

### First-passage times and solutions of the telegrapher equation with boundaries

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(Received 26 October 1992)

The first-passage-time distribution function (FPTDF) is derived for a relativistic random walk (RW) in one-dimensional (1D) space limited by one boundary. Thereby two configurations are considered with the start of the RW directed towards or away from the boundary. For each configuration the distribution function (DF) of the RW path ends is evaluated subjected to either absorption or reflection occurring at the boundary. The DF's are identical with the solutions of the telegrapher equation in 1D space under the same initial and boundary conditions. The calculus can be extended to two boundaries, where all combinations of reflecting and absorbing boundaries are possible, for which the Laplace transforms of the path-end DF's and the FPTDF's are presented. The derivation is demonstrated and cross-checked for the case of two absorbing boundaries.

PACS number(s): 02.50.-r, 03.40.Kf, 05.40.+j

#### I. INTRODUCTION

The solution of a partial differential equation in a finite medium requires the knowledge of the boundary values (BV's). As they are a part of the time-dependent solution, their time dependence must be known *a priori*, which is not the case for absorbing or reflecting boundaries. On the other hand, known stationary boundary conditions prove in most cases insufficient to solve the time-dependent problem. General aspects of the problem can be found in [1-3] and a survey is presented in [4], but only a few publications refer to the telegrapher equation (TE) [5,6] in one-dimensional (1D) space with absorbing boundaries, and symmetric initial conditions.

Here we present solutions of the TE in 1D space as well, but with a variety of one or two absorbing and/or reflecting boundaries for one-sided sources, from which all presently known solutions can be derived. Actually the solutions are obtained from a random walk (RW) model that allows the distinction of two directional components, which is not the case for the TE and its known solutions [7,8]: A particle moves with constant speed along the spatial coordinate  $x$ , where it reverses its flight direction at randomly distributed instants. The occurrence of these flips, equivalent to backscattering

events in the RW executed by the particle, is assumed to be Poisson distributed with the rate  $r$  (constant in time and space). The time-dependent distribution function (DF) of the path ends of the RW is identical with the known solution of the TE, naturally under the same initial and boundary conditions, i.e., for a point source emitting a source current of half the source strength in either  $x$  direction and for boundaries at  $x = \pm \infty$ . From this identity we conclude that the unknown solutions of the TE subjected to different initial and/or boundary conditions can be obtained likewise by the RW model, which entails that the first-passage-time distribution functions (FPTDF's) of the RW ought to be identical with the time-dependent BV's of the TE.

The TE with the reduced space coordinate  $q = x/c$ ,

$$\left[ \left( \frac{\partial}{\partial t} + r \right)^2 - r^2 - \frac{\partial^2}{\partial q^2} \right] \mathcal{L}(t, q) = 0, \tag{1}$$

is solved for a uniform medium with infinite extension and with a point source at  $t = q = 0$  that emits a current of unit strength equivalent to one particle in the positive  $q$  direction. The solution describes the flux (particle density times velocity) by a probability density function (PDF) [8]:

$$\mathcal{L}_+(t, q) = e^{-rt} \Theta(t) \left\{ \delta^+(t - q) + \frac{r}{2} \left[ I_0^-(\theta) + \left( \frac{t+q}{t-q} \right)^{1/2} I_1^+(\theta) \right] \Theta(t - |q| \right\} \text{ with } \theta = r(t^2 - q^2)^{1/2} \tag{2a}$$

$$= \mathcal{L}_{+,0}^+(t, q) + \sum_{k=0}^{\infty} [\mathcal{L}_{+,2k+1}^-(t, q) + \mathcal{L}_{+,2k+2}^+(t, q)] \tag{2b}$$

$$= \mathcal{L}_+^+(t, q) + \mathcal{L}_+^-(t, q). \tag{2c}$$

$\Theta(t)$  and  $\delta(t \mp q)$  have the usual meanings,  $I_k$  is the modified Bessel function of order  $k$ ,  $r$  is the scattering rate, and the subscripts  $\pm$  indicate the orientation of the source current in  $q$  space. The constant particle speed limits the flux PDF to the interval  $-t \leq q \leq t$ .

The same distribution is obtained for the path ends of a one-particle RW starting in the positive  $q$  direction, but it is only the latter that allows one to relate the three terms in (2a) to a free-flight term and contributions from an odd and

an even number of reversals, as described by (2b). Actually if we expand both Bessel functions into series, then the  $n$ th-order term in the overall sum (2b) represents the path-end DF of a path with  $n$  flips. Consequently a given starting direction, corresponding to a one-sided orientation of a one-particle source, makes it possible to attribute to any term of order  $n$  a flight direction, consequently two flight directions can be distinguished in the path-end PDF as indicated by the superscripts  $\pm$  in (2c).

Associated with these flight directions are two DF's for one-sided currents, one for a positive and one for a negative current component (PCC, NCC) [9]. Recalling the Poisson distribution of the scattering events, the time and space intervals between the flips form a renewal process and the process is stationary. Consequently the path-end PDF (2) can be interpreted as a transition probability (TP) expressed in terms of differences in time and space. And further we deduce from (2c) that  $\mathcal{L}_+^\pm(t, q)$  and  $\mathcal{L}_-^\pm(t, q)$  are TP's as well, with the current orientation additionally taken into account. Marking all currents or current components with their superscript, (2c) can be extended to its general form

$$\int_0^+ dt' \int_{+\infty}^+ dq' Q^+(t', q') \mathcal{L}_+^\pm(t-t', q-q') = \int_0^t dt' \int_{+\infty}^+ dq' Q^+(t', q') [\mathcal{L}_+^+(t-t', q-q') + \mathcal{L}_+^-(t-t', q-q')] , \quad (2d)$$

where  $Q^+(t, q)$  denotes the DF of a positive current and where (2d) reduces to (2c) by setting  $Q^+(t, q) = 1^+ \delta(t) \delta(q)$ .

