

First Passage Time in a Two-Layer System

Jysoo Lee¹ and Joel Koplik¹

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As a first step in the first passage problem for passive tracer in stratified porous media, we consider the case of a two-dimensional system consisting of two layers with different convection velocities. Using a lattice generating function formalism and a variety of analytic and numerical techniques, we calculate the asymptotic behavior of the first passage time probability distribution. We show analytically that the asymptotic distribution is a simple exponential in time for any choice of the velocities. The decay constant is given in terms of the largest eigenvalue of an operator related to a half-space Green's function. For the anti-symmetric case of opposite velocities in the layers, we show that the decay constant for system length L crosses over from L^{-2} behavior in the diffusive limit to L^{-1} behavior in the convective regime, where the crossover length L^* is given in terms of the velocities. We also have formulated a general self-consistency relation, from which we have developed a recursive approach which is useful for studying the short-time behavior.

KEY WORDS: First passage problem; convection-diffusion equation; layered system; asymptotic behavior.

1. INTRODUCTION

The motion of a passive tracer in a fluid under the combined action of molecular diffusion and convection arises in a variety of settings, such as fluid flows through porous media, fixed-bed catalytic reactors, and the dispersion of pollutant in oceans.⁽¹⁾ In many situations, the convection-diffusion equation (CDE) describing the variation of tracer concentration with space and time becomes inhomogeneous, i.e., the fluid velocity field and/or the diffusivity is not a constant, but a function of spatial position. One obvious method in the study of inhomogeneous systems is a perturbation technique^(2, 3). Here, one starts from a homogeneous version of the system,

¹ Benjamin Levich Institute and Department of Physics, City College of the City University of New York, New York, New York 10031.

which usually is solvable. The velocity or diffusivity is written as a sum of a homogeneous and an inhomogeneous term and the appropriate quantities are expressed as expansions involving the inhomogeneous term. The perturbative method is not immediately applicable when the magnitude of the disorder is strong, as many or an infinite number of terms are required, but in some cases, effective-medium theories may be used for an approximate summation.⁽⁴⁾ However, such techniques are certainly not suitable for systems whose disorder is strongly correlated in space, where usually only straightforward numerical simulation or, for problems with an appropriate geometry, network models⁽⁵⁾ are useful.

In this paper we are motivated by the particular case of tracer dispersion in porous geological systems such as aquifers and hydrocarbon reservoirs^(6, 7) and by the observation that such materials are very prominently stratified.⁽⁸⁾ In this context, Matheron and de Marsily⁽⁹⁾ first observed that when the number of layers is effectively infinite, the velocity fluctuations associated with the variation in structure and permeability of the layers could give rise to superdiffusive tracer motion. Several authors studied this problem further⁽¹⁰⁻¹²⁾ and by now there is a fair understanding of the tracer probability distribution for the case of a large number of horizontally infinite layers. Unfortunately, the results do not provide concrete statements about the most practical configuration, involving a source and sink of tracer at *finite* separation. One would like to solve the *first passage time* problem for a large number of horizontal layers of finite extent, with various boundary conditions (sink or reflection) at the system edges. As a first step in this direction, we consider the simple case of tracer motion in a geometry consisting of two two-dimensional, semi-infinite layers, where tracer is released in the interior point and is adsorbed at the edges. Although a great simplification compared to the case of an infinite number of layers, as we shall see this problem is already sufficiently difficult that only an approximate solution is available. (In fact, even in the ostensibly elementary problem of simple diffusion in two half-spaces with different diffusivities, a lengthy analysis has recently appeared.⁽¹³⁾)

The analysis to follow is based on an exact generating function formalism for biased random walks in the geometry of interest, and approximation schemes to extract the asymptotic behavior. More generally, we hope that our methods are pertinent to the problem of transport in systems with "block" disorder, for inhomogeneous materials which are naturally modeled as a collection of finite homogeneous sub-regions placed in contact.⁽¹⁴⁾ When the size of the sub-regions is much less than that of the system itself, or the wavelength of any probe, the disorder is short ranged and perturbation techniques are appropriate, but otherwise few methods beyond numerical simulation are available.

In this paper, we address the first passage time properties of passive tracer which convects and diffuses in a two-layer system, which is the simplest nontrivial case of layered structures. The system, shown in Fig. 1, consists of two semi-infinite blocks occupying the two-dimensional region $|x| \leq L$. The blocks are in physical contact, allowing tracer to pass between them, and inside each block different fluid flow fields convect the tracer. For simplicity, the tracer diffusivities are assumed to be equal. The two finite boundaries at $x = \pm L$ are taken to be perfect absorbers. Tracer is released at some point in the interior, and the time-dependent flux at the boundary is computed, which in this situation is identical to the first passage time probability distribution.

We begin in Section 2 with a precise formulation of the model as a random walk process, and by introducing appropriate generating functions, formulate an exact self-consistency relation for the first passage time distribution.² In Section 3, in order to obtain the asymptotic behavior at long time, we expand the first passage time distribution in terms of the number of times a tracer particle has crossed the interface between the blocks before reaching the boundaries. We then approximately sum the expansion, using the central limit theorem, to obtain the asymptotic distribution. We show analytically that *the asymptotic distribution decays as a simple exponential in time, for any choice of the velocity fields*, where the decay constant is given in terms of the largest eigenvalue of an operator which is related to a half-space Green's function. We estimate the decay constant for the special case of the "antisymmetric" model. For the limiting case of high velocities, we estimate the largest eigenvalue and find the decay constant behaves as $1/L$, which agrees with numerical simulations. In the opposite case of pure diffusion, the decay constant behaves as $1/L^2$, in good agreement with analytic estimates and numerical simulations. In Section 4, we consider the behavior in the intermediate-velocity regime, using two methods: an expansion method about the convective limit, and a more general scaling argument which predicts a crossover from a diffusive to a convective regime as L increases. The crossover length L^* is given in terms of the velocity, and the scaling argument is consistent with the above results as well as those of numerical simulations. We conclude in Section 5, with a summary and discussion of future possibilities. In Appendix A, we interpret the general self-consistency condition as a recursion relation, and obtain an expansion useful for obtaining the short-time behavior of the first passage time distribution. Appendix B solves the first passage time problem explicitly for the simple case of convection and diffusion in a single layer.

² One can study the problem using a continuous (time and/or space) random walk. However, that approach has not been pursued in this paper.

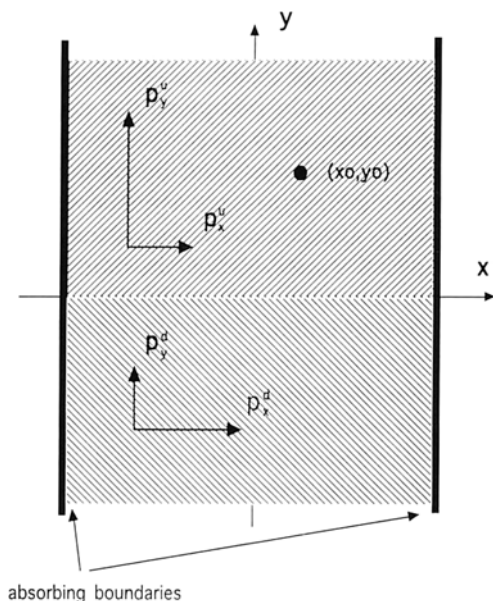


Fig. 1. System geometry: two semi-infinite blocks, $y > 0$ and $y \leq 0$, with different velocities, with absorbing boundaries at $x = \pm L$.

2. SELF-CONSISTENCY RELATION

2.1. Definition of the Model

Since the tracer motion is given by the convection-diffusion equation, one may equivalently think of it as a biased random walk on a spatial lattice in discrete time. Consider then a lattice of unit spacing in the x - y plane, where the velocity field takes on different values in the upper and lower half-planes, and where only the region $-L \leq x \leq L$ is relevant (see Fig. 1). The probability $P_n(x, y)$ that the particle is at position (x, y) at time n is given by the master equation

$$\begin{aligned}
 P_{n+1}(x, y) = & p_x(y-1) p_y(y-1) P_n(x-1, y-1) \\
 & + p_x(y+1)[1-p_y(y+1)] P_n(x-1, y+1) \\
 & + [1-p_x(y-1)] p_y(y-1) P_n(x+1, y-1) \\
 & + [1-p_x(y+1)][1-p_y(y+1)] P_n(x+1, y+1) \\
 & + \delta_{n+1,0} \delta_{x,x_0} \delta_{y,y_0}
 \end{aligned} \tag{1}$$

where p_x (p_y) are the hopping probabilities in the positive x (y) direction, which satisfy

$$p_{x/y}(y) = \begin{cases} p_{x/y}^u & \text{if } y \geq 1 \\ p_{x/y}^d & \text{otherwise} \end{cases} \tag{2}$$

and where the Kronecker deltas prescribe that the particle starts from (x_o, y_o) at time $n=0$. The master equation implies that each step is along the diagonal of a square, which is a particularly convenient hopping rule for the analysis to come, and in the limit of long time and distance, as good as any other. Indeed, by expanding the right-hand side in a Taylor series about (x, y) , it is easy to see that (1) is equivalent to a convection-diffusion equation with diffusion coefficient $1/2$ and velocity $(2p_x - 1, 2p_y - 1)$. (There are also higher-order terms involving the derivatives of $p_{x/y}$, which are not relevant in the cases considered subsequently.)

