

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/269636112>

Advection–Diffusion Equation with Absorbing Boundary

Article in *Journal of Statistical Physics* · December 2014

DOI: 10.1007/s10955-015-1257-2 · Source: arXiv

CITATIONS

8

READS

522

2 authors:



John Grant

The Open University (UK)

3 PUBLICATIONS 10 CITATIONS

[SEE PROFILE](#)



Michael Wilkinson

The Open University (UK)

149 PUBLICATIONS 3,501 CITATIONS

[SEE PROFILE](#)

Some of the authors of this publication are also working on these related projects:



Particles and waves in turbulence [View project](#)

John Grant and Michael Wilkinson

Advection diffusion equation with absorbing boundary

Received: date / Accepted: date

Abstract We consider a spatially homogeneous advection-diffusion equation in which the diffusion tensor and drift velocity are time-independent, but otherwise general. We derive asymptotic expressions, valid at large distances from a steady point source, for the flux onto a completely permeable boundary and onto an absorbing boundary. The absorbing case is treated by making a source of antiparticles at the boundary. In both cases there is an exponential decay as the distance from the source increases; we find that the exponent is the same for both boundary conditions.

Keywords Diffusion, advection, absorption

PACS 05.10.Gg, 05.40.-a, 05.45.Df

1 Introduction

In this paper we discuss the solution of the advection-diffusion equation with a point source of intensity $\sigma(t)$ located at \mathbf{x}_0 . In d spatial dimensions the particle density $\rho(\mathbf{x}, \mathbf{x}_0, t)$ at position \mathbf{x} at time t satisfies

$$\frac{\partial \rho}{\partial t} = - \sum_{i=1}^d v_i \frac{\partial \rho}{\partial x_i} + \sum_{i=1}^d \sum_{j=1}^d D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j} + \sigma(t) \delta(\mathbf{x} - \mathbf{x}_0) \quad (1)$$

where the v_i are components of the drift velocity \mathbf{v} , the D_{ij} are elements of the diffusion tensor \mathbf{D} and both \mathbf{v} and \mathbf{D} are independent of position and time.

Our objective is, for $d = 2$, to determine the particle flux, $J_a(x_2)$, from a steady source onto the boundary $x_1 = 0$ in the case where particles are absorbed on contact with the boundary at $\mathbf{x} = (0, x_2)$. Dealing with an absorbing boundary is difficult when there is both advection and diffusion because there is no simple local boundary condition which $\rho(\mathbf{x}, \mathbf{x}_0, t)$ must satisfy. For this reason we also consider a reference problem where the boundary is completely permeable and has no effect on particles, the flux in this case is denoted by $J_0(x_2)$.

The primary motivation for analysing this problem arose from studies of the structure of fractal measures generated by random dynamical systems which can serve as models for particles in turbulent flows [1, 2, 3]. A fractal measure can be characterised by the statistics of constellations of nearby points sampling the measure. The simplest case is where a constellation consisting of just two points is characterised by the distance δr between two trajectories. Defining $x_1 = -\ln(\delta r/\xi)$, where ξ is a correlation length of the flow, it is found that x_1 obeys an advection-diffusion equation when $x_1 \gg 0$

Department of Mathematics and Statistics,
 The Open University, Walton Hall,
 Milton Keynes, MK7 6AA,
 England.
 E-mail: m.wilkinson@open.ac.uk

[4,5]. The point $x_1 = 0$ is both the location of an absorbing boundary and a source for trajectories entering the region $x_1 > 0$. In the region $x_1 \gg 1$ the probability density of x_1 is an exponential function, which corresponds to a power-law distribution of δr . The exponent of this power-law determines the correlation dimension of the fractal [4,5]. If we consider a constellation formed by three trajectories, we can consider the shape statistics of triangles formed by triplets of points lying inside a small ball, of radius ϵ [6]. The shape of a triangle may be characterised by the parameter $z = \mathcal{A}/\mathcal{R}^2$, where \mathcal{A} is its area and \mathcal{R} its radius of gyration. For a fractal measure generated by a random flow we showed that the variables $x_1 = -\ln(\delta r/\xi)$ and $x_2 = -\ln z$ evolve according to an advection-diffusion process in the region $x_1 \gg 1$ and $x_2 \gg 1$, with an absorbing boundary on the line $x_1 = 0$, and we are led to consider the problem illustrated in figure 1. This approach, described in [6], can be extended to show that other variables characterising shapes of constellations of nearby points can be described by a suitable advection-diffusion equation.