Reading the notations in (2d) from left to right the transition of any initial state, given by the DF of a current directed towards  $q > 0$  (being either a one-sided current, or a current component alone, or the non-negative difference PCC minus NCC, see [9]) can be tracked down to the final or follow-up state, given by the DF's of two current components in opposite directions. Naturally subscripts and/or superscripts may be omitted if they are quoted redundantly or if they are of no interest. This is the case in many applications below, where superscripts are only retained to describe the current components of the final state, while currents of preceding states may show up only with their amplitude DF.

## II. THE ONE-BOUNDARY PROBLEM

The initial condition of a point source with unit strength at  $t=q=0$  oriented towards  $q > 0$  will be maintained throughout this paper; other source configurations are mentioned explicitly; see also Appendixes A and C.

Introducing an absorbing or reflecting boundary two alternatives have to be considered: Setting the boundary at  $q = -a < 0$  or at  $q = u > 0$ , the source would be directed away from or towards the boundary. In any case the boundary causes a disturbance which we ascribe to a secondary source at the site of the boundary. Evidently it will come into existence only with the arrival of the front of the undisturbed flux, i.e., for  $t \geq a$  or  $t \geq u$ . Furthermore we will require the disturbing flux to meet two (stationary boundary) conditions: The superposition of disturbing and undisturbed flux must vanish at the "rear side" of the boundary, while on its "front side" it must decrease or increase according to the absorbing or reflecting property of the boundary.

*Case (a1).* Considering an absorbing boundary at  $q = -a$ , the postulates above can be cast into two equations, describing the flux in the left (right) half space [lhs (rhs)] off the boundary:

$$\mathcal{L}_+(t, q) \Theta(-(q+a)) - \int_0^+ dt' \mathcal{A}^-(t', -a) \times \mathcal{L}_-(t-t', q+a) \Theta(-(q+a)) = 0 , \quad (3a)$$

$$\mathcal{L}_+(t, q) \Theta(q+a) - \int_0^t dt' \mathcal{A}^-(t', -a) \times \mathcal{L}_-(t-t', q+a) \Theta(q+a) = \mathcal{L}_+(t, q, -a) . \quad (3b)$$

The two terms in the sums (3a) and (3b) describe the original flux (2) and a disturbing flux. The effect of the absorbing boundary is equivalent to a source with "negative" amplitude  $-\mathcal{A}(t, -a)$ , i.e., a particle sink at  $q = -a$  that emits "missing" particles. As the emission is directed into the lhs  $q < -a$ , as indicated by the superscript, it entails a flux DF, which is expressed by the double convolution integral of the sink  $-\mathcal{A}^-(t, q)$  and the flux  $\mathcal{L}_-(t, q)$ , the mirror image of (2), see (A1).

In the lhs of the boundary the sum of the "negative" disturbing flux and the "positive" undisturbed flux cancel (3a), while in the rhs the particles absorbed at the boundary—it must be those that move to the left and that hit the boundary at its front side, a postulate that will be verified by (8)—cause a bleeding of the prevailing undisturbed flux, thus giving rise to the new distribution  $\mathcal{L}_+(t, q, -a)$  (3b). In (3a) and (3b) the convolution integral in space is already carried out while Laplace transforms (LT) are used to evaluate the convolution integral in time:

$$f_+(s, q) \Theta(-(q+a)) - A^-(s, -a) f_{-,L}(s, q+a) = 0 , \quad (4a)$$

$$f_+(s, q) \Theta(q+a) - A^-(s, -a) f_{-,R}(s, q+a) = f_+(s, q, -a) . \quad (4b)$$

$f_+(s, q)$  is the Laplace transform of  $\mathcal{L}_+(t, q)$  given by

$$\begin{aligned} f_+(s, q) &= \frac{1}{2\tau} [(r^- + \sigma^+ - \tau^+) e^{q\tau} \Theta(-q) \\ &\quad + (r^- + \sigma^+ + \tau^+) e^{-q\tau} \Theta(q)] \\ &= f_{+,L}(s, q) + f_{+,R}(s, q) \\ &\quad \text{with } \sigma = s + r, \quad \tau = (\sigma^2 - r^2)^{1/2} . \end{aligned} \quad (5)$$

Inserting (5) and the mirror image  $f_-(s, q)$  (A2) into (4a) furnishes all data—amplitude and orientation—of the sink

$$\begin{aligned} A^-(s, -a) &= k^- e^{-a\tau} \quad \text{with } k^- = \frac{f_{+,L}(s, q)}{f_{-,L}(s, q)} \\ &= \frac{(r^- + \sigma^+ - \tau^+)^-}{(r^+ + \sigma^- + \tau^-)} = \frac{(\sigma - \tau)^-}{r} , \end{aligned} \quad (6a)$$

$$A(s, -a) = k e^{-a\tau} \quad \text{with } k = \frac{(r + \sigma - \tau)}{(r + \sigma + \tau)} = \frac{(\sigma - \tau)}{r} , \quad (6b)$$

which are used in (4b) to evaluate the flux in the rhs  $q \geq -a$ :

$$f_+(s, q, -a) = \left[ f_+(s, q) - \left( \frac{(\sigma - \tau)^+}{2\tau} + \frac{(\sigma - \tau)^{2-}}{2r\tau} \right) \times e^{-(q+2a)\tau} \right] \Theta(q+a). \quad (7)$$

The flux at the boundary

$$f_+(s, q, -a)|_{q=-a} = \left[ \frac{r^-}{2\tau} - \frac{(\sigma - \tau)^{2-}}{2r\tau} \right] e^{-a\tau} = k^- e^{-a\tau} = A^-(s, -a) \quad (8)$$

has the same amplitude as the assumed sink but a positive sign and as its PCC vanishes while the NCC is identical with (6), the flux actually reduces to a current in the

negative  $q$  direction at  $q = -a$ . This complies with Mark's boundary conditions [10] and proves the identity of the boundary value  $A(s, -a)$  with the FPTDF  $A^-(s, -a)$ , naturally in consideration of the special configuration for source and boundary, which means that only particles moving to the left account for it.

