Diffusion through Permeable Interfaces: Fundamental Equations and their Application to First-Passage and Local Time Statistics - Supplemental Material

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SOLUTION OF THE MASTER EQUATION

Here we provide the solution to the Master equation, Eq. (1) of the main text. The solution follows the methodology of the defect technique [1], where one uses the free propagator of the defect-free Master equation, $\Psi_{m,n}(t)$, that is the solution for $\Delta = 0$ and $\Psi_{m,n}(0) = \delta_{m,n}$, to build the full solution of Eq. (1).

The defect technique allows one to obtain the formal relation between $\widetilde{\mathcal{P}}_m(\epsilon)$ and $\widetilde{\mathcal{P}}_r(\epsilon)$ and $\widetilde{\mathcal{P}}_{r+1}(\epsilon)$ ($\widetilde{f}(\epsilon) = \int_0^t f(t)e^{-\epsilon t}dt$ for any time-dependent function $f(t)$ with ϵ the Laplace variable) as follows,

$$\widetilde{\mathcal{P}}_{m,n}(\epsilon) = \widetilde{\Psi}_{m,n}(\epsilon) - \Delta[\widetilde{\mathcal{P}}_{r+1,n}(\epsilon) - \widetilde{\mathcal{P}}_{r,n}(\epsilon)][\widetilde{\Psi}_{m,r}(\epsilon) - \widetilde{\Psi}_{m,r+1}(\epsilon)], \tag{S1}$$

where we have used the notation $\widetilde{\mathcal{P}}_{m,n}(\epsilon)$ to indicate the initial condition $\mathcal{P}_{m,n}(0) = \delta_{m,n}$. By simply setting $m = r$ and $m = r + 1$ in Eq. (S1) we have a set of simultaneous equations that solve for $\widetilde{\mathcal{P}}_{r,m}(\epsilon)$ and $\widetilde{\mathcal{P}}_{r+1,m}(\epsilon)$. Solving for these and substituting back into Eq. (S1), we get the solution of Eq. (1) of the main text,

$$\widetilde{\mathcal{P}}_m(\epsilon) = \widetilde{\Psi}_{m-n}(\epsilon) - [\widetilde{\Psi}_{m-r}(\epsilon) - \widetilde{\Psi}_{m-r-1}(\epsilon)]\frac{\widetilde{\Psi}_{r+1-n}(\epsilon) - \widetilde{\Psi}_{r-n}(\epsilon)}{\frac{1}{\Delta} + \widetilde{\Psi}_1(\epsilon) - 2\widetilde{\Psi}_0(\epsilon) + \widetilde{\Psi}_{-1}(\epsilon)}, \tag{S2}$$

where we have used the translational invariance of the propagator, $\Psi_{m,n}(t) = \Psi_{m-n}(t)$. Using the form of the free propagator, $\widetilde{\Psi}_l(\epsilon) = e^{-\xi|l|}/(2F\sinh\xi)$, where $\cosh(\xi) = 1 + \epsilon/(2F)$ [2], and substituting into Eq. (S2), we find

$$\widetilde{\mathcal{P}}_{m,n}(\epsilon) = \frac{e^{-\xi|m-n|}}{2F\sinh(\xi)} + \frac{\Delta\left(e^{\xi}+1\right)\left(e^{\xi|m-r|} - e^{\xi|m-r-1|}\right)\left(e^{\xi|r-n|} - e^{\xi|r+1-n|}\right)e^{-\xi(|m-r|+|m-r-1|+|r-n|+|r+1-n|)}}{4F\left(Fe^{\xi} + F - 2\Delta\right)\sinh^2(\xi)}. \tag{S3}$$

Let us now take the continuum limit of Eq. (S3): with the lattice spacing $\alpha \to 0$, we let m, n, r, f, F become infinitely large such that $m\alpha \to x$, $n\alpha \to x_0$, $r\alpha \to x_b$, $f\alpha \to \kappa$, $F\alpha^2 \to D$ and $\mathcal{P}_m(t)/\alpha \to P(x,t)$. In this limit we have $F \to \infty$, thus $\xi \to \sqrt{\epsilon/F}$ and $\sinh(\xi) \to \sqrt{\epsilon/F}$, so we find

$$\widetilde{P}(x,\epsilon|x_0) = \begin{cases} \dfrac{1}{2}\left(\dfrac{e^{-|x-x_0|\sqrt{\epsilon/D}}}{\sqrt{D\epsilon}} + \dfrac{e^{-|x+x_0-2x_b|\sqrt{\epsilon/D}}}{\sqrt{D\epsilon}+2\kappa}\right), \ x, x_0 > x_b \text{ or } x, x_0 < x_b, \\[2ex] \dfrac{\kappa e^{-|x-x_0|\sqrt{\epsilon/D}}}{2\kappa\sqrt{D\epsilon} + D\epsilon}, \ x_0 < x_b < x \text{ or } x_0 > x_b > x. \end{cases} \tag{S4}$$