The first passage problem corresponds to absorbing boundaries at the system edges, so we put $P_n(x, y) = 0$ at $x = \pm L$, and define H_n^\pm to be the probability that the particle first reaches $x = \pm L$ at time n . Motivated by simplicity and previous work on the many-layer problem, we suppose the velocities are in the x direction, parallel to the layer boundaries, so that $p_y^u = p_y^d = 1/2$. For the same reasons, we assume that the net convective bias or average velocity vanishes, which implies that the probability of hopping to the right in the upper half plane equals the probability of hopping to the left in the lower half-plane, or $p_x^u = 1 - p_x^d$. We refer to this as the “anti-symmetric” model, and some results about the general case appear in Section 5. Lastly, in the remainder of this section, we simplify the analysis by further assuming $p_x^u = 1$ (and $p_x^d = 0$); so that particles in the upper (lower) half-plane always move to the right (left), and we refer to this as the “+/- model.” The latter restriction is lifted in Section 4.

2.2. Derivation of a Self-Consistency Relation

In this section, we derive some useful relations for the +/- model. The master equation (1) reduces to

$$P_{n+1}(x, y) = \begin{cases} (P_n(x-1, y-1) + P_n(x-1, y+1))/2, & y \geq 2 \\ (P_n(x-1, y+1) + P_n(x+1, y-1))/2, & y = 0, 1 \\ (P_n(x+1, y-1) + P_n(x+1, y+1))/2, & y \leq -1 \end{cases} + \delta_{n+1,0} \delta_{x,x_o} \delta_{y,y_o} \tag{3}$$

We define the following generating functions:

$$\begin{aligned}
 P(x, y, z) &\equiv \sum_{n=0}^{\infty} P_n(x, y) z^n \\
 G_+(x, \alpha, z) &\equiv \sum_{y=1}^{\infty} P(x, y, z) \alpha^y \\
 G_-(x, \alpha, z) &\equiv \sum_{y=-\infty}^0 P(x, y, z) \alpha^y
 \end{aligned} \tag{4}$$

Substituting Eq. (4) in Eq. (3), we obtain

$$\begin{aligned}
 G_+(x, \alpha, z) &= \frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) G_+(x-1, \alpha, z) \\
 &\quad + \frac{z}{2} (P(x+1, 0, z) \alpha - P(x-1, 1, z)) \\
 &\quad + \delta_{x, x_0} \alpha^{y_0}
 \end{aligned} \tag{5}$$

and

$$\begin{aligned}
 G_-(x, \alpha, z) &= \frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) G_-(x+1, \alpha, z) \\
 &\quad + \frac{z}{2} (P(x-1, 1, z) - P(x+1, 0, z) \alpha)
 \end{aligned} \tag{6}$$

where we assume $y_0 \geq 1$ without the loss of generality.

The functions G_+ and G_- can be expressed in terms of simple Green's functions. We define the Green's function in the upper block ($y \geq 1$) to be the solution of

$$g_+(x; x', \alpha, z) = \frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) g_+(x-1; x', \alpha, z) + \delta_{x, x'} \tag{7}$$

which is

$$g_+(x; x', \alpha, z) = \begin{cases} \left[\frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) \right]^{x-x'} & \text{if } -L < x' \leq x < L \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

Similarly, the Green's function for the lower block ($y \leq 0$), is the solution of

$$g_-(x; x', \alpha, z) = \frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) g_-(x+1; x', \alpha, z) + \delta_{x, x'} \tag{9}$$

which is

$$g_-(x; x', \alpha, z) = \begin{cases} \left[\frac{z}{2} \left(\alpha + \frac{1}{\alpha} \right) \right]^{x'-x} & \text{if } -L < x \leq x' < L \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

Using these Green's functions, we can express G_{\pm} as

$$G_+(x, \alpha, z) = \frac{z}{2} \sum_{x'=-L+1}^{L-1} g_+(x; x', \alpha, z) [P(x'+1, 0, z) \alpha - P(x'-1, 1, z)] + g_+(x; x_o, \alpha, z) \alpha^{y_o} \quad (11)$$

and

$$G_-(x, \alpha, z) = \frac{z}{2} \sum_{x'=-L+1}^{L-1} g_-(x; x', \alpha, z) [P(x'-1, 1, z) - P(x'+1, 0, z) \alpha] \quad (12)$$

There is a simple way to understand Eqs. (11)–(12). The Green's function g_+ (g_-) is the solution of the homogeneous convection equation $P_x = 1$ (0) for a particle starting from $(x', 0)$. The second term in Eq. (11) corresponds to the original particle which starts from (x_o, y_o) . The first term of the equation is due to the existence of the boundary. It subtracts the contribution of the particle [$P(x, 1, z)$ term] which leaves the block, and adds the contribution of the particle [$P(x, 0, z)$ term] which enters the block. The equation for the lower block, Eq. (12), has essentially the same structure, except that it lacks the second term due to the absence of a starting particle in the block.

We are interested in the first passage properties which can be calculated from H_n^{\pm} . They are related to G_{\pm} by

$$\begin{aligned} H^+(z) &= zG_+(L-1, 1, z) \\ H^-(z) &= zG_-(-L+1, 1, z) \end{aligned} \quad (13)$$

where $H^{\pm}(z)$ is defined to be $\sum_{n=0}^{\infty} H_n^{\pm} z^n$. In Eqs. (11)–(12), G_{\pm} are expressed in terms of two unknown functions $P(x, 0, z)$ and $P(x, 1, z)$, which again can be calculated from G_{\pm} themselves as follows. We expand Eq. (11) as a series of α . The terms proportional to α , from the definition of $G_+(x, \alpha, z)$, are exactly $P(x, 1, z) \alpha$. In other words,

$$\begin{aligned}
 P(x, 1, z) = & \frac{z}{2} \sum_{x'=-L+1}^x \left(\frac{z}{2}\right)^{x-x'} \binom{x-x'}{(x-x')/2} P(x'+1, 0, z) \\
 & - \frac{z}{2} \sum_{x'=-L+1}^x \left(\frac{z}{2}\right)^{x-x'} \binom{x-x'}{(x-x'+1)/2} P(x'-1, 1, z) \\
 & + \left(\frac{z}{2}\right)^{x-x_0} \binom{x-x_0}{(x-x_0+y_0-1)/2} \quad (14)
 \end{aligned}$$

Similarly, $P(x, 0, z)$ can be expressed as

$$\begin{aligned}
 P(x, 0, z) = & \frac{z}{2} \sum_{x'=x}^{L-1} \left(\frac{z}{2}\right)^{x'-x} \binom{x'-x}{(x'-x)/2} P(x'-1, 1, z) \\
 & - \frac{z}{2} \sum_{x'=x}^{L-1} \left(\frac{z}{2}\right)^{x'-x} \binom{x'-x}{(x'-x-1)/2} P(x'+1, 0, z) \quad (15)
 \end{aligned}$$

where $\binom{x}{y}$ is the binomial coefficient. Here, we also define $\binom{x}{y} = 0$, if x or y is not a nonnegative integer, or if $x < y$. Thus, the problem of calculating the first passage property is reduced to solving the self-consistency equations (14)–(15). This is the key result in this section, and it will later serve as a basis for an iteration scheme. It is not unnatural that we end up with self-consistent relations rather than explicit solutions. The boundary conditions we have to satisfy at the interface between the two blocks are (1) continuity and (2) flux conservation. Since these conditions are only implicit [i.e., they are relations among the fields $P(x, y, z)$], they result in implicit relations between $G(x, \alpha, z)$, which are the self-consistency conditions.