Equation (8) agrees with the situation at a medium-vacuum interface, with the vacuum for  $q < -a$ , where particles having crossed the boundary continue their flight as a current and never return to the boundary (compare [9]):

$$j_+(s, q, -a)|_{q < -a} = -A^-(s, -a)e^{(q+a)s}\Theta(-(q+a))\mathbf{e}, \quad (9)$$

where  $\mathbf{e}$  is the unit vector in the positive  $q$  direction.

For the sake of completeness we present the originals of the LT's of (6), (7), and (9):

$$\begin{aligned} \mathcal{A}(t, -a) &= \frac{r}{2} e^{-r\theta} \Theta(t) \left[ I_0(\theta) - \frac{t+q}{t-q} I_2(\theta) \right] \Theta(t - |q|)|_{q=-a} \\ &= \frac{2}{r} abs \left[ \frac{\partial}{\partial q} \mathcal{L}_+^+(t, q)|_{q=-a} \right], \end{aligned} \quad (10)$$

$$\begin{aligned} j_+(t, q, -a)|_{q < -a} &= - \int_0^t dt' \int_{-\infty}^{+\infty} dq' \mathcal{A}^-(t', q') \delta(q'+a) \delta^-(t-t'+q-q') \Theta(t-t') \mathbf{e} \\ &= - \frac{r}{2} e^{-r\eta} \Theta(t) \left[ I_0^-(\eta) - \frac{t_1-a}{t_1+a} I_2^-(\eta) \right] \Theta(t_1-a) \Theta(-(q+a)) \mathbf{e} \end{aligned} \quad (11)$$

with  $t_1 = t + q + a$ ,  $\eta = r(t_1^2 - a^2)^{1/2}$ ,

$$\begin{aligned} \mathcal{L}_+(t, q, -a) &= \left\{ \mathcal{L}_+(t, q) - \frac{r}{2} e^{-r\theta} \Theta(t) \left[ \left( \frac{t-\ddot{a}}{t+\ddot{a}} \right)^{1/2} I_1^+(\omega) + \frac{t-\ddot{a}}{t+\ddot{a}} I_2^-(\omega) \right] \theta(t - |\ddot{a}|} \right\} \Theta(q+a) \\ &\text{with } \ddot{a} = q + 2a \text{ and } \omega = r(t^2 - \ddot{a}^2)^{1/2}. \end{aligned} \quad (12)$$

We notice that the flux (12) is described by the undisturbed flux (2) and a disturbing flux, where the latter is defined in the domain

$$\begin{aligned} \mathcal{D}(t, q, -a) &= \Theta(t) \Theta(t - \ddot{a}) \Theta(q + a) \\ &= \Theta(t - a) \Theta((t - a) - (q + a)) \Theta(q + a) \\ &= \Theta(t) \Theta(t - |\ddot{a}|) \Theta(q + a). \end{aligned}$$

The second alternative expresses explicitly its existence for  $t \geq a$  in agreement with (9), while the third one makes it look like it is coming from a mirror image source  $\mathcal{A}(t, -2a)$  that exists for  $t \geq 0$  at the double distance  $q = -2a$  behind the boundary.

The corresponding survival probability (SP) is given by the space integral of (7) or (12), leading to the simple expression

$$S_+(s, -a) = [1 - A(s, -a)]/s, \quad (13)$$

$$\mathcal{S}_+(t, -a) = \Theta(t) - \int_0^t dt' \Theta(t') \mathcal{A}(t - t', -a) \quad (14)$$

that verifies plausibly the tight connection with the FPTDF.

*Case (a2).* If the boundary at  $q = -a$  reflects the particle, the reflective property of the boundary shall be marked by a caret placed above the boundary coordinate—Eqs. (3a) and (4a) still remain valid, whereas (3b) and (4b) are replaced by

$$\begin{aligned} \mathcal{L}_+(t, q) \Theta(q + a) + \int_0^t dt' \mathcal{A}^+(t', -a) \mathcal{L}_+(t - t', q + a) \\ \times \Theta(q + a) = \mathcal{L}_+(t, q, -\hat{a}), \end{aligned} \quad (3c)$$

$$\begin{aligned} f_+(s, q) \Theta(q + a) + A^+(s, -a) f_{+,R}(s, q + a) \\ = f_+(s, q, -\hat{a}). \end{aligned} \quad (4c)$$

The reflecting boundary acts like a particle source with positive amplitude given by the FPTDF  $A(t, -a)$  oriented towards the rhs off  $q = -a$ . Inserting (5) and  $A(s, -a)$  from (6) in (4c) leads to

$$f_+(s, q, -\hat{a}) = \left[ f_+(s, q) + \frac{r^+ + \sigma^- - \tau^-}{2\tau} e^{-(q+2a)\tau} \right] \times \Theta(q+a), \quad (15)$$

$$\begin{aligned} \mathcal{L}_+(t, q, -\hat{a}) = & \left\{ \mathcal{L}_+(t, q) \right. \\ & + \frac{r}{2} e^{-rt} \Theta(t) \\ & \times \left[ I_0^+(\omega) + \left[ \frac{t-\ddot{a}}{t+\ddot{a}} \right]^{1/2} I_1^-(\omega) \right] \\ & \left. \times \Theta(t-\ddot{a}) \right\} \Theta(q+a). \quad (16) \end{aligned}$$

For  $q = -a$  the PCC and NCC contribute equal amounts, so the flux (15) or (16) is exactly twice the amplitude of the undisturbed flux (5), respectively (2), while the net current is zero, compare [9]. The corresponding SP is  $\Theta(t)$ .

