{\infty} dt\, \frac{ka}{\sqrt{4\pi D t^3}}\, \frac{e^{-(kh)^2/4Dt}}{\mathrm{erf}(kh/\sqrt{4Dt})}\, \exp\left\{\sum_{n=1}^{\infty} \ln\Big[\mathrm{erf}(nh/\sqrt{4Dt})\Big]\right\}, \tag{B.1}$$

we introduce the variable $u = h/\sqrt{4Dt}$, to rewrite Eq. (B.1) as

$$G_k = \frac{2k}{\sqrt{\pi}}\int_0^{\infty} du\, \frac{e^{-(ku)^2}}{\mathrm{erf}\,(ku)}\, \exp\Big\{\sum_{n=1}^{\infty} \ln\left[\mathrm{erf}\,(nu)\right]\Big\}. \tag{B.2}$$

For $k \gg 1$, the two dominant factors in the integrand are $e^{-k^2u^2}$ and $e^{\Psi(u)}$, where $\Psi(u) = \sum_{n=1}^{\infty} \ln\left[\mathrm{erf}\,(nu)\right]$.

The factor $e^{-(ku)^2}$ vanishes rapidly for $u \gg 1/k$, while e^{Ψ} vanishes rapidly for $u \to 0$ so that we can evaluate the integral by the Laplace method. The determination of the asymptotic behavior of $\Psi(u)$ is a bit involved because $\ln\mathrm{erf}\,(nu)$ changes rapidly with n for small u. Consequently, replacing the sum for Ψ by an integral leads to errors in the subleading terms that ultimately contribute to the power-law prefactor in the expression for G_k. Thus we split the sum as follows:

$$\Psi(u) = \sum_{n=1}^{N} \ln\left[\mathrm{erf}\,(nu)\right] + \sum_{n=N+1}^{\infty} \ln\left[\mathrm{erf}\,(nu)\right]\,, \tag{B.3}$$

and choose N so that $N \gg 1$ but $Nu \ll 1$. The latter inequality allows us to replace $\mathrm{erf}\,(nu)$ by $(2/\sqrt{\pi})\,nu$ in the first sum. Then the first sum, which we denote by $\Psi_1(u,N)$, is

$$\Psi_1(u,N) = N \ln \frac{2}{\sqrt{\pi}} + N \ln u + \ln N!\,.$$

Using the Stirling's formula for the last term leads to

$$\Psi_1(u,N) \simeq N \ln \frac{2}{\sqrt{\pi}} + N \ln u + N \ln N - N + \ln \sqrt{2\pi N}\,. \tag{B.4}$$

In the second sum in Eq. (B.3), which we denote by $\Psi_2(u,N)$, we can indeed replace the sum by the integral. Accounting for the Euler-Maclaurin correction, we obtain

$$\Psi_2(u,N) = \frac{1}{u}\int_{Nu}^{\infty} dz\, \ln(\mathrm{erf}\, z) - \frac{1}{2}\ln[\mathrm{erf}\,(Nu)] \simeq \frac{1}{u}\int_{Nu}^{\infty} dz\, \ln(\mathrm{erf}\, z) - \frac{1}{2}\ln\left(\frac{2Nu}{\sqrt{\pi}}\right). \tag{B.5}$$

For the integral on the right hand side of Eq. (B.5) we can write

$$\int_{Nu}^{\infty} dz\, \ln(\mathrm{erf}\, z) = \int_{0}^{\infty} dz\, \ln(\mathrm{erf}\, z) - \int_{0}^{Nu} dz\, \ln(\mathrm{erf}\, z) = -E_\infty - \int_{0}^{Nu} dz\, \ln(\mathrm{erf}\, z).$$

The remaining integral can be easily evaluated at $Nu \ll 1$, by again using $\mathrm{erf}\, z = (2/\sqrt{\pi})\, z + \ldots$, and we obtain

$$\Psi_2(u) \simeq -\frac{E_\infty}{u} - N\ln(Nu) + N \ln \frac{\sqrt{\pi}}{2} + N - \frac{1}{2}\ln\left(\frac{2Nu}{\sqrt{\pi}}\right). \tag{B.6}$$

Adding the two contributions Ψ_1 and Ψ_2, we obtain

$$\Psi(u) \simeq -\frac{E_\infty}{u} - \ln\sqrt{u} + \ln\, \pi^{3/4}.$$

As it must, the result for Ψ does not depend on the cutoff N. Returning to Eq. (B.2), its large-k asymptotic behavior is described by

$$G_k \simeq \frac{2k}{\sqrt{\pi}}\int_0^\infty du\, \frac{e^{-(ku)^2}}{\mathrm{erf}\,(ku)} \times \frac{\pi^{3/4}}{\sqrt{u}}\, e^{-E_\infty/u}\,. \tag{B.7}$$

The product of the two competing exponents in the relevant region of u can be written as $e^{-H(u)}$, where

$$H(u) = (ku)^2 + \frac{E_\infty}{u}. \tag{B.8}$$

The maximum contribution to the integral comes from the region near the minimum of $H(u)$. This occurs at $u_* = (E_\infty/2)^{1/3}\, k^{-2/3}$, while the minimum value is $H(u_*) = 3(E_\infty/2)^{2/3}\, k^{2/3}$. The fact that $u_* \to 0$ as $k \to \infty$ justifies *a posteriori* the assumption $Nu \sim Nu_* \ll 1$ that we made in evaluating $\Psi(u)$. Now we expand

$$H(u) = H(u_*) + \tfrac{1}{2}H''(u_*)\,(u-u_*)^2 + \ldots\,. \tag{B.9}$$

Since $H''(u_*) = 6k^2$, the width of the peak of the integrand at $u = u_*$ scales as $\sim 1/k$, and so it is smaller (by a factor of $k^{1/3} \gg 1$) than the peak position $u_* \sim k^{-2/3}$. Thus the relative width of the peak vanishes for $k \to \infty$. Thus for large k we can neglect higher-order corrections in the expansion (B.9), expand the integration range in (B.7) to $(-\infty, \infty)$, and evaluate the slowly-varying factors $[\sqrt{u}\,\mathrm{erf}\,(ku)]^{-1}$ at $u = u_*$. Computing the resulting Gaussian integral gives final result that is quoted in Eq. (26). This formula is in excellent agreement with the numerical evaluation of the exact expression (B.2), with a relative error that is less than 1% already at $k = 12$. As expected, there is disagreement as small k. For example, for $k = 1$ Eq. (26) yields $0.44011\ldots$, whereas the exact value that we computed numerically is $G_1 = 0.6146\ldots$.

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