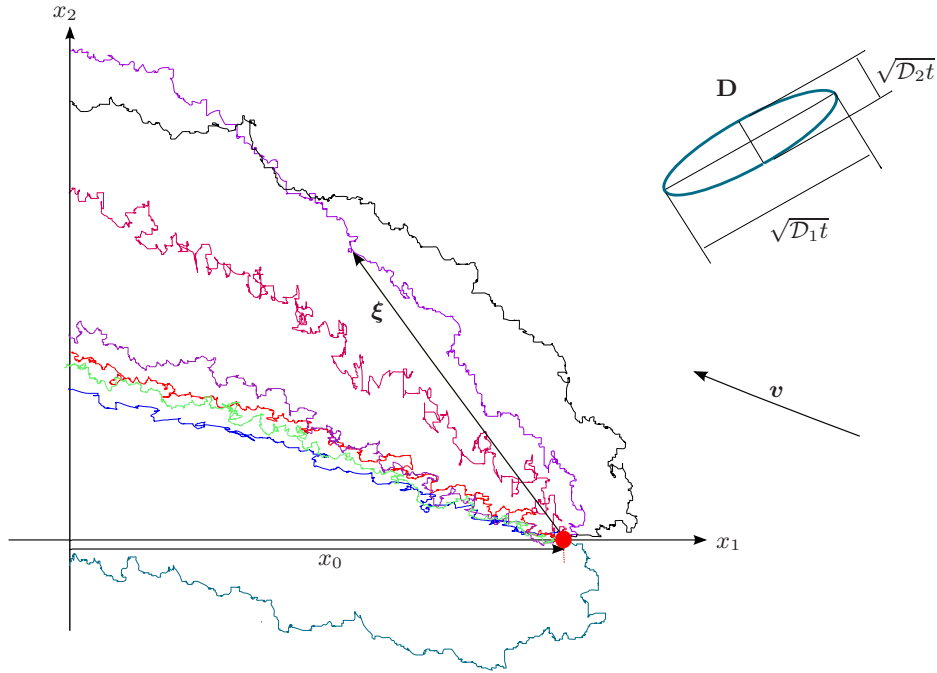


Fig. 1 (Colour online). Particles created by a steady unit source at $(x_0, 0)$ undergo advection with velocity \mathbf{v} and diffusion with diffusion tensor \mathbf{D} . The displacement of a particle from the source is denoted by $\boldsymbol{\xi}$. The eigenvalues of \mathbf{D} are \mathcal{D}_1 and \mathcal{D}_2 and the principal axes of diffusion are the major and minor axes of the ellipse $\mathbf{x}^T \cdot \mathbf{D} \mathbf{x} = 1$. In the absence of advection, after a time t a ‘droplet’ comprising many particles initially concentrated at a point would occupy an ellipse with the orientation and dimensions shown in the figure. We wish to determine the flux density onto the absorbing boundary $x_1 = 0$ at $(0, x_2)$, for large x_2 .

A second reason for studying this absorption problem is its relevance to the modelling of fallout plumes from events such as volcanic eruptions. The study of dispersion of dust and smoke in the atmosphere has a long history (see [7,8]). Ermak [9] appears to have been the first author to treat settling and deposition (that is drift and absorption) as well as diffusive dispersion. Stockie [10] gives a recent review of this area. Our calculation would be relevant to fallout when the diffusive dispersion is anisotropic.

We investigate the flux onto the boundary $x_1 = 0$ at position $(0, x_2)$, from a steady point source at $(x_0, 0)$. At large distance from the source the flux onto an absorbing boundary has magnitude

$$J_a(x_2) \sim A_a(x_2) \exp[-\Phi_0(x_2)] \quad (2)$$

where $\Phi_0(x_2)$ and $A_a(x_2)$ both depend upon the source position x_0 . We find that $\Phi_0(x_2)/x_2$ approaches finite limits as $x_2 \rightarrow \pm\infty$ and that $A_a(x_2)$ is asymptotic to a power law as $x_2 \rightarrow \pm\infty$. For a transparent boundary the flux is of the same form, with $A_a(x_2)$ replaced by another function $A_0(x_2)$ which decays

more slowly as $|x_2| \rightarrow \infty$. Somewhat surprisingly, the exponent $\Phi_0(x_2)$ is the same for the transparent and absorbing boundary cases.

This paper is organised as follows. In section 2, we determine the density and flux for a permeable boundary, for general \mathbf{v} and \mathbf{D} . The resulting expressions appear to be singular whenever \mathbf{D} is a singular matrix, but in section 2.3 we show that they give finite values even when \mathbf{D} is a rank-one matrix. We consider the effect of an absorbing boundary in section 3, showing how an implicit expression for the flux can be written in terms of a source of ‘antiparticles’ which are created on the boundary. The one-dimensional case is solved explicitly, and we show that the method is in accord with results from the theory of first-passage time processes, discussed in [11,12]. In section 4 the results from sections 2 and 3 are combined to obtain the flux, in two dimensions, from a steady source at $\mathbf{x}_0 = (x_0, 0)$ onto an absorbing boundary along the x_2 axis. A surprising cancellation ensures that the exponent $\Phi_0(x_2)$ is the same as that for the completely permeable boundary treated in section 2. We conclude in section 5 with some numerical illustrations of the quality of the approximations and some comments on the structure of our asymptotic results.

2 Particle density and flux for a permeable boundary

In this section we consider the problem of calculating the steady state particle density and the corresponding flux arising from a steady point source. We then apply the results in two dimensions to calculate the density and flux along a line, the x_2 axis. The line has no effect on the particles: it is a completely permeable or ‘transparent’ boundary and the particles may cross it multiple times and at different locations.

2.1 Particle flux for a non-singular diffusion tensor

In d dimensions the free space propagator or Green’s function for (1) (that is, the probability density for a particle released at \mathbf{x}_0 at time zero to reach \mathbf{x} at time t) is

$$G_0(\mathbf{x}, \mathbf{x}_0, t) = \left[\frac{\exp[-S(\boldsymbol{\xi}, t)]}{\sqrt{\det(\mathbf{D}) (4\pi t)^d}} \right] \Theta(t) \quad (3)$$

where $\Theta(t)$ is the Heaviside step function, $\boldsymbol{\xi}$ is the displacement vector $\mathbf{x} - \mathbf{x}_0$ and

$$S(\boldsymbol{\xi}, t) = \frac{(\boldsymbol{\xi} - \mathbf{v}t) \cdot \mathbf{D}^{-1}(\boldsymbol{\xi} - \mathbf{v}t)}{4t} . \quad (4)$$

The particle density at point \mathbf{x} at time t is therefore

$$\rho_0(\mathbf{x}, \mathbf{x}_0, t) = \int_{-\infty}^t dt' \sigma(t') G_0(\mathbf{x}, \mathbf{x}_0, t - t') . \quad (5)$$

The flux vector $\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0, t)$ is

$$\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0, t) = \rho_0(\mathbf{x}, \mathbf{x}_0, t) \mathbf{v} - \mathbf{D} \nabla \rho_0(\mathbf{x}, \mathbf{x}_0, t) \quad (6)$$

where the gradient is with respect to \mathbf{x} . Now consider the steady-state density $\rho_0(\mathbf{x}, \mathbf{x}_0)$ and flux $\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0)$ due to a steady source $\sigma(t) = \sigma_0$. Using (5) and employing (3), (4) to evaluate the gradient,

$$\mathbf{D} \nabla \rho_0(\mathbf{x}, \mathbf{x}_0, t) = \sigma_0 \int_{-\infty}^0 dt' \mathbf{D} \nabla G_0(\mathbf{x}, \mathbf{x}_0, t - t') = -\sigma_0 \int_{-\infty}^0 dt' G_0(\mathbf{x}, \mathbf{x}_0, t - t') \frac{1}{2(t - t')} (\boldsymbol{\xi} - \mathbf{v}(t - t')) \quad (7)$$

giving

$$\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0) = \sigma_0 \int_{-\infty}^0 dt G_0(\mathbf{x}, \mathbf{x}_0, t) \mathbf{v}_{\text{eff}}(\mathbf{x}, \mathbf{x}_0, t) \quad (8)$$

where the effective velocity is

$$\mathbf{v}_{\text{eff}}(\mathbf{x}, \mathbf{x}_0, t) \equiv \frac{1}{2} \left(\frac{\mathbf{x} - \mathbf{x}_0}{t} + \mathbf{v} \right) . \quad (9)$$