Cases (b1), (b2). In the same way the flux DF is derived for one absorbing or one reflecting boundary at  $q = u > 0$ . In both cases the flux behind the boundary will disappear according to

$$\mathcal{L}_+(t, q) \Theta(q-u) - \int_0^t dt' \mathcal{B}^+(t', u) \mathcal{L}_+(t-t', q-u) \times \Theta(q-u) = 0, \quad (17a)$$

which is just Siegert's formula [1], while the flux DF's for

$$\begin{aligned} \mathcal{B}(t, u) = & e^{-rt} \Theta(t) [(r^2 q / \theta) I_1(\theta) \Theta(t - |q|) + \delta(t - q)]|_{q=u} \\ = & \frac{2}{r} \text{abs} \left[ \frac{\partial}{\partial q} \mathcal{L}_+(t, q)|_{q=u} \right], \quad (21) \end{aligned}$$

$$\mathcal{L}_+(t, q, u) = \left\{ f_+(t, q) - \frac{r}{2} e^{-rt} \Theta(t) \left[ I_0^-(\beta) + \left[ \frac{t+\ddot{u}}{t-\ddot{u}} \right]^{1/2} I_1^+(\beta) \right] \Theta(t - |\ddot{u}|) \right\} \Theta(-(q-u)), \quad (22)$$

$$\begin{aligned} \mathcal{L}_+(t, q, \hat{u}) = & [\mathcal{L}_+(t, q) + \mathcal{L}_-(t, \ddot{u})] \Theta(-(q-u)) \\ = & \left\{ \mathcal{L}_+(t, q) + e^{-rt} \Theta(t) \left[ \frac{r}{2} \left[ I_0^+(\beta) + \left[ \frac{t+\ddot{u}}{t-\ddot{u}} \right]^{1/2} I_1^-(\beta) \right] \Theta(t - |\ddot{u}|) + \delta(t + \ddot{u}) \right] \right\} \Theta(-(q-u)) \end{aligned}$$

with  $\ddot{u} = q - 2u$  and  $\beta = r(t^2 - \ddot{u}^2)^{1/2}$ . (23)

Again fluxes and currents at  $q = u$  can be calculated from the two last expressions as in the previous cases with the corresponding SP's given by

$$\mathcal{S}_+(t, u) = \Theta(t) - \int_0^t dt' \Theta(t') \mathcal{B}(t-t', u), \quad (24)$$

$$\mathcal{S}_+(t, \hat{u}) = \Theta(t). \quad (25)$$

Equations (10) and (21) in their last versions express the linear dependence of the FPTDF on the absolute value of the gradient of that current component in the undisturbed flux (2) that is directed away from the boundary. As this relation is independent of the source-boundary configuration it may be a general feature of the FPTDF, worthwhile for further investigation.

Applying rule [11] to the LT's (7) and (19) reproduces the expressions (17) and (18) derived in [5].

$q \leq u$  are derived from the equations

$$\mathcal{L}_+(t, q) \Theta(-(q-u)) - \int_0^t dt' \mathcal{B}^+(t', u) \mathcal{L}_+(t-t', q-u) \times \Theta(-(q-u)) = f_+(t, q, u), \quad (17b)$$

$$\mathcal{L}_+(t, q) \Theta(-(q-u)) + \int_0^t dt' \mathcal{B}^-(t', u) \mathcal{L}_-(t-t', q-u) \times \Theta(-(q-u)) = \mathcal{L}_+(t, q, \hat{u}). \quad (17c)$$

Proceedings as before the LT's of the FPTDF and the fluxes are

$$B(s, u) = e^{-u\tau}, \quad (18)$$

$$\begin{aligned} f_+(s, q, u) = & f_+(s, q) \Theta(-(q-u)) \\ & - B^+(s, u) f_{+,L}(s, q-u) \\ = & \left[ f_+(s, q) - \frac{r^- + \sigma^+ - \tau^+}{2\tau} e^{(q-2u)\tau} \right] \\ & \times \Theta(-(q-u)), \quad (19) \end{aligned}$$

$$\begin{aligned} f_+(s, q, \hat{u}) = & f_+(s, q) \Theta(-(q-u)) \\ & + B^-(s, u) f_{-,L}(s, q-u) \\ = & \left[ f_+(s, q) + \frac{r^+ + \sigma^- + \tau^-}{2\tau} e^{(q-2u)\tau} \right] \\ & \times \Theta(-(q-u)), \quad (20) \end{aligned}$$

with the corresponding original DF's of FPTDF and fluxes

### III. THE TWO-BOUNDARY PROBLEM

The same procedure can be used to evaluate the flux DF between two boundaries together with the BV [12] at either boundary, thereby any combination of reflecting and absorbing boundaries is possible. Here we derive the DF between two absorbing boundaries, as for this case the result can be cross-checked with its counterpart under stationary conditions.

Starting with the same initial conditions for source and boundaries as before [cases (a1) and (a2)] we split the original flux coming from the particle source in two one-sided branches and follow up the development of each flux branch in accordance with the successive encounters with the boundaries.

The flux branch propagating in the negative  $q$  direction

hits the absorbing boundary at  $q = -a$  first. The absorption gives rise to a primary disturbance that makes the flux vanish for  $q < -a$ , (26a), while it spreads for  $q \geq -a$  towards the opposite boundary  $q = u$ , (26b). For  $t \geq 2a + u$  this boundary gives rise to a secondary disturbance (a disturbance of the disturbance) that makes the primary disturbance vanish for  $q > u$ , (27a), while it propagates for  $q \leq u$  back to the other boundary at  $q = -a$ , (27b). With its arrival at  $t = 3a + 2u$  a third-order disturbance develops, cancelling the secondary disturbance for  $q < -a$ , (28a), and spreading on the other side again towards  $q = u$ , (28b), and so forth:

$$f_{+,L}(s,q)\Theta(-(q+a)) - A_1^- f_{-,L}(s,q+a) = 0, \quad (26a)$$

$$f_{+,L}(s,q)\Theta(q+a) - K^- e^{u\tau} f_{-,R}(s,q+a) = f_{+,1}(s,q,-a), \quad (26b)$$