Unfortunately, these conditions are essentially $4L - 2$ coupled linear equations, which are nontrivial to solve. We have developed an iterative scheme useful in getting the short-time behaviors ($n \sim L$), which is discussed in Appendix A. We now develop an alternative method which can give the information about the asymptotic ($n \gg L$) behavior.

3. ASYMPTOTIC BEHAVIOR

3.1. Expansion of $H_+(z)$

We turn to an alternative method for obtaining the first passage time. We expand quantities in terms of the number of times the particle has crossed the interface between the blocks before reaching the boundary. Consider the $+/-$ model again, Eq. (3), and recall the previous definitions

of $P(x, y, z)$ and $H_+(z)$, Eqs. (4) and (13). We now define "half-space" Green's functions g_{\pm}^h as

$$g_+^h(x, y, x', y', z) = \left(\frac{z}{2}\right)^{x-x'} \left\{ \binom{x-x'}{(x-x'+y-y')/2} - \binom{x-x'}{(x-x'+y+y')/2} \right\}$$

$$g_-^h(x, y, x', y', z) = \left(\frac{z}{2}\right)^{x'-x} \left\{ \binom{x'-x}{(x'-x+y-y')/2} - \binom{x'-x}{(x'-x+y+y')/2} \right\}$$

(16)

where $\binom{x}{y}$ is defined as in Eq. (15). Here, g_+^h (g_-^h) is the Green's function in the upper (lower) block with absorbing boundary at $y=0$ ($y=1$). Due to the boundary condition, the functions g_{\pm}^h do not contain contributions from the particles which leave the block, a property which will be useful subsequently.

We define $H_+^{(n)}(z)$, the part of $H_+(z)$ corresponding to particles which have crossed the interface n times. Using the definition of g_+^h , we have

$$H_+^{(0)}(z) = \sum_y z g_+^h(L-1, y, x_o, y_o, z) \tag{17}$$

where we assume $y_o > 0$ without loss of generality. We now calculate the flux of particles out of the upper block. Define $P^{(n)}(x, y, z)$ to be the part of $P(x, y, z)$ corresponding to particles which have crossed the interface n times. At the edge of the upper block (the $y=1$ line),

$$P^{(0)}(x, 1, z) = g_+^h(x, 1, x_o, y_o, z) \tag{18}$$

Half $(1-p_y^n)$ of these particles will jump to $(x+1, 0)$. Therefore, the influx at the edge of the lower block ($y=0$ line) is

$$P_{in}^{(1)}(x, 0, z) \equiv \frac{z}{2} P^{(0)}(x-1, 1, z) \tag{19}$$

We define the operator $T_{\pm}(x, x', z)$ as

$$\frac{z}{2} v(x \pm 1, z) \equiv \sum_{x'} T_{\pm}(x, x', z) v(x, z') \tag{20}$$

where $v(x, z)$ is a vector. Thus, Eq. (19) in operator form is

$$P_{in}^{(1)}(0, z) = T_-(z) P^{(0)}(1, z) \tag{21}$$

where we dropped the indices x and x' .

We have to know what fraction of the flux will go back to the upper block. We first obtain

$$P^{(1)}(x, 0, z) = \sum_{x'} g_-^h(x, 0, x', 0, z) P_{\text{in}}^{(1)}(x', 0, z) \tag{22}$$

Again, half (p_y^d) of the particles will cross the interface and jump to $(x - 1, 1)$,

$$P_{\text{in}}^{(2)}(x, 1, z) \equiv \frac{z}{2} P^{(1)}(x + 1, 0, z) = T_+(z) P^{(1)}(0, z) \tag{23}$$

Since $H_+^{(2)}$ arises from from the walkers which have crossed the interface twice, its sole contribution comes from $P_{\text{in}}^{(2)}$ which is

$$H_+^{(2)}(z) = z \sum_y \sum_{x'} g_+^h(L - 1, y, x', 1, z) P_{\text{in}}^{(2)}(x', 1, z) \tag{24}$$

We then calculate the fraction of $P_{\text{in}}^{(2)}$ which jumps back to the lower block, thus completing the cycle. At the edge of the upper block,

$$P^{(2)}(x, 1, z) = \sum_{x'} g_+^h(x, 1, x', 1, z) P_{\text{in}}^{(2)}(x, 1, z) \tag{25}$$

and half of these will jump to $(x + 1, 0)$

$$P_{\text{in}}^{(3)}(0, z) = T_-(z) P^{(2)}(1, z) \tag{26}$$

The above results can be written in a more compact form. We first define several operators

$$\begin{aligned} (g_+^o(z))_{x, x'} &\equiv g_+^h(x, 1, x', 1, z) \\ (g_-^o(z))_{x, x'} &\equiv g_-^h(x, 0, x', z) \\ (h_+^o(z))_{x, x'} &\equiv z \sum_y g_+^h(L - 1, y, x', 1, z) \end{aligned} \tag{27}$$

in terms of which the above results can be written as

$$\begin{aligned} P_{\text{in}}^{(2)}(1, z) &= T_+(z) g_-^o(z) T_-(z) P^{(0)}(1, z) \\ H_+^{(2)}(z) &= h_+^o(z) P_{\text{in}}^{(2)}(1, z) \end{aligned} \tag{28}$$

Furthermore, by repeating the above procedure, we can show that

$$\begin{aligned} P_{\text{in}}^{(2i)}(1, z) &= T_+(z) g_-^o(z) T_-(z) g_+^o(z) P_{\text{in}}^{(2i-2)}(1, z) \\ H_+^{(2i)} &= h_+^o(z) P_{\text{in}}^{(2i)}(1, z) \end{aligned} \tag{29}$$

With the definitions

$$\begin{aligned}
 u(z) &= T_+(z) g_-^o(z) T_-(z) g_+^o(z) \\
 u_1(z) &= T_+(z) g_-^o(z) T_-(z)
 \end{aligned}
 \tag{30}$$

we arrive at the key result of this section:

$$H_+(z) = H_+^{(0)}(z) + \sum_{i=1}^{\infty} h_+^o(z) u^i(z) u_1(z) P^{(0)}(1, z)
 \tag{31}$$

The validity of the expansion has been checked by comparing $H_+(z)$ obtained above with that obtained by numerical simulations. Details of the simulations will be discussed later.

3.2. Asymptotic Form of H_+^n

In this section, we derive the asymptotic form of the first passage time distribution, starting from Eq. (31). Recall the definition $H_+(z) \equiv \sum_n H_+^n z^n$. In general, $H_+(z)$ is an infinite-order polynomial in z , where H_+^n , the coefficient of z^n , is the hitting probability at time n . We now consider the various terms in Eq. (31). Using Eq. (17), we can show that the degree of $H_+^{(0)}(z)$ cannot be larger than $2L - 1$. Since it does not give a contribution to $H_+(z)$ in the asymptotic $n \gg L$ regime, we can ignore this term. Next, in the summand of the equation, the same operator $u(z)$ has been repeatedly applied to a vector $u^i(z) P^{(0)}(1, z)$. Thus, we can approximate $u^i(z)$ with $\lambda^i(z)$, where $\lambda(z)$ is the largest eigenvalue of $u(z)$. If the operator in question is self-adjoint and diagonalizable, this approximation would surely be justified, at least for $i \gg 1/[\lambda(z) - \lambda_2(z)]$, where $\lambda_2(z)$ is the second largest eigenvalue of $u(z)$, but in this instance this step is an assumption, which, however, is supported by the numerical results below. We now ask whether the asymptotic behavior will be changed by the approximation. The maximum degree of z for the terms in the summand can be calculated from Eq. (16). The maximum degree of $h_+^o(z)$, $u(z)$, $u^i(z)$ and $P^{(0)}(1, z)$ cannot be larger than $2L - 1$, $4L - 2$, $2L$, and $2L - 2$, respectively. In the sum, the term containing $u^i(z)$ contributes for $n \leq i(2L - 1) + 6L - 3$. Therefore, the terms for which the eigenvalue approximation is not valid ($i < i_o$, and i_o is finite) give a contribution only up to finite time, and will not change the asymptotic behavior. Thus,

$$H_+(z) \sim \sum_{i=0}^{\infty} \lambda^i(z) \cdot [h_+^o(z) u^i(z) P^{(0)}(1, z)]
 \tag{32}$$