2.2 Asymptotic values of particle density and flux

It is not possible to express the integrals in equations (5) and (8) exactly in a closed form. However, for large $|\boldsymbol{\xi}| = |\mathbf{x} - \mathbf{x}_0|$, these integrals are dominated by contributions from a neighbourhood of the critical point t^* at which $S(\boldsymbol{\xi}, t)$ has a minimum. The method of Laplace can be applied to estimate these integrals (we comment later on the identity of the large parameter of the theory). The Laplace method gives the following estimates for the steady-state density and flux with a permeable boundary

$$\begin{aligned}\rho_0(\mathbf{x}, \mathbf{x}_0) &\sim \gamma \sigma_0 G_0(\mathbf{x}, \mathbf{x}_0, t^*) \\ \mathbf{J}_0(\mathbf{x}, \mathbf{x}_0) &\sim \rho_0(\mathbf{x}, \mathbf{x}_0) \mathbf{v}_{\text{eff}}(\mathbf{x}, \mathbf{x}_0, t^*) .\end{aligned}\quad (10)$$

where γ is the Gaussian integral

$$\gamma = \int_{-\infty}^{\infty} du \exp \left[-\frac{1}{2} \frac{\partial^2 S(\boldsymbol{\xi}, t^*)}{\partial t^2} u^2 \right] . \quad (11)$$

The condition that S be stationary with respect to t is

$$\frac{\partial S}{\partial t}(\boldsymbol{\xi}, t^*) = \frac{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v} (t^*)^2 - \boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}}{4(t^*)^2} = 0 \quad (12)$$

giving

$$t^* = \sqrt{\frac{\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}}{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v}}} . \quad (13)$$

Since \mathbf{D} is symmetric

$$S(\boldsymbol{\xi}, t^*) = \frac{1}{2} \left(\sqrt{\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}} \sqrt{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v}} - \boldsymbol{\xi} \cdot \mathbf{D}^{-1} \mathbf{v} \right) \quad (14)$$

Also, the second derivative and the Gaussian integral (11) are

$$\frac{\partial^2 S}{\partial t^2}(\boldsymbol{\xi}, t^*) = \frac{1}{2} \mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v} \sqrt{\frac{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v}}{\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}}} , \quad \gamma = \frac{2\sqrt{\pi} (\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi})^{\frac{1}{4}}}{(\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v})^{\frac{3}{4}}} . \quad (15)$$

Substituting these results into (10) gives

$$\rho_0(\mathbf{x}, \mathbf{x}_0) \sim \sigma_0 A_0(\mathbf{x}, \mathbf{x}_0) \exp[-\Phi_0(\mathbf{x}, \mathbf{x}_0)] \quad (16)$$

where

$$\Phi_0(\mathbf{x}, \mathbf{x}_0) = S(\boldsymbol{\xi}, t^*) , \quad A_0(\mathbf{x}, \mathbf{x}_0) = \frac{(\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi})^{\left(\frac{1-d}{4}\right)} (\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v})^{\left(\frac{d-3}{4}\right)}}{\sqrt{\det(\mathbf{D})} (4\pi)^{(d-1)}} . \quad (17)$$

From equation (10) when $|\boldsymbol{\xi}|$ is large the asymptotic value of the steady state flux can be written as

$$\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0) \sim \frac{\sigma_0}{2} A_0(\mathbf{x}, \mathbf{x}_0) \left[\mathbf{v} + \left(\sqrt{\frac{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v}}{\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}}} \right) \boldsymbol{\xi} \right] \exp[-\Phi_0(\mathbf{x}, \mathbf{x}_0)] . \quad (18)$$

On the streamline *directly* downwind of the source the displacement vector $\boldsymbol{\xi} = \mathbf{x} - \mathbf{x}_0 = \lambda \mathbf{v}$ for some $\lambda > 0$ so that $\Phi_0(\mathbf{x}, \mathbf{x}_0) = 0$, $P_0(\mathbf{x}, \mathbf{x}_0) \sim \sigma_0 A_0(\mathbf{x}, \mathbf{x}_0)$ and $\mathbf{J}_0(\mathbf{x}, \mathbf{x}_0) \sim \sigma_0 A_0(\mathbf{x}, \mathbf{x}_0) \mathbf{v}$. Therefore, directly downwind of the source point, there is no exponential reduction of the steady state particle density or the particle flux and the flux is directed along the drift vector. However, there is an algebraic reduction in both as the distance $|\boldsymbol{\xi}|$ from the source increases. On any other ray starting from \mathbf{x}_0 then as $|\boldsymbol{\xi}|$ increases Φ_0 increases and the particle density and flux undergo the same exponential reduction along the ray. The algebraic coefficients in the particle density and the flux are asymptotic to the same power law: $|\boldsymbol{\xi}|^{\frac{1-d}{2}}$.

The Laplace method provides an estimate of integrals of the form

$$I(\lambda) = \int_a^b d\tau f(\tau) \exp[-\lambda S(\tau)] \quad (19)$$

in the limit as $\lambda \rightarrow \infty$, which assumes that $S(\tau)$ has a minimum in the interval $[a, b]$ at τ^* . It is not immediately clear that (5) is in this form. To see the connection define $\tau = t/t^*$, where t^* was given by (13). Equation (5) can then be expressed in a form similar to (19), where the large parameter is

$$\lambda = \sqrt{\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi}} \sqrt{\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v}} . \quad (20)$$

In the two-dimensional case, which is our primary concern, the magnitude of the flux onto the boundary $x_1 = 0$ is the magnitude of first component of \mathbf{J}_0 . At position x_2 , this is

$$J_0(x_2) \equiv |[\mathbf{J}_0(x_2)]_1| = A_0(x_2) \exp[-\Phi_0(x_2)] \quad (21)$$

where $\Phi_0(x_2) \equiv \Phi_0((0, x_2), (x_0, 0))$, and where

$$A_0(x_2) \sim \frac{1}{\sqrt{|x_2|}} . \quad (22)$$

2.3 Rank-one diffusion tensor

The expressions for the density and flux which we have obtained contain \mathbf{D}^{-1} , the inverse of the diffusion tensor. We might therefore expect the analysis in the preceding sections to be valid only when \mathbf{D} is nonsingular. However we now show that the results continue to hold for the case where \mathbf{D} is a rank one matrix.