$$-A_1^- f_{-,R}(s,q+a)\Theta(q-u) + A_2^+ f_{+,R}(s,q-u) = 0, \quad (27a)$$

$$-K^- e^{u\tau} f_{-,R}(s,q+a)\Theta(-(q-u)) + K^{2+} e^{u\tau} f_{+,L}(s,q-u) = f_{+,2}(s,q,u), \quad (27b)$$

$$A_2^+ f_{+,L}(s,q-u)\Theta(-(q+a)) - A_3^- f_{-,L}(s,q+a) = 0, \quad (28a)$$

$$K^{2+} e^{u\tau} f_{+,L}(s,q-u)\Theta(q+a) - K^{3-} e^{u\tau} f_{-,R}(s,q+a) = f_{+,3}(s,q,-a), \quad (28b)$$

$$-A_3^- f_{-,R}(s,q+a)\Theta(q-u) + A_4^+ f_{+,R}(s,q-u) = 0, \quad (29a)$$

$$-K^{3-} e^{u\tau} f_{-,R}(s,q+a)\Theta(-(q-u)) + K^{4+} e^{u\tau} f_{+,L}(s,q-u) = f_{+,4}(s,q,u). \quad (29b)$$

Equations (26a) and (26b) are quasi-identical with (4a) and (4b);  $-A_1 = -A_1(s,-a)$ ,  $+A_2 = +A_2(s,u)$ ,  $-A_3 = -A_3(s,-a)$ , ... stand for the sinks and sources (the latter have to be interpreted as sinks of missing particles) at the boundaries that come into existence successively as indicated by their indexes. In every second equation  $-A_1, A_2, -A_3, \dots$  is replaced by its explicit value  $-Ke^{u\tau}, +K^2e^{u\tau}, -K^3e^{u\tau}, \dots$  with  $K = k\epsilon$ ,  $\epsilon = e^{-(a+u)\tau}$ , obtained from the previous equation.

The other positive branch of the original flux encounters the boundaries in the reverse order  $q = u, -a, u, \dots$ ; they give rise to the sinks (sources)  $-B_1 = -B_1(s,u)$ ,  $+B_2 = +B_2(s,-a)$ , ... and to disturbances in the flux distribution, described by (30a)–(32b) and so forth:

$$f_{+,R}(s,q)\Theta(q-u) - B_1^+ f_{+,R}(s,q-u) = 0, \quad (30a)$$

$$f_{+,R}(s,q)\Theta(-(q-u)) - 1^+ e^{-b\tau} f_{+,L}(s,q-u) = f_{+,1}(s,q,u), \quad (30b)$$

$$-B_1^+ f_{+,L}(s,q-u)\Theta(-(q+a)) + B_2^- f_{-,L}(s,q+a) = 0, \quad (31a)$$

$$-1^+ e^{-u\tau} f_{+,L}(s,q-u)\Theta(q+a) + K^- e^{-u\tau} f_{-,R}(s,q+a) = f_{+,2}(s,q,-a), \quad (31b)$$

$$B_2^- f_{-,R}(s,q+a)\Theta(q-u) - B_3^+ f_{+,R}(s,q-u) = 0, \quad (32a)$$

$$K^- e^{-u\tau} f_{-,R}(s,q+a)\Theta(-(q-u)) - K^{2+} e^{-u\tau} f_{+,L}(s,q-u) = f_{+,3}(s,q,u). \quad (32b)$$

The two original flux branches plus the infinite sum of all their follow-up disturbances contribute to the time-dependent flux DF within and at the boundaries, see Appendix B:

$$f_+(s,q,-a,u) = \frac{1}{2\tau M} \{ (1 - e^{-2u\tau}) [k^- e^{-2a\tau} (r^+ + \sigma^- - \tau^-) e^{-q\tau} - 1^+ (r^- + \sigma^+ - \tau^+) e^{q\tau}] \Theta(-q) \Theta(q+a) + (k^2 e^{-2a\tau} - 1) [1^+ e^{-2u\tau} (r^- + \sigma^+ - \tau^+) e^{q\tau} - 1^+ (r^- + \sigma^+ + \tau^+) e^{-q\tau}] \Theta(q) \Theta(-(q-u)) \}, \quad (33)$$

$$f_+(s,q,-a,u)|_{q=-a} = \frac{k^- e^{-a\tau} (1 - e^{-2u\tau})}{M} = \sum_{k=0}^{\infty} (A_{2k+1}^- - B_{2k+2}^-) = \frac{A^-(1 - B^2)}{(1 - A^2 B^2)}, \quad (34a)$$

$$f_+(s,q,-a,u)|_{q=u} = \frac{1^+ e^{-u\tau} (1 - k^2 e^{-2a\tau})}{M} = \sum_{k=0}^{\infty} (B_{2k+1}^+ - A_{2k+2}^+) = \frac{B^+(1 - A^2)}{(1 - A^2 B^2)}, \quad (34b)$$

where  $A$  and  $B$  are identical with the expressions (6) and (18).

Again we can derive the SP either from the space integral of (33) or from the FPTDF's (34a) and (34b) in analogy to (13) and (14) or (24):

$$S_+(s,-a,u) = \frac{[1 - (A + B)/(1 + AB)]}{s}, \quad (35)$$

$$\mathcal{S}_+(t, -a, u) = \Theta(t) - \int_0^t dt' \Theta(t') [\mathcal{L}_+(t-t', q, -a, u)|_{q=-a} + \mathcal{L}_+(t-t', q, -a, u)|_{q=u}] . \tag{36}$$