The product $h_+^o(z) u'(z) P^{(0)}(1, z)$ is also a polynomial of finite order, and ignoring the product changes only the amplitude of the asymptotic behavior. We thus arrive at simple expression

$$H_+(z) \sim \frac{1}{1 - \lambda(z)} = \sum_{i=0}^{\infty} \lambda^i(z) \tag{33}$$

We define the coefficient of the z^j term of $\lambda(z)$ to be c_j^1 . We can interpret $\lambda(z)$ as a generating function for a random walk process—the probability to jump j steps forward is given by the coefficient c_j^1 . The fraction of random walkers which survive after one step is $s_o \equiv \lambda(1)$. The average displacement after one step is $s_1 \equiv \lambda'(1)/\lambda(1)$, and the average of the square of the displacement after one step is $s_2 \equiv \lambda''(1)/\lambda(1)$, where

$$\begin{aligned} \lambda'(z) &= z \frac{d}{dz} \lambda(z) \\ \lambda''(z) &\equiv \left[z \frac{d}{dz} \right]^2 \lambda(z) \end{aligned} \tag{34}$$

We also define the variance $\sigma^2 \equiv s_1^2 - s_2$. Following the interpretation, the coefficient c_j^i of the z^j term for $\lambda^i(z)$ forms the distribution of the displacement of the random walker after i steps. The fraction of random walkers which survive for i steps is s_o^i , the average displacement is is_1 , and the variance is $i\sigma^2$. Since the second moment s_2 is finite, we can apply the central limit theorem. Thus for large i , the coefficient c_j^i becomes

$$c_j^i \sim \frac{s_o^i}{(2\pi i \sigma^2)^{1/2}} \exp \left[-\frac{(j - is_1)^2}{2i\sigma^2} \right] \tag{35}$$

Substituting this into the equation for $H_+(z)$, Eq. (33), we obtain

$$H_+^n \sim \sum_{i=0}^{\infty} \frac{s_o^i}{(2\pi i \sigma^2)^{1/2}} \exp \left[-\frac{(n - is_1)^2}{2i\sigma^2} \right] \tag{36}$$

which can be evaluated by the method of the steepest descent to be

$$\begin{aligned} H_+^n &\sim \exp \left[\ln s_o \cdot \frac{n}{s_1} \cdot \frac{1 - \ln s_o \cdot (\sigma/s_1)^2/2}{1 - \ln s_o \cdot (\sigma/s_1)^2} \right] \\ &\equiv \exp[-c(L)n] \end{aligned} \tag{37}$$

where $c(L)$ is a size-dependent decay constant. Even though the equation is derived for the $+/-$ model, its derivation only assumes the existence of

the half-space Green's functions similar to Eq. (16). *Since these functions exist for the most general situation of the two block system, the asymptotic distribution is always simple exponential.* Below, we compare the above results with an exact enumeration method, and find good agreement.

3.3. Estimation of the Eigenvalue

The problem of finding the asymptotic behavior of the first passage time distribution is reduced to finding $\lambda(z)$, the largest eigenvalue of the operator $u(z)$. Unfortunately, there is no known method to calculate the analytic expression of the eigenvalues of an arbitrary matrix, and the complicated structure of $u(z)$ does not help matters. We present two methods to estimate $\lambda(z)$. These methods are not expected to produce exact numbers, but are intended to give some idea of the parameter L -dependences of the first passage time distribution.

The first method is to express $\lambda(z)$ in terms of the average of the elements of $u(z)$. We start from the matrix $T_+(z)g_-^o(z)$, whose largest eigenvalue $\lambda_+(z)$ is approximated as

$$\lambda_+(z) \sim \frac{1}{2L-1} \sum_{x=-L+1}^{L-1} \sum_{x'=-L+1}^{L-1} (T_+(z)g_-^o(z))_{x,x'} \quad (38)$$

where $2L-1$ is the size of the matrix. This approximation is motivated by the numerical fact that the eigenvector $v_+(z)$ corresponding to $\lambda_+(z)$ is close to being uniform, i.e., $(v_+(z))_x = v_o(z)$ for all x . Note that if the eigenvector is uniform, Eq. (38) becomes exact. We then obtain

$$\lambda_+(z) \sim \frac{1}{2L-1} \left(\frac{z}{2}\right) (2L-2) + \frac{1}{2L-1} \sum_{k=1}^{L-1} \left(\frac{z}{2}\right)^{2k+1} (2L-2k-2) \left\{ \binom{2k}{k} - \binom{2k}{k+1} \right\} \quad (39)$$

The expression can be further simplified to

$$\lambda_+(z) \sim \frac{z}{2} + \frac{1}{(4\pi)^{1/2}} \sum_{k=1}^L z^{2k} k^{-3/2} \left(1 - \frac{k}{L}\right) \quad (40)$$

where we assume $L \gg 1$. The largest eigenvalue $\lambda_-(z)$ of the matrix $T_-(z)g_+^o(z)$ can also be estimated by the same method. It turns out that

$$\lambda_-(z) \sim \lambda_+(z) \quad (41)$$

The matrix $u(z)$ is given by the product of the two matrices $T_+(z)g_-^o(z)$ and $T_-(z)g_+^o(z)$. We further approximate the largest eigenvalue of the

product of two matrices as the product of the largest eigenvalues of the two matrices, which implies

$$\lambda(z) \sim \lambda_-(z) \lambda_+(z) \sim \lambda_+^2(z) \quad (42)$$

We calculate $\lambda_+(1)$, $\lambda'_+(1)$, and $\lambda''_+(1)$, where the primed values are defined in the same way in Eq. (34). By evaluating the integral in Eq. (40), we obtain

$$\begin{aligned} \lambda_+(1) &\sim \left(\frac{1}{2} + \frac{1}{\sqrt{\pi}}\right) - \frac{2}{\sqrt{\pi}} L^{-1/2} + \mathcal{O}\left(\frac{1}{L}\right) \\ \lambda'_+(1) &\sim \frac{4}{3\sqrt{\pi}} L^{1/2} + \left(\frac{1}{2} - \frac{2}{\sqrt{\pi}}\right) + \mathcal{O}\left(\frac{1}{L}\right) \\ \lambda''_+(1) &\sim \frac{8}{15\sqrt{\pi}} L^{3/2} + \left(\frac{1}{2} - \frac{4}{3\sqrt{\pi}}\right) + \mathcal{O}\left(\frac{1}{L}\right) \end{aligned} \quad (43)$$

The second approximation method is based on the interpretation that $\lambda(z)$ is related to a certain generating function for a random walk. Consider the matrix $T_-(1)g'_+(1)$. The matrix gives the probability to reach points on $y=0$, starting from points on $y=1$ with an absorbing boundary at $y=0$. Thus, $\lambda_+(z)$ is roughly the generating function of the hitting probability on the line $y=0$ for a walk starting from $y=1$. For simplicity, consider a walker starting from $(0, 1)$. Since the only effect of convection in the x direction is to remove all the walkers which do not reach $y=0$ until time step L , we only have to deal with a one-dimensional problem. The corresponding one-dimensional problem is treated by ignoring the x axis and limiting the maximum time step to be L . Then $\lambda_+(z)$ is

$$\lambda_+(z) \sim \int_1^L dn \frac{z^n}{(2\pi n)^{1/2}} (1 - e^{-8/n}) \quad (44)$$

where the integrand is the flux to $y=0$ at step n , and we have approximated the sum by an integral. The eigenvalue $\lambda_+(1)$ is

$$\lambda_+(1) \sim \int_1^\infty dn \frac{1}{(2\pi n)^{1/2}} (1 - e^{-8/n}) - \int_L^\infty dn \frac{1}{(2\pi n)^{1/2}} (1 - e^{-8/n}) \quad (45)$$

The first integral is the probability to hit $y=0$ during an infinite period of time, which is unity. After simplifying the second integral for $L \gg 1$ we have

$$\lambda_+(1) \sim 1 - \frac{16}{(2\pi)^{1/2}} L^{-1/2} \quad (46)$$

The second approximation, compared to Eq. (43), has the same dependence on L , but different numerical coefficients. This supports the previous suggestion that the coefficients obtained by these methods are not reliable. However, the fact that two very different methods give the same dependence on L gives some support to the validity of the form. The leading term in $\lambda_+(1)$, which is the value of $\lambda_+(1)$ in the limit $L \rightarrow \infty$, deserves special attention. It is the probability that an unbiased random walker hits the $y = 0$ line during an infinite period of time, which is equal to unity. Even in the case that the matrix is applied to the exact eigenvector, the random walker eventually has to be absorbed at the $y = 0$ boundary for $L \rightarrow \infty$, implying $\lambda_+(1) = 1$. Therefore, we set $\lim_{L \rightarrow \infty} \lambda_+(1) = 1$ from now on.