In general since \mathbf{D} is symmetric it may be diagonalised by a suitable rotation of the axes. Because we are, at this point, still considering a permeable boundary we can apply a rotation to diagonalise \mathbf{D} without loss of generality. We will therefore consider the case where \mathbf{D} is of the form

$$\mathbf{D} = \begin{bmatrix} D_{11} & 0 \\ 0 & \epsilon \end{bmatrix} \quad (23)$$

and take the limit as $\epsilon \rightarrow 0$. This limiting case corresponds to diffusive motion with drift in the x_1 direction, with a diffusion constant D_{11} and drift velocity v_1 , together with drift with velocity v_2 , and almost no diffusion, in the x_2 direction.

With \mathbf{D} given by (23) and ϵ small but non-zero, then using equation (16) to calculate the particle density far from the source we find that the terms in ϵ^{-1} cancel. Neglecting terms of order ϵ^2 we find that the result is independent of ϵ . At $(0, x_2)$ the density is

$$\rho_0(x_2) \sim \frac{\sigma_0}{2\sqrt{\pi D_{11} x_2 v_2}} \exp \left[-\frac{x_2 v_1^2}{4 D_{11} v_2} \right] . \quad (24)$$

We now show that this is in fact equal to the probability density for the case where $\epsilon = 0$. If $\epsilon = 0$ the displacement from x_0 in the x_1 direction is due to one-dimensional diffusion with drift, with diffusion coefficient D_{11} and drift velocity v_1 . The propagator for the x_1 component of the motion is therefore

$$G_0(x_1, x_0, t) = \frac{1}{\sqrt{4\pi D_{11} t}} \exp \left[-\frac{(x_1 - x_0 - v_1 t)^2}{4 D_{11} t} \right] \Theta(t) . \quad (25)$$

Further, when $\epsilon = 0$ there is no diffusion in the x_2 direction and, at time t , the x_2 coordinate of the particle is given by $x_2 = v_2 t$. The propagator for the two dimensional motion when $\epsilon = 0$ is therefore

$$G((x_1, x_2), (x_0, 0), t) = G_0(x_1, x_0, t) \delta(x_2 - v_2 t) . \quad (26)$$

From (5), for a source of intensity $\sigma(t) = \sigma_0 \Theta(t)$ the particle density at $\mathbf{x} = (x_1, x_2)$ from a steady source at \mathbf{x}_0 is

$$\begin{aligned} \rho_0(\mathbf{x}, \mathbf{x}_0) &= \frac{\sigma_0}{\sqrt{4\pi D_{11}}} \int_0^\infty \frac{dt'}{\sqrt{t'}} \exp \left[-\frac{(x_1 - x_0 - v_1 t')^2}{4 D_{11} t'} \right] \delta(x_2 - v_2 t') \\ &= \frac{\sigma_0}{\sqrt{4\pi D_{11} x_2 v_2}} \exp \left[-\frac{v_2 (x_1 - x_0 - v_1 x_2 / v_2)^2}{4 D_{11} x_2} \right] \end{aligned} \quad (27)$$

and on the boundary far from the source, since $x_1 = 0$ and $x_2 \gg x_0$, this reduces to (24).

3 Antiparticle method for an absorbing boundary

3.1 Integral equation for the absorption flux

It is straightforward to perform a Monte Carlo simulation of the advection diffusion process with an absorbing boundary: the particles are simply removed from the simulation whenever they cross the boundary. In contrast when solving a Fokker-Planck equation, such as equation (1) for a particle density, it is not possible to write down a local boundary condition which implies that particles colliding with a boundary are absorbed. However, we can add an additional source term to the Fokker-Planck equation and, in principle, this allows us to describe an absorbing boundary by adding a suitable source of ‘antiparticles’ at the boundary. After emission at the boundary the antiparticles propagate in the same way as particles do but, to model absorption, the antiparticle density is subtracted from the particle density. Since this approach does not rely on any geometrical symmetries of the system it is more general than approaches which use the method of images.

In the two-dimensional case suppose that position on the boundary Σ can be parameterised by the arc length s and let $j(\mathbf{x}', t')$ be the rate of antiparticle creation *per unit length* at point \mathbf{x}' and time t' . Then the element, ds of the boundary at point \mathbf{x}' is a source of antiparticles with intensity $j(\mathbf{x}', t')ds$ and the antiparticles created at the boundary contribute an amount

$$- \int_{\Sigma} ds \int_{-\infty}^t dt' j(\mathbf{x}', t') G_0(\mathbf{x}, \mathbf{x}', t - t') \quad (28)$$

to the overall density at point \mathbf{x} at time t .

Each antiparticle is created in response to the *first arrival* of a particle at the boundary. The intensity of the antiparticle source is therefore

$$j(\mathbf{x}', t') = \mathbf{n}(\mathbf{x}') \cdot \mathbf{J}_a(\mathbf{x}', \mathbf{x}_0, t') \quad (29)$$

where $\mathbf{J}_a(\mathbf{x}', \mathbf{x}_0, t')$ is the absorption flux at \mathbf{x}' and t' due to a particle source at \mathbf{x}_0 and $\mathbf{n}(\mathbf{x})$ is the unit normal on the boundary at \mathbf{x}' , pointing out of the region of diffusion-advection. The particle density in the presence of an absorbing boundary $\rho_a(\mathbf{x}, \mathbf{x}_0, t)$ is therefore

$$\rho_a(\mathbf{x}, \mathbf{x}_0, t) = \rho_0(\mathbf{x}, \mathbf{x}_0, t) - \int_{\Sigma} ds \int_{-\infty}^t dt' \mathbf{n}(\mathbf{x}') \cdot \mathbf{J}_a(\mathbf{x}', \mathbf{x}_0, t') G_0(\mathbf{x}, \mathbf{x}', t - t') . \quad (30)$$

3.2 Exact absorption flux in one dimension

We illustrate the solution of the integral equation (30) in one dimension and derive an exact expression for the flux density $\mathbf{J}_a(0, x_0, t)$ of particles absorbed at the origin, $x = 0$, arising from a source of strength $\sigma(t) = \delta(t)$ localised at x_0 , with $x_0 > 0$.