For the special case of a symmetric unit source, see rule [11], with the boundaries at  $q = \pm a$  the flux DF is symmetric in  $q$ ,

$$f_R(s, q, -a, a) = \frac{(1+k)}{4\tau(1+ke^{-2a\tau})} [(r^- + \sigma^+ + \tau^+)e^{-q\tau} - e^{-2a\tau}(r^- + \sigma^+ - \tau^+)e^{q\tau}] \Theta(q) \Theta(-(q-a)) , \tag{37}$$

$$f(s, q, -a, a)|_{q=\pm a} = 1^\pm (1+k)e^{-a\tau} / 2(1+ke^{-2a\tau}) , \tag{38}$$

where the denominator in (37) and (38) refers to a series of equidistant ( $\Delta t = 2a$ ) alternating steps in the original. Consequently the latter can be expressed only implicitly by means of a convolution integral, e.g., for (38)

$$\begin{aligned} & \int_0^t dt' \mathcal{L}(t-t', q, -a, a)|_{q=\pm a} \Theta(t') \left[ \delta(t') + \frac{r}{2} e^{-r't'} \left[ I_0(\theta') - \frac{t'-q}{t'+q} I_2(\theta') \right] \Theta(t'-q) \right]_{q=2a} \\ &= \frac{1}{2} e^{-r't} \Theta(t) \left\{ \delta^+(t-q) + \frac{r}{2} \left[ \left[ \frac{2rq}{\theta} \right] I_1^+(\theta) + I_0^+(\theta) - \frac{t-q}{t+q} I_2^+(\theta) \right] \Theta(t-2) \right\} \Big|_{q=a} \quad \text{with } \theta' = r(t'^2 - q^2)^{1/2} , \end{aligned} \tag{39a}$$

which in turn can be expressed by FPTDF's such as (10) and (21),

$$\int_0^t dt' f(t-t', q, -a, a)|_{q=\pm a} [\delta(t') + \mathcal{A}(t'-2a)] = \mathcal{B}^+(t, a) + \mathcal{A}^+(t, -a) . \tag{39b}$$

For simplicity the presentation of the originals of (33), (34), and (37) is omitted as it would involve convolution integrals similar to the one in (39).

Three more DF's together with their BV's for various combinations of absorbing and reflecting boundaries are listed in Appendix C.

*Proof.* In order to confirm the results above we present a proof with its main steps. It is easily shown that (2) is the forced response solution of

$$\begin{aligned} & \left[ \left[ \frac{\partial}{\partial t} + r \right]^2 - r^2 - \frac{\partial^2}{\partial q^2} \right] f_+(t, q) \\ &= \left[ \frac{\partial^+}{\partial t} + r^+ + r^- - \frac{\partial^+}{\partial q} \right] \delta(t) \delta(q) , \end{aligned} \tag{40}$$

where according to the superscripts the terms in the differential operator on the rhs of (40) give rise to the two current components in (2) and (5). This one-to-one correspondence permits the derivation of fluxes, currents, and current components, etc. straight from the TE, respectively, its Green's function by choosing the appropriate differential operator on the rhs of (40). For example, rule [11] provides for the solution of (1) for a symmetric source with unit strength at  $t = q = 0$ ; similarly it can be derived from the TE (40) augmented by its mirror image. Likewise all DF's deduced from the RW model are solutions of the TE, irrespective of the presence or absence of fully or partially absorbing and/or reflecting boundaries, subject to any kind of source emission (one-sided, non-symmetric, or symmetric).

If the RW is extended to include forward and backward scattering (with equal rate  $r$ ) and absorption as well (with the rate  $\alpha$ , which corresponds to a trapping rate), only  $r$  out of  $(\alpha + 2r)$  collision events entail a backscatter-

ing. This leads to modifications in the TE's:  $\partial/\partial t \rightarrow \partial/\partial t + \alpha$ ; the distributions:  $\exp(-rt) \rightarrow \exp[-(\alpha + r)t]$ ; and the corresponding LT's:  $s \rightarrow s + \alpha$ . Introducing the new parameters  $\Sigma_a = \alpha/c$ ,  $\Sigma_s = 2r/c$  [13],  $1/D = \Sigma_t = \Sigma_a + \Sigma_s = (\alpha + 2r)/c$ , where  $\Sigma_a$ ,  $\Sigma_s$ , and  $\Sigma_t$  denote the macroscopic absorption, scattering, and transport cross section and  $D$  the diffusion coefficient, and assuming a symmetric unit source at  $t = x = 0$  the TE reads in spatial representation

$$\begin{aligned} & \left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \left[ \Sigma_a + \frac{1}{D} \right] \frac{\partial}{c \partial t} + \frac{\Sigma_a}{D} - \frac{\partial^2}{\partial x^2} \right] \mathcal{L}(ct, x) \\ &= \left[ \frac{\partial}{c \partial t} + \frac{1}{D} \right] \delta(ct) \delta(x) . \end{aligned} \tag{41}$$

The stationary solution of (41) with absorbing boundaries at  $x = \pm a$  is

$$\begin{aligned} \mathcal{L}(x, -a, a) &= \frac{e^{-\kappa|x|} - e^{-2\kappa(a+d)} e^{\kappa|x|}}{2\kappa D (1 + e^{-2\kappa(a+d)})} \\ &\quad \text{with } \kappa = \left[ \frac{\Sigma_a}{D} \right]^{1/2} \end{aligned} \tag{42}$$

[14], where  $d$  is the extrapolation distance defined by

$$\frac{1}{d} = - \frac{\nabla \mathcal{L}(x, -a, a)}{\mathcal{L}(x, -a, a)} \Big|_{x=a} . \tag{43a}$$

At the extrapolated boundary the flux (42) vanishes:  $\mathcal{L}(x = a + d, -a, a) = 0$ . As the flux at the boundary actually reduces to a current and as Fick's law ought to be valid there as well, (43a) can be written as

$$\frac{1}{D} = - \frac{\nabla \mathcal{L}(x, -a, a)}{\mathcal{J}(x, -a, a)} \Big|_{x=a} , \tag{43b}$$

which implies  $d = D$  (correct in 1D space). Inserting (42) in (43b) gives

$$(1 - \kappa D) / (1 + \kappa D) = e^{-2\kappa d} . \tag{44}$$

Referring to (37) for  $q > 0$ , including absorption, taking the stationary limit  $s \rightarrow 0$ , and changing to spatial representation with the new parameters

$$f_R(x, -a, a) = \frac{e^{-\kappa x} - Ee^{-2\kappa a}e^{\kappa x}}{2\kappa D(1 + Ee^{-2\kappa a})} \Theta(x)\Theta(-(x-a))$$

with  $E = \frac{(1-\kappa D)}{(1+\kappa D)}$ . (45)

Comparison of (45) and (42) confirms (44) straightaway.