We now proceed to calculate $c(L)$. The expressions for s_o , s_1 and s_2 can be obtained from Eqs. (43) and (42):

$$\begin{aligned}
 s_o &\sim \lambda_+^2(1) \simeq 1 - \frac{4}{\sqrt{\pi}} L^{-1/2} + \mathcal{O}\left(\frac{1}{L}\right) \\
 s_1 &\sim 2 \frac{\lambda'_+(1)}{\lambda_+(1)} \simeq \frac{8}{3\sqrt{\pi}} L^{1/2} + \mathcal{O}(1) \\
 s_2 &\sim 2 \frac{\lambda''_+(1)}{\lambda_+(1)} + 2 \left(\frac{\lambda'_+(1)}{\lambda_+(1)}\right)^2 \simeq \frac{16}{15\sqrt{\pi}} L^{3/2} + \mathcal{O}(L) \\
 \sigma^2 &\sim s_2 - s_1^2 \sim \frac{16}{15\sqrt{\pi}} L^{3/2} + \mathcal{O}(L)
 \end{aligned}
 \tag{47}$$

Finally, we can calculate $c(L)$ using the definition in Eq. (37),

$$\begin{aligned}
 c(L) &\equiv -\frac{\ln s_o}{s_1} \frac{1 - \ln s_o(\sigma/s_1)^2/2}{1 - \ln s_o(\sigma/s_1)^2} \\
 &\sim \frac{39}{32} L^{-1}
 \end{aligned}
 \tag{48}$$

3.4. Numerical Check

We have calculated the decay constant $c(L)$ in three major steps. First, we expand $H_+(z)$ in terms of the number of times a random walker has crossed the interface [Eq. (31)]. We then calculate its asymptotic distribution in terms of the eigenvalue $\lambda(z)$ with the help of the central limit theorem [Eq. (37)]. We then estimate $\lambda(z)$ and $c(L)$ [Eqs. (47)–(48)]. In this section, we check the validity of these results by comparing them with those of numerical simulations. It will serve as an intermediate check

before we proceed to a more general situation, where we will continue to use the methods developed above.

We start with the exact sum, Eq. (31). We calculate the first few moments of $H_+(z)$ from the equation, which are easier to compare. The zeroth moment $H_+(1)$ is rather easy to evaluate. Consider the i th term in the sum. We just have to calculate the product $h_+(1) u(1) P_{in}^{(2i+2)}(1, 1)$, where we know all the individual terms. Furthermore, the $(i + 1)$ th term can be obtained by replacing $P_{in}^{(2i+2)}(1, 1)$ by $P_{in}^{(2i+4)}(1, 1) = u(1) P_{in}^{(2i+2)}(1, 1)$. We sum these terms in the increasing order of i , until the magnitude of the new term is smaller than a certain value, which is chosen to be 10^{-20} . The higher moments are slightly more complicated to calculate. Consider again the i th term in the sum. The first moment can be calculated by using the chain rule

$$\begin{aligned}
 & [h_+(z) u(z) P_{in}^{(2i+2)}(1, z)]' \\
 &= h_+'(z) u(z) P_{in}^{(2i+2)}(1, z) + h_+(z) u'(z) P_{in}^{(2i+2)}(1, z) \\
 &+ h_+(z) u(z) P_{in}'^{(2i+2)}(1, z)
 \end{aligned} \tag{49}$$

where the primed values are defined in the same way as in Eq. (34). Also the $(i + 1)$ th term can be obtained by replacing

$$\begin{aligned}
 P_{in}^{(2i+2)}(1, z) &\rightarrow P_{in}^{(2i+4)}(1, z) = u(z) P_{in}^{(2i+2)}(1, z) \\
 P_{in}'^{(2i+2)}(1, z) &\rightarrow P_{in}'^{(2i+4)}(1, z) = u'(z) P_{in}^{(2i+2)}(1, z) + u(z) P_{in}'^{(2i+2)}(1, z)
 \end{aligned} \tag{50}$$

Higher-order moments are calculated in same way with the heavy use of the identity

$$[A(z) B(z)]^{(n)} = \sum_{k=0}^n \binom{n}{k} A^{(k)}(z) B^{(n-k)}(z) \tag{51}$$

where $A^{(n)}(z)$ is the n th derivative of the function $A(z)$. We compare the first five moments with those obtained by an exact enumeration method (see, e.g., ref. 15). For several values of $L = 10-100$ and several initial conditions, the values obtained by the two methods are essentially identical.

We check the next step, the asymptotic form of the hitting probability distribution, Eq. (37). The form is simple exponential, and the decay constant $c(L)$ is given in terms of $\lambda(z)$. We directly calculate the distribution H_+^n by the exact enumeration method for $L = 10-300$. In Fig. 2, we show the distribution for $L = 100$. It is clear that H_+^n is an exponential after some transition period. This is also true for the other sizes we have studied, and the length of the transition period is of the order L .

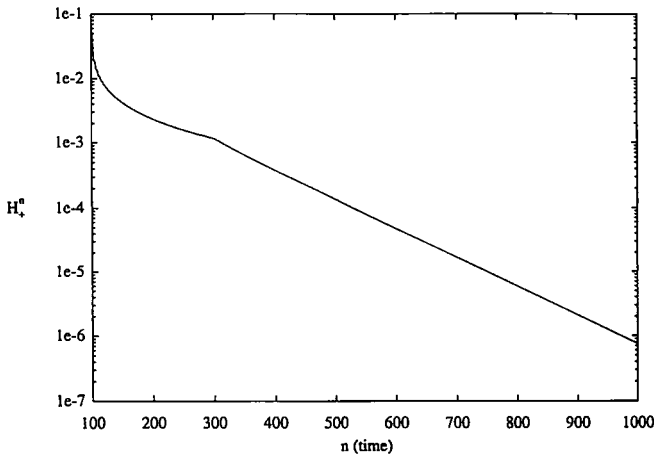


Fig. 2. The hitting probability distribution H_+^n for $L = 100$ obtained by the exact enumeration. An exponential behavior in the asymptotic regime is evident.

We check the value of the decay constant $c(L)$. Since the theoretical value of $c(L)$ is given in terms of $\lambda(z)$, we have to know the value of $\lambda(z)$ in order to compare. To calculate the eigenvalue numerically, we go back to the discussion in the previous paragraph about calculating the moments of $H_+(z)$. We consider $\lambda(1)$ first. Since the matrix $u(1)$ has been repeatedly applied to the vector $P_{in}^{(1i+2)}(1, 1)$ to obtain $P_{in}^{(2i+4)}(1, 1)$, we have

$$\lambda(1) = \lim_{i \rightarrow \infty} P_{in}^{(2i+4)}(1, 1) / P_{in}^{(2i+2)}(1, 1) \tag{52}$$

We find that the ratio hardly changes for $i > 50$, so we take the ratio at $i = 100$ as $\lambda(1)$. For higher moments, start from the relation

$$\lambda(z) = \lim_{i \rightarrow \infty} P_{in}^{(2i+4)}(1, z) / P_{in}^{(2i+2)}(1, z) \tag{53}$$

Taking the derivative and multiplying by z on both sides, we obtain

$$\lambda'(1) = \lim_{i \rightarrow \infty} \frac{P_{in}^{(2i+4)}(1, 1) P_{in}^{(2i+2)}(1, 1) - P_{in}^{(2i+4)}(1, 1) P_{in}^{(2i+2)}(1, 1)}{[P_{in}^{(2i+2)}(1, 1)]^2} \tag{54}$$

The higher-order terms [e.g., $\lambda''(1)$] can be calculated in a similar way. Finally, using these $\lambda(1)$, $\lambda'(1)$, and $\lambda''(1)$ we calculate the decay constant $c(L)$ from Eq. (37). In Fig. 3, we show the values of $c(L)$ just obtained as well as those obtained by numerical simulations, for several values of L . The simulational values are obtained by least-square fitting the last one-half or one-third part of the numerically obtained H_+^n , like the one in

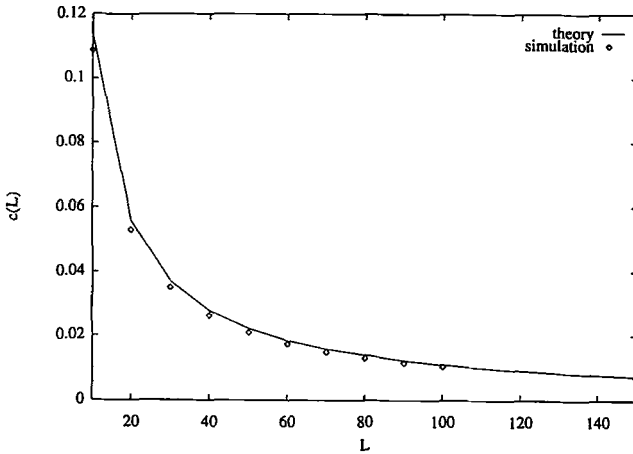


Fig. 3. The decay constant $c(L)$ for the $+/-$ model given by the eigenvalue approximation (solid line) compared to the value obtained by the exact enumeration (diamonds).