If D is the diffusion coefficient and $\mathbf{v} = -v\mathbf{i}$ is the drift velocity (so that the particles drift towards the left) then for $t > 0$ the free propagator, representing propagation without absorption, is

$$G_0(x, x_0, t) = \frac{1}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x - x_0 + vt)^2}{4Dt} \right] \Theta(t) \quad (31)$$

and the corresponding free flux density is $\mathbf{J}_0(x, x_0, t) \equiv -J_0(x, x_0, t)\mathbf{i}$ where the flux *onto* the boundary (i.e. to the left) is

$$\begin{aligned} J_0(x, x_0, t) &= vG_0(x, x_0, t) + D \frac{\partial G_0}{\partial x}(x, x_0, t) \\ &= \frac{1}{\sqrt{4\pi Dt}} \left(\frac{x_0 - x + vt}{2t} \right) \exp \left[-\frac{(x - x_0 + vt)^2}{4Dt} \right] . \end{aligned} \quad (32)$$

The one-dimensional form of (30), giving the particle density at point x at time t for a system with an absorbing boundary at $x = 0$, is

$$\rho_a(x, x_0, t) = \rho_0(x, x_0, t) - \int_0^t dt' J_a(0, x_0, t') G_0(x, 0, t - t') . \quad (33)$$

The corresponding flux is

$$J_a(x, x_0, t) = v\rho_a(x, x_0, t) + D \frac{\partial \rho_a}{\partial x}(x, x_0, t) \quad (34)$$

and using (33) in (34) gives

$$J_a(x, x_0, t) = J_0(x, x_0, t) - \int_0^t dt' J_a(0, x_0, t') J_0(x, 0, t - t') . \quad (35)$$

This equation expresses the absorption flux at time t from an ejection of particles at $t = 0$ as the sum of a direct flux from the source and a term resulting from the creation of ‘antiparticles’ due to the flux which reached the boundary at the earlier time t' . Since $J_0(x, x_0, t)$ is known (from (32)), equation (35) is a linear Volterra integral equation of the second kind for $J_a(x, x_0, t)$, with kernel $J_0(x, 0, t)$. It may be solved for J_a using the method of Laplace transforms. Noting that the integral in the equation is a convolution, the Laplace transform of (35), in the time variable, is

$$\bar{J}_a(x, x_0, s) = \bar{J}_0(x, x_0, s) - \bar{J}_a(0, x_0, s) \bar{J}_0(x, 0, s) \quad (36)$$

where \bar{J}_a and \bar{J}_0 are the Laplace transforms of J_a and J_0 , respectively.

Since $x = 0$ is an absorbing boundary we must have $J_a(x, x_0, t) = 0$ for $x < 0$, therefore, to determine $J_a(0, x_0, t)$, we consider

$$\bar{J}_a(\epsilon, x_0, s) = \bar{J}_0(\epsilon, x_0, s) - \bar{J}_a(0, x_0, s) \bar{J}_0(\epsilon, 0, s) \quad (37)$$

in the limit as $\epsilon \rightarrow 0^+$. The Laplace transform of $J_0(x, x_0, t)$ is

$$\bar{J}_0(x, x_0, s) = \left(\frac{1 \mp \alpha}{2\alpha} \right) \exp \left[- \left(\frac{\xi v}{2D} \right) (1 \pm \alpha) \right] \quad (38)$$

according as $\xi = x - x_0$ is \pm ve and where

$$\alpha \equiv \sqrt{1 + \frac{4Ds}{v^2}} . \quad (39)$$

So equation (37) becomes

$$\bar{J}_a(\epsilon, x_0, s) + \bar{J}_a(0, x_0, s) \left(\frac{1 - \alpha}{2\alpha} \right) \exp \left[- \frac{\epsilon v}{2D} (1 + \alpha) \right] = \left(\frac{1 + \alpha}{2\alpha} \right) \exp \left[- \frac{(\epsilon - x_0)v}{2D} (1 - \alpha) \right] \quad (40)$$

and in the limit as $\epsilon \rightarrow 0^+$ this gives

$$\bar{J}_a(0, x_0, s) = \exp \left[- \frac{x_0 v}{2D} (\alpha - 1) \right] = \exp \left[- \frac{x_0 v}{2D} \left(\sqrt{1 + \frac{4Ds}{v^2}} - 1 \right) \right] . \quad (41)$$

Alternatively, we can consider the limit as $\epsilon \rightarrow 0^-$: in this case there is no absorption flux at $x = 0^-$ because particles reaching $x = 0$ have been absorbed, and (37) is replaced by

$$0 = \bar{J}_0(\epsilon, x_0, s) - \bar{J}_a(0, x_0, s) \bar{J}_0(\epsilon, 0, s) . \quad (42)$$

It is readily verified that using (42) instead of (37) leads to the same result.

Inverting the Laplace transform gives the exact expression for the rate of absorption onto the boundary:

$$J_a(0, x_0, t) = \frac{1}{\sqrt{4\pi D}} \frac{x_0}{t^{3/2}} \exp \left[- \frac{(x_0 - vt)^2}{4Dt} \right] . \quad (43)$$

Distributions of this form are in a class which are sometimes referred inverse Gaussian or Wald distributions.

4 Flux onto an absorbing boundary in two dimensions

4.1 The method of calculation

We now apply the results derived in sections (2.3) and (3.2) to the case of absorption on a line in two dimensions. Absorption at the point $(0, x_2)$ requires that the particle *first* arrives at the boundary $x_1 = 0$ at ordinate x_2 . We will consider the problem in terms of the first arrival time at the boundary and the distribution of the absorption ordinate conditional on that arrival time.