*Note added.* After completion of this paper I got to know about the work [15], in which the expressions for two FPTDF's (one-boundary problem with absorbing boundary) were presented as well. Different expressions were obtained for a source directed away from the boundary, Eq. (10) in this paper, (18) in [15].

**APPENDIX A**

Analogous to (2a) and (5) the flux PDF and its LT subsequent to a source oriented in the opposite ( $q < 0$ ) direction is given by

$$f_+(s, q, -a, u) = \frac{1}{2\tau M} [M^+(r^- + \sigma^+ - \tau^+)e^{q\tau}\Theta(-q) + K^{2+}e^{u\tau}(r^- + \sigma^+ - \tau^+)e^{(q-u)\tau}$$

$$- K^-e^{u\tau}(r^+ + \sigma^- - \tau^-)e^{-(q+a)\tau} + M^+(r^- + \sigma^+ + \tau^+)e^{-q\tau}\Theta(q)$$

$$- K^-e^{-u\tau}(r^+ + \sigma^- - \tau^-)e^{-(q+a)\tau} + 1^+e^{-u\tau}(r^- + \sigma^+ - \tau^+)e^{(q-u)\tau}] \Theta^*$$

with  $\Theta^* = \Theta(q+a)\Theta(-(q-u))$  and  $M = 1 - K^2$ . (B1)

Rearranging (B1) as a sum of two one-sided DF's

$$= \frac{1}{2\tau M} \{ [M^+(r^- + \sigma^+ - \tau^+)e^{q\tau} + k^{2+}\epsilon^2(r^- + \sigma^+ - \tau^+)e^{q\tau} - k^-e^{-2a\tau}(r^+ + \sigma^- - \tau^-)e^{-q\tau}$$

$$- l^+e^{-2u\tau}(r^- + \sigma^+ - \tau^+)e^{q\tau} + k^-\epsilon^2(r^+ + \sigma^- - \tau^-)e^{-q\tau}] \Theta(-q)\Theta(q+a)$$

$$+ [M^+(r^- + \sigma^+ + \tau^+)e^{-q\tau} - l^+e^{-2u\tau}(r^- + \sigma^+ - \tau^+)e^{q\tau} + k^-\epsilon^2(r^+ + \sigma^- - \tau^-)e^{-q\tau}$$

$$+ k^{2+}\epsilon^2(r^- + \sigma^+ - \tau^+)e^{q\tau} - k^-e^{-2a\tau}(r^+ + \sigma^- - \tau^-)e^{-q\tau}] \Theta(q)\Theta(-(q-u)) \}$$

with  $M = 1 - k^2\epsilon^2$ , (B2)

inserting for  $M$  and using the relation  $(r^+ + \sigma^- - \tau^-) = k^+(r^- + \sigma^+ + \tau^+)$ , derived from the mirror image equation of (4a) in the eighth term of (B2), as well as  $(r^- + \sigma^+ - \tau^+) = k^-(r^+ + \sigma^- + \tau^-)$  from (6) in the first and fourth terms leads to (33).

**APPENDIX C**

With the source configuration leading to (2a) the LT's of the flux DF's within and at the boundaries, i.e., for one absorbing and one reflecting, respectively, for two reflecting boundaries become

$$f_+(s, q, -a, \hat{u})$$

$$= \frac{1}{2\tau N} \{ (k + e^{-2u\tau}) [1^-(r^+ + \sigma^- - \tau^-)e^{q\tau} - k^+e^{-2a\tau}(r^- + \sigma^+ + \tau^+)e^{-q\tau}] \Theta(-q)\Theta(q+a)$$

$$+ (1 - k^2e^{-2a\tau}) [1^+(r^- + \sigma^+ + \tau^+)e^{-q\tau} + 1^-e^{-2u\tau}(r^+ + \sigma^- + \tau^-)e^{q\tau}] \Theta(q)\Theta(-(q-u)) \}$$

with  $N = 1 + k\epsilon^2$ , (C1)

$$f_+(s, q, -a, \hat{u})|_{q=-a} = 1^-e^{-a\tau}(k + e^{-2u\tau})/N, \tag{C2a}$$

$$f_+(s, q, -a, \hat{u})|_{q=u} = e^{-u\tau}(1 - k^2e^{-2a\tau})[(r^- + \sigma^+ + \tau^+) + (r^+ + \sigma^- + \tau^-)]/2\tau N, \tag{C2b}$$

$$f_+(s, q, -\hat{a}, u) = \frac{1}{2\tau N} \{ (1 - e^{-2u\tau}) [1^+(r^- + \sigma^+ - \tau^+)e^{q\tau} + k^+e^{-2a\tau}(r^- + \sigma^+ + \tau^+)e^{-q\tau}] \Theta(-q)\Theta(q+a)$$

$$+ (1 + ke^{-2a\tau}) [1^+(r^- + \sigma^+ + \tau^+)e^{-q\tau} - 1^+e^{-2u\tau}(r^- + \sigma^+ + \tau^+)e^{q\tau}] \Theta(q)\Theta(-(q-u)) \}, \tag{C3}$$

$$f_-(t, q) = e^{-rt}\Theta(t) \left\{ \delta^-(t+q) + \frac{r}{2} \left[ I_0^+(\theta) + \left( \frac{t-q}{t+q} \right)^{1/2} I_1^-(\theta) \right] \times \Theta(t-|q|) \right\}, \tag{A1}$$

$$f_-(s, q) = \frac{1}{2\tau} [(r^+ + \sigma^- + \tau^-)e^{q\tau}\Theta(-q) + (r^+ + \sigma^- - \tau^-)e^{-q\tau}\Theta(q)]$$