Fig. 2. There are in general good agreements between these two values except for very small values of L , where several approximations made to get the theoretical value may not be justified.

We proceed to the last step of the calculation, the estimation of the decay constant $c(L)$. In Fig. 4, we show the values of $c(L)$ given by Eq. (48) and those obtained by the exact enumeration. The values by the enumeration are identical to those shown in Fig. 3. It is clear that the numerical

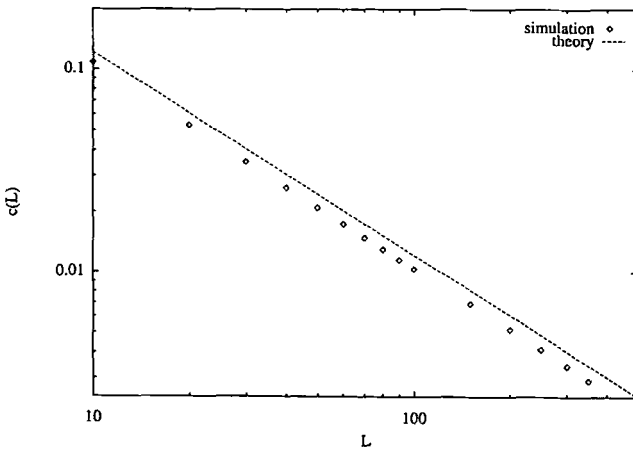


Fig. 4. The decay constant $c(L)$ for the $+/-$ model given by Eq. (48) (dashed line) and that obtained by the exact enumeration (diamonds).

data show the $1/L$ behavior as predicted by the theory. On the other hand, the measured prefactor (~ 1) is a little smaller than the predicted value (39/32). These are all in accord with the expectation that the prediction of the $1/L$ dependence is reliable, but that of the prefactor is not. It is unexpected that the value of the prefactor obtained by the enumeration method is so close to that of the theory.

We have checked the steps to reach the decay constant $c(L)$. The errors involved in the eigenvalue approximation are well controlled, and the approximation seems to be well justified for obtaining the asymptotic properties. Even though we do not have the same level of rigor in estimating the eigenvalues $\lambda(z)$, we still have enough control to predict the correct dependence of L .

4. THE GENERAL ANTISYMMETRIC MODEL

Having obtained a reasonable understanding of the asymptotic behavior of the $+/-$ model, we turn to the general antisymmetric model. We now allow an arbitrary horizontal bias $0 \leq p_x^u \leq 1$, and due to the symmetry in the system, we can restrict ourselves to $p_x^u \geq 1/2$ without loss of generality.

4.1. The Diffusive Limit: $p_x^u = 1/2$

We consider the antisymmetric model with no bias ($p_x^u = 1/2$), first using the formalism developed for the $+/-$ model. We now have a different operator $u(z)$, and therefore a different eigenvalue $\lambda(z)$. The asymptotic distribution of H_+^n is still a simple exponential, and the decay constant $c(L, p_x^u)$ is given in terms of $\lambda(z)$ [Eq. (48)]. In Section 3.3 one estimate was based on transforming the problem into a one-dimensional diffusion problem with an absorbing boundary. In the transformation, one determines the average time required for the particles to be absorbed at the external boundaries at $x = \pm L$. In the $+/-$ model, the transport in the horizontal direction is a purely convective process, so that the time is identical to the length L . Now, the transport in the horizontal direction is purely diffusive, so the time is $2L^2$. Substituting into Eq. (48), we obtain

$$c(L, p_x^u) \sim \frac{29}{64} L^{-2} \tag{55}$$

The L^{-2} dependence is also consistent with the calculation for the one-block case with no convection. In Fig. 5, we plot $c(L, p_x^u)$ determined by the above equation as well as those determined by the exact enumeration.

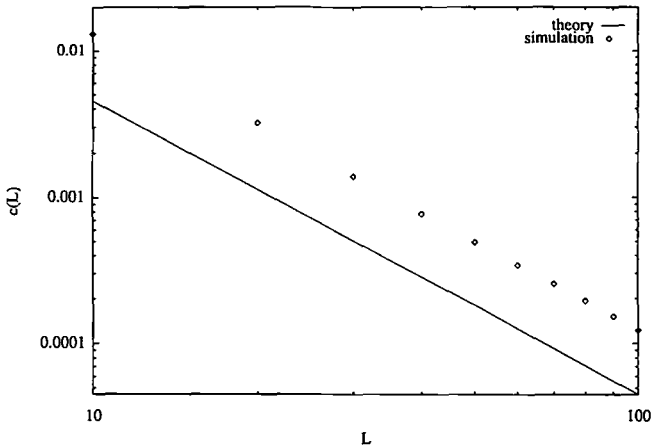


Fig. 5. The decay constant $c(L, p_x^u)$ for the antisymmetric model with $p_x^u = 1/2$ given by Eq. (48) (solid line) and that obtained by the exact enumeration (diamonds).

The numerical data clearly show the $1/L^2$ dependence with the prefactor about twice that given in Eq. (55).

A more direct check of these results is obtained by noting that in this case we are considering pure diffusion in a two-dimensional strip of width $2L$, and one expects an exponential decay of tracer concentration with a time constant $O(L^2)$. More precisely, a straightforward solution of the diffusion equation for this geometry in Appendix B gives $H_n^+ \sim \exp[-(\pi^2/8L^2)n]$, in good agreement with the above simulation.

4.2. The Neighborhood of $p_x^u = 1$

It is useful to consider explicitly the case $p_x^u = 1 - \varepsilon$ to first order of ε , where the formalism developed for the $+/-$ model can be used with only minor changes. Starting from the master equation (1), it is straightforward to show that the half-space Green's functions g_+^h, g_-^h of Eq. (16) must be modified to

$$\begin{aligned}
 g_+^h(x, y; x', y', z) &= (1 - (x - x')\varepsilon) \left(\frac{z}{2}\right)^{x-x'} \\
 &\times \left\{ \left(\binom{x-x'}{(x-x'+y-y')/2} \right) - \left(\binom{x-x'}{(x-x'+y-y')/2} \right) \right\} \\
 &+ (x - x' + 2) \varepsilon \left(\frac{z}{2}\right)^{x-x'+2}
 \end{aligned}$$

$$\begin{aligned}
 & \times \left\{ \binom{x-x'+2}{(x-x'+y-y'+2)/2} \right. \\
 & \left. - \binom{x-x'+2}{(x-x'+y+y'+2)/2} \right\} \\
 g_-^h(x, y; x', y', z) &= (1 - (x' - x)\varepsilon) \left(\frac{z}{2}\right)^{x'-x} \\
 & \times \left\{ \binom{x'-x}{(x'-x+y-y')/2} - \binom{x'-x}{(x'-x+y-y'-2)/2} \right\} \\
 & + (x' - x + 2) \varepsilon \left(\frac{z}{2}\right)^{x'-x+2} \\
 & \times \left\{ \binom{x'-x+2}{(x'-x+y-y'+2)/2} - \binom{x'-x+2}{(x'-x+y+y')/2} \right\}
 \end{aligned} \tag{56}$$

where terms of order ε^2 are ignored. The above equation reduces to Eq. (16) for $\varepsilon = 0$, which suggests that the perturbation is not singular. The eigenvalue $\lambda(z)$ for the matrix $u(z)$ can be obtained by following the same procedure as in the $+/-$ model. We first calculate the eigenvalue $\lambda_+(z)$ of the matrix $T_-(z)g_+(z)$,