In the following we introduce several probability density functions. We shall adopt the convention that the probability density function (PDF) of a random variable x is denoted by a function P_x , so that the probability that x lies in the interval $[x, x + dx]$ is $P_x(x) dx$. The first arrival time is determined by the x_1 component of the motion alone. This is a one-dimensional advection-diffusion process, with diffusion constant D_{11} , drift velocity $v_1 = -v$ and starting from initial point x_0 . The PDF for the first arrival time is the flux obtained above. In this context equation (43) becomes

$$P_t(t) = \frac{x_0}{\sqrt{4\pi D_{11} t^3}} \exp \left[-\frac{(x_0 - v_1 t)^2}{4D_{11} t} \right]. \quad (44)$$

The absorption ordinate is a random variable, x_2 , whose PDF may be obtained from $P_{x_2|t}(x_2, t)$, the probability density for x_2 conditional upon the first arrival time t :

$$P_{x_2}(x_2) = \int_0^\infty dt P_{x_2|t}(x_2, t) P_t(t). \quad (45)$$

The conditional PDF in this expression can be obtained from the propagator $G_0(\mathbf{x}, \mathbf{x}_0, t)$, which is a joint probability density for x_1 and x_2 conditional upon t , by dividing by the appropriate marginal density of x_1 :

$$P_{x_2|t}(x_2, t) = \frac{G_0((0, x_2), (x_0, 0), t)}{\int_{-\infty}^\infty dx_2 G_0((0, x_2), (x_0, 0), t)}. \quad (46)$$

Using equation (3), since $t \geq 0$, we can write this as

$$P_{x_2|t}(x_2, t) = \frac{\exp[-S(\boldsymbol{\xi}, t)]}{I(x_0, t)} \quad (47)$$

where $\boldsymbol{\xi} = (-x_0, x_2)$ and

$$I(x_0, t) \equiv \int_{-\infty}^\infty dx_2 \exp[-S(\boldsymbol{\xi}, t)]. \quad (48)$$

Then equation (45) becomes

$$P_{x_2}(x_2) \sim \frac{x_0}{\sqrt{4\pi D_{11}}} \int_0^\infty \frac{dt}{t^{3/2}} \left[\frac{1}{I(\boldsymbol{\xi}_1, t)} \exp \left(-S(\boldsymbol{\xi}, t) - \frac{(x_0 - v_1 t)^2}{4D_{11} t} \right) \right]. \quad (49)$$

In the steady state the x_1 component of the particle flux onto the boundary has magnitude $J_a(x_2) = \sigma_0 P_{x_2}(x_2)$.

4.2 Estimates using the method of Laplace

For large $|\boldsymbol{\xi}|$ (i.e. for large $|x_2|$) both of the integrals in equation (49) can be approximated by the method of Laplace. This allows us to determine the asymptotic form of the PDF of the ordinate of the absorption point, $P_{x_2}(x_2)$ and, thereby, the magnitude of the absorption flux $J_a(x_2)$.

For any given values of ξ_1 and t the dominant contribution to $I(x_0, t)$ arises from a neighbourhood of the critical value ξ_2^* , at which $S(\boldsymbol{\xi}, t)$ has a minimum with respect to x_2 and

$$I(x_0, t) \sim \exp[-S((\xi_1, \xi_2^*), t)] \int_{-\infty}^\infty d\xi_2 \exp \left[-\frac{(\xi_2 - \xi_2^*)^2}{2} \frac{\partial^2 S}{\partial \xi_2^2}((\xi_1, \xi_2^*), t) \right]. \quad (50)$$

Writing $\boldsymbol{\xi}^* = (\xi_1, \xi_2^*)$, the critical value ξ_2^* satisfies

$$\frac{\partial S}{\partial \xi_2}(\boldsymbol{\xi}^*, t) = \frac{D_{11}\xi_2^* - D_{12}\xi_1 - (D_{11}v_2 - D_{12}v_1)t}{2 \det(\mathbf{D})t} = 0 \quad (51)$$

so that

$$\xi_2^* = \frac{D_{12}}{D_{11}}(\xi_1 - v_1t) + v_2t \quad (52)$$

and

$$\boldsymbol{\xi}^* - \mathbf{v}t = \left[(\xi_1 - v_1t), \frac{D_{12}}{D_{11}}(\xi_1 - v_1t) \right]^T \quad (53)$$

giving

$$S(\boldsymbol{\xi}^*, t) = \frac{(\xi_1 - v_1t)^2}{4D_{11}t} \quad (54)$$

and

$$\frac{\partial^2 S}{\partial \xi_2^2}(\boldsymbol{\xi}^*, t) = \frac{D_{11}}{2 \det(\mathbf{D})t} . \quad (55)$$

Substituting these results into equation (50) gives

$$I(x_0, t) \sim \exp \left[-\frac{(\xi_1 - v_1t)^2}{4D_{11}t} \right] \int_{-\infty}^{\infty} d\xi_2 \exp \left[-\frac{D_{11}(\xi_2 - \xi_2^*)^2}{4 \det(\mathbf{D})t} \right] \quad (56)$$

and evaluating the Gaussian integral we have

$$I(x_0, t) \sim \sqrt{\frac{4\pi \det(\mathbf{D})t}{D_{11}}} \exp \left[-\frac{(\xi_1 - v_1t)^2}{4D_{11}t} \right] . \quad (57)$$

Equation (49) now gives

$$P_{x_2}(x_2) \sim \frac{x_0}{4\pi\sqrt{\det(\mathbf{D})}} \int_0^\infty \frac{dt}{t^2} \left[\exp \left(-S(\boldsymbol{\xi}, t) - \frac{(x_0 - v_1t)^2}{4D_{11}t} + \frac{(\xi_1 - v_1t)^2}{4D_{11}t} \right) \right] . \quad (58)$$

Since $\xi_1 = -x_0$ on the boundary the last two terms in the exponent sum to a constant value giving

$$P_{x_2}(x_2) \sim \frac{x_0}{4\pi\sqrt{\det(\mathbf{D})}} \exp \left(\frac{x_0 v_1}{D_{11}} \right) \int_0^\infty \frac{dt}{t^2} \exp [-S(\boldsymbol{\xi}, t)] . \quad (59)$$