$$= f_{-,L}(s, q) + f_{-,R}(s, q). \tag{A2}$$

**APPENDIX B**

In (26a)–(29b) and (30a)–(32b) the portions of the DF's lying within the interval  $-a \leq q \leq u$ , i.e., all first terms in the equations with "b" in the equation numbers, give to two terms plus four infinite series with the sum

$$f_+(s, q, -\hat{a}, u)|_{q=-a} = ke^{-u\tau}(1 - e^{-2u\tau})[(r^- + \sigma^+ + \tau^+) + (r^+ + \sigma^- + \tau^-)]/2\tau N, \quad (\text{C4a})$$

$$f_+(s, q, -\hat{a}, u)|_{q=u} = 1^+ e^{-u\tau}(1 + ke^{-2a\tau})/N, \quad (\text{C4b})$$

$$f_+(s, q, -\hat{a}, \hat{u}) = \frac{1}{2\tau L} \{ (k + e^{-2u\tau})[1^-(r^+ + \sigma^- + \tau^-)e^{q\tau} + 1^+ e^{-2a\tau}(r^- + \sigma^+ + \tau^+)e^{-q\tau}] \Theta(-q) \Theta(q+a) \quad (\text{C4c})$$

$$+ (1 + ke^{-2a\tau})[1^+(r^- + \sigma^+ + \tau^+)e^{-q\tau} + 1^- e^{-2u\tau}(r^+ + \sigma^- + \tau^-)e^{q\tau}] \Theta(q) \Theta(-(q-u)) \} \\ \text{with } L = 1 - \epsilon^2, \quad (\text{C5})$$

$$f_+(s, q, -\hat{a}, \hat{u})|_{q=-a} = e^{-a\tau}(k + e^{-2u\tau})[(r^- + \sigma^+ + \tau^+) + (r^+ + \sigma^- + \tau^-)]/2\tau L, \quad (\text{C6a})$$

$$f_+(s, q, -\hat{a}, \hat{u})|_{q=u} = e^{-u\tau}(1 + ke^{-2a\tau})[(r^- + \sigma^+ + \tau^+) + (r^+ + \sigma^- + \tau^-)]/2\tau L. \quad (\text{C6b})$$

For a symmetric source and two reflecting boundaries at  $q = \pm a$

$$f_R(s, q, -\hat{a}, \hat{a}) = \frac{(1+k)}{4\tau(1 - e^{-2a\tau})} [(r^- + \sigma^+ + \tau^+)e^{-q\tau} + e^{-2a\tau}(r^+ + \sigma^- + \tau^-)e^{q\tau}] \Theta(q) \Theta(-(q-a)), \quad (\text{C7})$$

$$f(s, q, -\hat{a}, \hat{a})|_{q=\pm a} = (1+k)e^{-a\tau}[(r^- + \sigma^+ + \tau^+) + (r^+ + \sigma^- + \tau^-)]/4\tau(1 - e^{-2a\tau}). \quad (\text{C8})$$

As in (39a) the original can be expressed only by a convolution integral:

$$\int_0^t dt' \mathcal{L}(t-t', q, -\hat{a}, \hat{a})|_{q=\pm a} \{ \delta(t') - e^{-r't'} \Theta(t') [\delta(t'-q) + (r^2 q / \theta') I_1(\theta') \Theta(t'-q)]|_{q=2a} \} \\ = e^{-r't} \Theta(t) \{ \delta(t-q) + r [I_0(\theta) + (rt/\theta) I_1(\theta)] \Theta(t-q) \}|_{q=a} \quad (\text{C9a})$$

or in other terms

$$\int_0^t dt' \mathcal{L}(t-t', q, -\hat{a}, \hat{a})|_{q=\pm a} [\delta(t') - \mathcal{B}(t', 2a)] = \left[ \frac{\partial}{\partial t} + 2r \right] [e^{-r't} \Theta(t) I_0(\theta) \Theta(t-q)]|_{q=a}. \quad (\text{C9b})$$

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- [9] The difference PCC minus NCC is the (net) current  $\mathbf{j}_+(t, q) = [\mathcal{L}_+^\dagger(t, q) - \mathcal{L}_+^-(t, q)] \mathbf{e}$  ( $\mathbf{e}$  denotes the unit vector in the positive  $q$  direction) that satisfies the consistency equation  $\partial \mathcal{L}_+^\dagger(t, q) / \partial q + (2r + \partial / \partial t) \mathcal{L}_+^\dagger(t, q) = \mathbf{0}$  and the continuity equation. Solving this set of coupled equations for  $\mathcal{L}_+^\dagger(t, q)$  gives (1).
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- [11] The DF's after unit point sources oriented in opposite directions, leaving the boundary coordinates unaltered,

can be obtained one from another by changing the superscripts, the sign of  $q$ , and by interchanging  $a$  with  $u$ . The rule applies for boundaries with equal boundary conditions, e.g., for  $\mathcal{L}_+(t, q, -a, u)$  and  $\mathcal{L}_-(t, q, -a, u)$ ; different boundary conditions must switch the side together with the reversal of the source direction, e.g.,  $\mathcal{L}_+(t, q, -a, \hat{u})$  and  $\mathcal{L}_-(t, q, -\hat{a}, u)$ . This rule allows the construction of DF's  $\mathcal{L}(t, q)$  (without  $\pm$  subscript) subsequent to symmetric unit sources.

- [12] One can speak of FPTDF's—in the proper sense of the word—only in connection with absorbing boundaries; for reflecting boundaries this expression would be incorrect as the particle may rebound repetitively off the reflecting boundary. Therefore we use the expression BV's, whenever reflecting boundaries are involved, as it is pertinent in both cases.
- [13] As this setting leads to the equivalence of (42) and (45) it answers, at least in 1D space, the question in [5] about the “correct physics for diffusion with forward-scattering effects included.”
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