$$\begin{aligned}
 \lambda_+(z) &\sim \lambda_+(z)|_{\varepsilon=0} \\
 &+ \frac{2\varepsilon}{2L-1} \sum_{k=1}^{L-1} (2k+1) \left(\frac{z}{2}\right)^{2k+1} \left\{ \binom{2k}{k} - \binom{2k}{k-1} \right\}
 \end{aligned} \tag{57}$$

where $\lambda_+(z)|_{\varepsilon=0}$ is the value of $\lambda_+(z)$ at $\varepsilon = 0$, and $g_+(z)$ is defined as in Eq. (27). Replacing the sum by an integral, we obtain

$$\begin{aligned}
 \lambda_+(1) &\sim 1 - \frac{2}{\sqrt{\pi}} (1 - \varepsilon) L^{-1/2} + \mathcal{O}\left(\frac{1}{L}\right) \\
 \lambda'_+(1) &\sim \frac{4}{3\sqrt{\pi}} (1 + \varepsilon) L^{1/2} + \mathcal{O}(1) \\
 \lambda''_+(1) &\sim \frac{8}{15\sqrt{\pi}} (1 + 3\varepsilon) L^{3/2} + \mathcal{O}(L^{1/2})
 \end{aligned} \tag{58}$$

where we have set $\lim_{L \rightarrow \infty} \lambda_+(1) = 1$ as discussed above. Similarly, the eigenvalue $\lambda_-(z)$ of the matrix $T_+(z)g_-(z)$ is determined to be

$$\lambda_-(z) \sim \lambda_+(z) \tag{59}$$

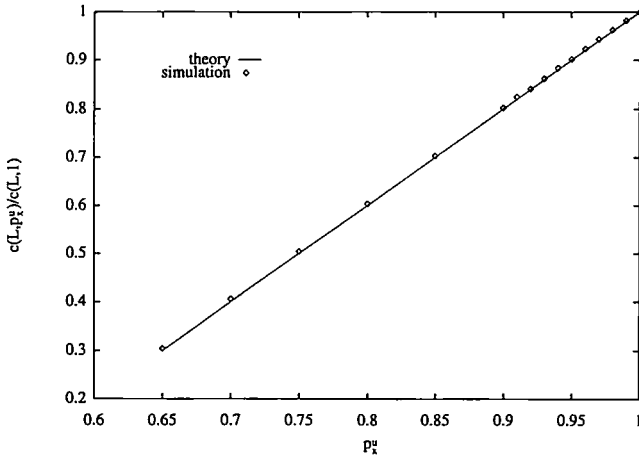


Fig. 6. The normalized decay constant $c(L, p_x^u)$ for the symmetric model predicted by the theory (solid line), and data obtained by the enumeration for $L = 100$ and several values of p_x^u (diamonds). There is good agreement even down to $p_x^u = 0.65$.

Combining these relations, we can write the eigenvalue $\lambda(z)$ as

$$\lambda(z) \sim \lambda_-(z) \lambda_+(z) \sim \lambda_+^2(z) \tag{60}$$

From $\lambda(z)$, the decay constant $c(L, p_x^u)$ is determined to be

$$c(L, p_x^u) \sim \frac{39}{32} (1 - 2\varepsilon) L^{-1} \tag{61}$$

which is the same as the $\varepsilon = 0$ result aside from the factor $1 - 2\varepsilon$, whose origin is easy to understand. When we estimate the eigenvalue by mapping into a one-dimensional problem, the average absorption time is required. For pure convection, this time is the length L divided by the horizontal velocity. In general, this velocity is given by $2p_x^u - 1 = 1 - 2\varepsilon$. Therefore, in the absence of diffusion, $c(L, p_x^u)$ has to be modified by replacing L by $L/(1 - 2\varepsilon)$, which is precisely what we find by the expansion. In Fig. 6, we show $c(L, p_x^u)$ for $L = 100$ and several values of p_x^u , where $c(L, p_x^u)$ is divided by the value at $p_x^u = 1$. We also show the corresponding result by the expansion, Eq. (61). There is a good agreement between the two, and not only is the expansion valid near $p_x^u = 1$ but there is no systematic deviation down to $p_x^u = 0.65$.

4.3. Scaling Argument for General p_x^u

The half-space Green's functions (16) have served as a starting point in the calculation of the decay constant at $p_x^u = 1$ and its neighborhood. For

other values of p_x^u , unfortunately, we are unable to find them in closed form. Although we can still show that the asymptotic distribution of H_+^n is a simple exponential, without explicit knowledge of the Green's functions, we no longer can use the same method to estimate the eigenvalue and the decay constant.

However, since we know the behavior for the two extreme cases of the antisymmetric model ($p_x^u = 1/2$ and 1), we can try to bridge the gap by a simple scaling argument. We propose a scaling ansatz

$$c(L, p_x^u) = L^{-2} f\left(\frac{L}{L^*}\right) \tag{62}$$

where $f(x)$ is a scaling function which satisfies

$$f(x) \sim \begin{cases} 1 & \text{if } x \ll 1 \\ x & \text{if } x \gg 1 \end{cases} \tag{63}$$

where we have defined a crossover length $L^* = 1/(2p_x^u - 1)$. (Recall that the lattice spacing has been set to one.) To verify that the ansatz is in accord with previous results, note first that for $p_x^u = 1$, $L^* = 1$, and since we are interested in $L \gg 1$, (63) gives $c(L, p_x^u) \sim L^{-1}$ as before. Next, for $p_x^u = 1/2$, $L^* \rightarrow \infty$ and $c(L, p_x^u) \sim L^{-2}$, again in agreement. Finally, for $p_x^u = 1 - \epsilon$, $L^* = 1/(1 - 2\epsilon)$, and for small ϵ , $L/L^* \gg 1$, so the decay constant becomes $(1 - 2\epsilon)/L$, which is exactly Eq. (61). To verify the ansatz away from the limiting cases, we have used numerical simulation. In Fig. 7, we show the

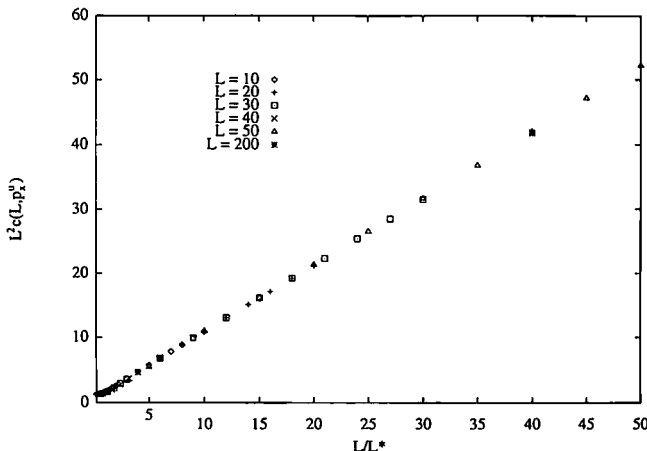


Fig. 7. The rescaled decay constant $c(L, p_x^u)$ obtained by the exact enumeration versus rescaled L . Data for several different values of $L = 10-200$ and $p_x^u = 0.5-1.0$ collapse onto one curve, which is the scaling function $f(x)$.

rescaled $c(L, p_x^u)$ obtained by exact enumeration versus, the rescaled L , for several values of $L = 10\text{--}200$ and $p_x^u = 0.5\text{--}1.0$. The data collapse onto one scaling curve, which approaches a constant as $x \rightarrow 0$ and is linear for large x , precisely as expected from Eq. (63). Thus the scaling ansatz provides an excellent description of the general antisymmetric model.

5. CONCLUSIONS

We have studied the first passage time distribution H_+^n of a two-layer system of width L , and determined its asymptotic form to be a simple exponential decay in time. For the special case of an antisymmetric model, the decay constant is calculated using several techniques, and is found to cross over from the expected L^{-2} behavior in the pure-diffusion regime to an L^{-1} behavior at high velocities.

The origin of the L^{-1} behavior in the convective regime is not intuitively obvious to us. It arises as the result of two contributions—one $L^{-1/2}$ factor from the $\ln s_o$ term, and another $L^{-1/2}$ factor from the $1/s_1$ term. As discussed in Section 3, s_o is roughly an eventual absorption probability of a one-dimensional random walk, and s_1 is the mean distance traveled before the absorption. This differs from a naive expectation that the L^{-1} behavior results from the mean distance s_1 behaving as L in the convective regime.