The remaining integral may be estimated as in section (2.2) giving

$$[\mathbf{J}_a(x_2)]_1 = \sigma_0 P_{x_2}(x_2) \sim \sigma_0 A_a(x_2) \exp [-\Phi_0(\mathbf{x}, \mathbf{x}_0)] \quad (60)$$

where Φ_0 is as given by equation (14) and

$$A_a(x_2) = \left[\frac{x_0 \exp(x_0 v_1 / D_{11})}{2\sqrt{\pi \det(\mathbf{D})}} \right] \frac{(\mathbf{v} \cdot \mathbf{D}^{-1} \mathbf{v})^{\frac{1}{4}}}{(\boldsymbol{\xi} \cdot \mathbf{D}^{-1} \boldsymbol{\xi})^{\frac{3}{4}}} . \quad (61)$$

On the x_2 axis far from the source $A_a(x_2) \sim |x_2|^{-3/2}$ so that A_a , and the flux onto an absorbing boundary, $J_a(x_2)$, decays more rapidly than the flux onto a permeable boundary, J_0 , as $|x_2|$ increases. However, surprisingly, the exponent Φ_0 in J_a is the same as that in J_0 .

5 Discussion of results

The above derivation depends upon using the Laplace method to estimate integrals, and it is instructive to assess the accuracy by comparison with Monte Carlo simulations. The particle paths can be generated using the Euler iterative scheme

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}\delta t + \sqrt{2\mathbf{D}\delta t}\boldsymbol{\eta}_n \quad (62)$$

with starting value \mathbf{x}_0 , where δt is a small time increment and each $\boldsymbol{\eta}_n$ is a d -dimensional vector of independent normally distributed random variables with zero mean and unit variance.

Figure 2 shows comparative plots of the magnitudes of the steady state absorption flux, $J_a(x_2)$, and the particle density $\rho_0(x_2)$ for a permeable boundary (the flux $J_0(x_2)$ onto a permeable boundary is obtained by multiplying $\rho_0(x_2)$ by an effective drift velocity: see equation (10)). The values of the source location \mathbf{x}_0 , drift velocity \mathbf{v} and diffusion tensor \mathbf{D} are given in each of the plots, which display the same data on linear and semi-logarithmic scales side-by-side. Both $J_a(x_2)$ and $\rho_0(x_2)$ are displayed as normalised distributions: in the case of $J_a(x_2)$ this corresponds to the source intensity σ_0 being equal to unity. The value of $\rho_0(x_2)$ computed from (8) by numerical integration is also shown.

In plots (a)-(f) $\mathbf{v} = [-1, 2]^T$ and since $v_2 \neq 0$ the distributions are skewed. Plots (g) and (h) illustrate the conclusion from section (2.3) that our analysis remains valid even if \mathbf{D} has rank one. The curves in the log-linear plots become parallel at large x_2 showing that, asymptotically, the exponential decay is the same whether or not there is an absorbing boundary.

In the case of the non-absorbing boundary, equation (18) is expected to serve as a precise asymptotic estimate of $\rho_0(x_2)$ as $|x_2| \rightarrow \infty$, and the plots in figure (2) show that this formula is indeed very accurate. In the case of the absorbing boundary, the status of equations (60) and (61) is more complicated, because there are two Laplacian integrations involved in their derivation. These equations are not precise asymptotes for $J_a(x_2)$ as $|x_2| \rightarrow \infty$ because this limit does not play a role in the estimate for the normalisation factor of the integral in the denominator of equation (46), (i.e. equation (57)). Equations (60), (61) are only precise asymptotic estimates when we take $x_0 \rightarrow \infty$ as well as $|x_2| \rightarrow \infty$. Our numerical results illustrate this: in the case of an absorbing boundary the quality of the asymptotic approximation improves as x_0 becomes larger. However the results also show that in practice equations (60) and (61) are accurate even for quite small x_0 and that they predict the correct scaling of $A_a(x_2)$.

In order to obtain $J_a(x_2)$ we have used an ‘antiparticle’ approach to determine the distribution of first contact times for the boundary, and combined this with a calculation of the distribution $P_{x_2|t}$ of the coordinate x_2 conditional upon the first contact time t . It is natural to ask whether the ‘antiparticle’ picture could lead to a more direct evaluation of $J_a(x_2)$ in the case where the distance of the source from the boundary, x_0 , is small. In that case most of the particles emitted from the source at $\mathbf{x}_0 = (x_0, 0)$ will be absorbed by the boundary at a point downstream of the source, $\mathbf{x}_d = \mathbf{x}_0 + \mathbf{v}x_0/v_1$. One might expect that the flux at \mathbf{x} would then be given by a dipole approximation

$$\begin{aligned} J_a(\mathbf{x}, \mathbf{x}_0) &\sim J_0(\mathbf{x}, \mathbf{x}_0) - J_0(\mathbf{x}, \mathbf{x}_d) \\ &\sim (\mathbf{x}_0 - \mathbf{x}_d) \cdot \nabla_{\mathbf{x}_0} J_0(\mathbf{x}, \mathbf{x}_0) \end{aligned} \quad (63)$$

however we were not able to produce a valid estimate of $J_a(x_2)$ using this type of dipolar approximation.

In conclusion, we have investigated the flux $J_a(x_2)$ onto an absorbing boundary, as a function of the coordinate x_2 measuring the distance from the source. We find that $J_a(x_2) \sim A_a(x_2) \exp[-\Phi_0(x_2)]$, where the exponent $\Phi_0(x_2)$ grows linearly as $x_2 \rightarrow \infty$ and is the same as the exponent for the flux onto a permeable boundary. The function $A_a(x_2)$ was shown to have an algebraic decay: $A_a(x_2) \sim |x_2|^{-3/2}$ for the absorbing boundary, compared to $A_0(x_2) \sim |x_2|^{-1/2}$ for a permeable boundary. These results will be directly relevant to extending recent studies [6] of the geometry of constellations of points sampling fractal measures.

This research was supported by the NORDITA program *Dynamics of Particles in Flows*.

References

1. G. Falkovich, K. Gawedzki and M. Vergassola, *Particles and fields in turbulence*, *Rev. Mod. Phys.*, **73**, 913-975, (2000).
2. J. Bec, K. Gawedzki and P. Horvai, *Multifractal clustering in compressible flows*, *Phys. Rev. Lett.*, **92**, 224501, (2004).
3. A. Pumir, B. Shraiman and M. Chertkov, *Geometry of Lagrangian dispersion in turbulence*, *Phys. Rev. Lett.*, **85**, 5324, (2000).
4. M. Wilkinson, B. Mehlig and K. Gustavsson, *Correlation dimension of inertial particles in random flows*, *Europhys. Lett.*, **89**, 50002, (2010).
5. M. Wilkinson, B. Mehlig, K. Gustavsson and E. Werner, *Clustering of exponentially separating trajectories*, *Eur. Phys. J. B*, **85**, 18, (2012).
6. M. Wilkinson and J. Grant, *Triangular constellations in fractal measures*, *Europhys. Lett.*, **107**, 50006, (2014).
7. O. F. T. Roberts, *The theoretical scattering of smoke in a turbulent atmosphere*, *Phil. Trans. Roy. Soc. Lond. A*, **104**, 640-54, (1924).
8. O. G. Sutton, *A theory of eddy diffusion in the atmosphere*, *Proc. Roy. Soc. Lond. A*, **135**, 143-65, (1932).
9. D. L. Ermak, *An analytical model for air pollutant transport and deposition from a point source*, *Atmos. Environ.*, **11**, 231-37, (1977).
10. J. M. Stockie, *The mathematics of atmospheric dispersion modelling*, *SIAM Rev.*, **53**, 349-72, (2011).
11. S. Redner, *A Guide to First Passage Processes*, Cambridge, University Press, (2001).
12. Z. Schuss, *Theory and Applications of Stochastic Processes: An Analytical Approach*, *Applied Mathematical Sciences* vol. 170, Springer (2010).
13. F. J. Dyson, *The S matrix in quantum electrodynamics*, *Phys. Rev.*, **75**, 1736, (1949).

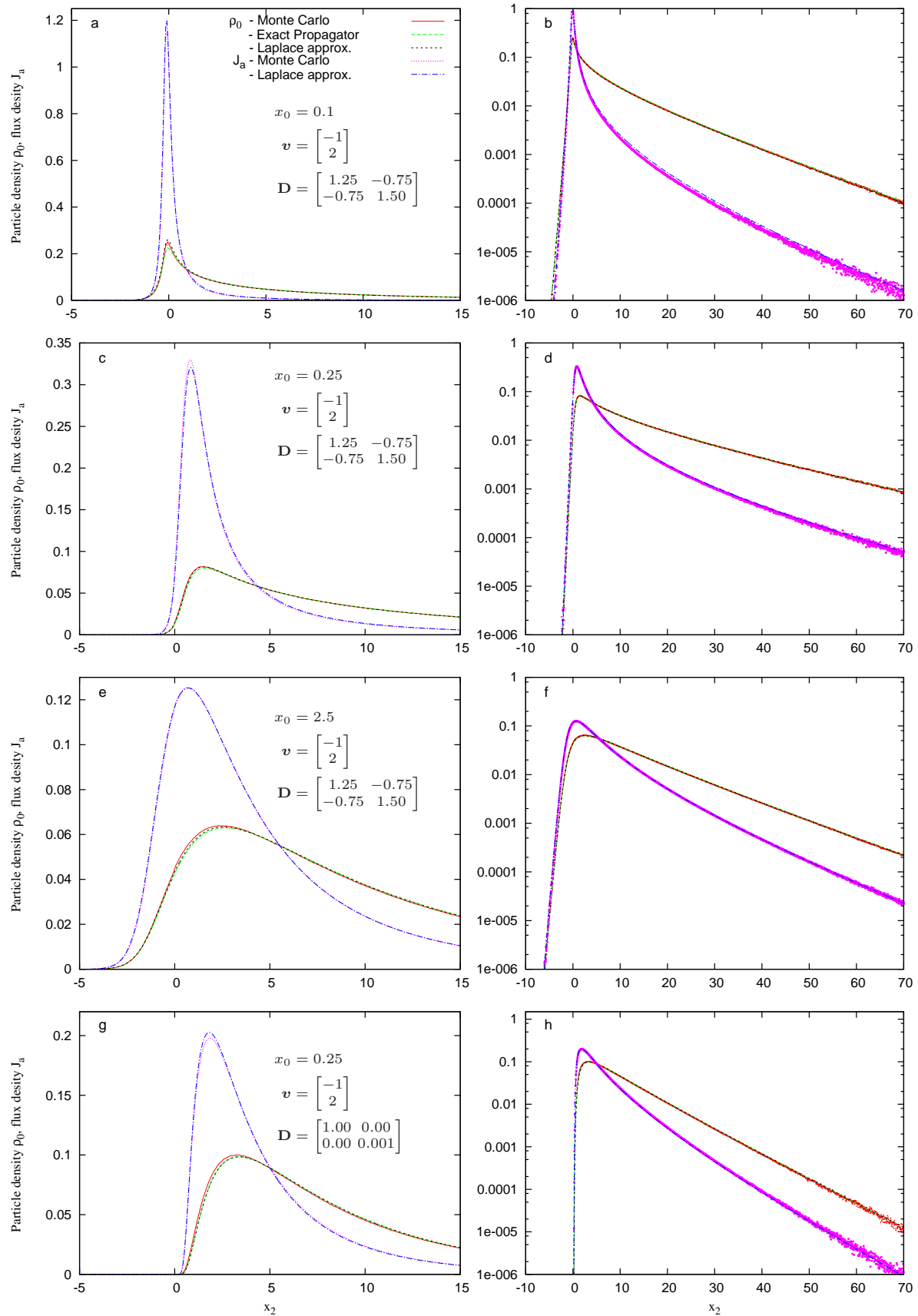


Fig. 2 (Colour online). Linear and log-linear plots of the magnitudes of the steady state particle density for a permeable boundary, $\rho_0(x_2)$, and the steady-state flux for an absorbing boundary, $J_a(x_2)$. The plots show normalised densities or fluxes at $(0, x_2)$ from a steady source at $(x_0, 0)$, for various values of v and D and x_0 .