Evidently, we have only considered the more tractable special cases in a two-layer system. It would be desirable to go beyond the antisymmetric limit of zero average velocity. In terms of the $p_x^u\text{--}p_x^d$ plane, the antisymmetric model corresponds to the line $p_x^u = 1 - p_x^d$, and the (elementary) one-block case to the line $p_x^u = p_x^d$. Due to the symmetries, the remaining region is bounded by the two cases with $1/2 \leq p_x^u \leq 1$. Of course, one would like to consider convection in two directions as well multiple layers, but these rather more difficult problems must await further work.

APPENDIX A. ITERATIVE METHOD FOR SHORT-TIME BEHAVIOR

We discuss an iterative scheme to obtain an approximate solution of the self-consistency equations (14)–(15), based on interpreting them as a recursion relation. We input a trial solution of $P(x, 0, z)$ and $P(x, 1, z)$ to the equations and obtain a (hopefully) improved approximation. In principle, we repeat this procedure until it converges to the correct solution.

We start from a trial solution

$$\begin{aligned} P^{(0)}(x, 0, z) &= 0 \\ P^{(0)}(x, 1, z) &= 0 \end{aligned} \tag{A1}$$

where the superscript indicates the number of iterations. For simplicity, we set $x_o = 0$ and $y_o = 1$. As shown in Eq. (13), the hitting probability H_+ is related to G_+ via $H_+(z) = zG_+(L - 1, 1, z)$. Also, using Eq. (11), we can write $G_+(L - 1, 1, z)$ as

$$\begin{aligned} G_+(L - 1, 1, z) &= \frac{1}{2} \sum_{x' = -L+1}^{L-1} z^{L-x'} (P(x' + 1, 0, z) - P(x' - 1, 1, z)) \\ &\quad + z^{L-1} \end{aligned} \tag{A2}$$

Combining these relations, we obtain

$$H_+^{(0)}(z) = z^L \tag{A3}$$

This rather trivial result is due to the fact that the presence of the second block is ignored in the zeroth-order approximation.

The next-order values of $P(x, 0, z)$ and $P(x, 1, z)$ can be calculated by inserting the trial values into Eqs. (14)–(15) to obtain

$$\begin{aligned} P^{(1)}(x, 0, z) &= 0 \\ P^{(1)}(x, 1, z) &= \left(\frac{z}{2}\right)^x \binom{x}{x/2} \end{aligned} \tag{A4}$$

where we define $\binom{x}{y} \equiv 0$, if x or y is not a nonnegative integer, or if $x < y$. Similarly, we obtain

$$H_+^{(1)}(z) = z^L - \frac{1}{2} z^L \sum_{x'=0}^{L-2} \left(\frac{1}{2}\right)^{x'} \binom{x'}{x'/2} \tag{A5}$$

Using Stirling’s formula, and replacing the sum by an integral, we find

$$H_+^{(1)}(z) \simeq z^L \left[1 - \left(\frac{2}{\pi}\right)^{1/2} L^{1/2} \right] \tag{A6}$$

The above result is unphysical, since H_+ becomes negative for large L . The deficiency is due to the fact that we only include the flux *out* of the upper block and not the flux *into* the block, while both fluxes are of the same order of magnitude. This problem will be resolved in the calculation at next order. The second-order iterations of $P(x, 0, z)$ and $P(x, 1, z)$ are

$$\begin{aligned}
 P^{(2)}(x, 0, z) &= \frac{z}{2} \sum_{x'=\max(x, 1)}^{L-1} \left(\frac{z}{2}\right)^{x'-x} \binom{x'-x}{(x'-x)/2} \left(\frac{z}{2}\right)^{x'-1} \binom{x'-1}{(x'-1)/2} \\
 P^{(2)}(x, 1, z) &= \left(\frac{z}{2}\right)^x \binom{x}{x/2} \\
 &\quad - \frac{z}{2} \sum_{x'=1}^x \left(\frac{z}{2}\right)^{x-x'} \binom{x-x'}{(x-x'+1)/2} \left(\frac{z}{2}\right)^{x'-x} \binom{x'-1}{(x'-1)/2} \quad (A7)
 \end{aligned}$$

Again using Stirling’s formula and replacing the sum by an integral, we obtain

$$\begin{aligned}
 P^{(2)}(x, 0, z) &= \frac{1}{\pi} \int_{\max(x, 1)}^{L-1} dx' z^{2x'-x} \frac{1}{[(x'-x)(x'-1)]^{1/2}} \\
 P^{(2)}(x, 1, z) &= z^x \left(\frac{2}{\pi x}\right)^{1/2} - \frac{z^x}{\pi} \int_1^x dx' \frac{1}{[(x-x')(x'-1)]^{1/2}} \quad (A8)
 \end{aligned}$$

and $H_+^{(2)}$ becomes

$$\begin{aligned}
 H_+^{(2)}(z) &= z^L \\
 &\quad - \frac{z^L}{(2\pi)^{1/2}} \int_1^{L-1} dx \frac{1}{(x-1)^{1/2}} \\
 &\quad + \frac{z^L}{2\pi} \int_2^{L-1} dx \int_1^{x-1} dx' \frac{1}{[(x-1-x')(x'-1)]^{1/2}} \\
 &\quad + \frac{z^L}{2\pi} \int_{-L+1}^0 dx \int_1^{L-1} dx' z^{2x'-2x} \frac{1}{[(x'-x-1)(x-1)]^{1/2}} \\
 &\quad + \frac{z^L}{2\pi} \int_1^{L-1} dx \int_{x+1}^{L-1} dx' z^{2x'-2x} \frac{1}{[(x'-x-1)(x-1)]^{1/2}} \quad (A9)
 \end{aligned}$$

Although the integrals in the equation cannot be evaluated in closed form, we can understand their structure. The first term is the contribution of tracer which did not cross the boundary. The second and the third terms are amount of flux going out of the first block. Thus, these three terms are proportional to z^L . The fourth and fifth terms are contributions from walkers which return to the upper block. Since the time to reach the boundary ($x = L$) depends on the where the walker exits (x') and reenters (x) the upper block, these terms contain different orders of z .

APPENDIX B. THE SINGLE-LAYER SYSTEM

To provide some feeling for the more difficult case of a nonzero average velocity, we calculate the first passage time distribution for a single layer. Consider tracer moving between adsorbing boundaries at $x = \pm L$ in the presence of a constant velocity field $v\hat{x}$. The motion in the y -direction is simple diffusion, completely decoupled from that along x , and the problem effectively is one-dimensional. We have

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \quad \text{with } c(\pm L, t) = 0 \tag{B1}$$

with the simple initial condition $c(x, 0) = \delta(x)$. Taking the Laplace transform via $\int_0^\infty dt e^{-st}$, we have

$$sc - \delta(x) + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \tag{B2}$$

which is readily solved for $x \neq 0$ as

$$c^\pm(x, s) = A^\pm e^{px/L} \sinh \left[(p^2 + \sigma)^{1/2} \left(1 \mp \frac{x}{L} \right) \right] \tag{B3}$$

Here the superscripts refer to $x > 0$ and $x < 0$, respectively, and we have defined $p = vL/2D$ and $\sigma = sL^2/D$. The coefficients A^\pm are determined by the conditions $c^+ = c^-$ and $\partial c^+/\partial x - \partial c^-/\partial x = -1/D$ at $x = 0$, which follow from the differential equation, so that

$$A^+ = A^- = \frac{L}{2D(p^2 + \sigma)^{1/2} \cosh[(p^2 + \sigma)^{1/2}]} \tag{B4}$$

The Laplace transform of the flux leaving the system at $x = \pm L$, which is identical to the first passage time probability distribution, is

$$J^\pm(s) = -D \frac{\partial c(\pm L, s)}{\partial x} = \frac{e^{\pm p}}{2 \cosh[(p^2 + \sigma)^{1/2}]} \tag{B5}$$

The long-time asymptotic behavior of J^\pm is controlled by the rightmost singularities of the Laplace transform in the complex- s plane, in this case the poles where $(p^2 + \sigma)^{1/2} = \pm i\pi/2$ or $s = s^* = -\pi^2 D/4L^2 - v^2/4D$. Thus, for $t \sim \infty$, $J^\pm(t) \sim \exp(s^*t)$. In the pure-diffusion limit, we set $v = 0$ and recall that $D = 1/2$ and identify t with step number n , so that $H_n^+ = J^+(n) \sim \exp(-\pi^2 n/8L^2)$. In the opposite limit of large velocity, we see that $J^+(t) \sim \exp(-v^2 t/4D)$, which coincides with the long-time behavior at a fixed spatial point of the usual Gaussian solution of the CDE.

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