The inverse Laplace transforms are found to be [3],

$$P(x,t|x_0) = \begin{cases} \dfrac{e^{\frac{-(x+x_0-2x_b)^2}{4Dt}} + e^{\frac{-(x-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}} - \dfrac{\kappa}{D}e^{2\kappa(|x+x_0-2x_b|+2\kappa t)/D}\operatorname{erfc}\left(\frac{|x+x_0-2x_b|+4\kappa t}{2\sqrt{Dt}}\right), \ x, x_0 > x_b \text{ or } x, x_0 < x_b, \\[2ex] \dfrac{\kappa}{D}e^{2\kappa(|x-x_0|+2\kappa t)/D}\operatorname{erfc}\left(\frac{|x-x_0|+4\kappa t}{2\sqrt{Dt}}\right), \ x_0 < x_b < x \text{ or } x_0 > x_b > x. \end{cases} \tag{S5}$$

It is a straightforward exercise to verify that Eq. (S5) solves the diffusion equation with the permeable boundary condition, Eq. (2) of the main text, and the localized initial condition [4–6].

SOLUTION OF THE INHOMOGENEOUS DIFFUSION EQUATION

Using the free propagator of the diffusion equation, $G_0(x,t|x_0)$, we may write the solution to the inhomogeneous diffusion equation, displayed in Eq. (3) of the main text, as

$$P(x,t)=\int_{-\infty}^{\infty}dyG_0(x,t|y)P(y,0)+\frac{D}{\kappa}\int_0^t ds\int_{-\infty}^{\infty}dyG_0(x,t-s|y)\delta'(y-x_b)J(x_b,s). \tag{S6}$$

After Laplace transforming, and using the fact $\int_{-\infty}^{\infty}dx\delta'(x)h(x)=-\int_{-\infty}^{\infty}dx\delta(x)h'(x)$ (for some generic function $h(x)$), for $P(x,0)=\delta(x-x_0)$ we have

$$\widetilde{P}(x,\epsilon|x_0)=\widetilde{G}_0(x,\epsilon|x_0)-\frac{D}{\kappa}\partial_{x_0}\widetilde{G}_0(x,\epsilon|x_b)\widetilde{J}(x_b,\epsilon|x_0), \tag{S7}$$

where $\partial_x h(y)=\frac{\partial}{\partial x}h(x)|_{x=y}$, for a generic function $h(x)$. Through differentiating Eq. (S7) with respect to x and setting $x=x_b$, we find the relation

$$\widetilde{J}(x_b,\epsilon|x_0)=\frac{\widetilde{J}_0(x_b,\epsilon|x_0)}{1+\frac{D}{\kappa}\partial_{x_0}\widetilde{J}_0(x_b,\epsilon|x_b)}. \tag{S8}$$

After substituting Eq. (S8) back into Eq. (S7), we obtain the solution $\widetilde{P}(x,\epsilon|x_0)$, presented in Eq. (4) of the main text. To obtain the solutions for the survival probability, Eq. (10) of the main text, and for the local time distribution, Eq. (16) of the main text, one follows a similar procedure.

RADIATION BOUNDARY

Here we show how by placing a perfectly absorbing boundary at the same location as a permeable barrier one recovers a radiation boundary [7–10]. We show this in the free diffusive case. A radiation boundary describes the phenomena of an incident particle being absorbed or reflected, controlled by the parameter λ (dimensions of velocity), such that the condition is written as

$$J(x_b,t|x_0)=\pm\lambda P(x_b,t|x_0), \tag{S9}$$

with the $+$ and $-$ sign correseponding to $x_0<x_b$ and $x_0>x_b$, respectively. Using, $G_0(x,t|x_0)$, we satisfy an absorbing boundary, through the method of images, by writing $G(x,t|x_0)=G_0(x,t|x_0)-G_0(x,t|2x_b-x_0)$. Substituting this expression into Eq. (4) of the main text, we obtain the solution,

$$\widetilde{P}(x,\epsilon|x_0)=\frac{e^{-|x-x_0|\sqrt{\frac{\epsilon}{D}}}}{2\sqrt{D\epsilon}}+\frac{e^{-|x+x_0-2x_b|\sqrt{\frac{\epsilon}{D}}}(\sqrt{D\epsilon}-\kappa)}{2\sqrt{D\epsilon}(\sqrt{D\epsilon}+\kappa)}, \tag{S10}$$

whose inverse Laplace transform is given by [3],

$$P(x,t|x_0)=\frac{e^{\frac{-(x+x_0-2x_b)^2}{4Dt}}+e^{\frac{-(x-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}}-\frac{\kappa}{D}e^{\kappa(|x+x_0-2x_b|+\kappa t)/D}\,\mathrm{erfc}\left(\frac{|x+x_0-2x_b|+2\kappa t}{2\sqrt{Dt}}\right). \tag{S11}$$

Upon insertion into Eq. (S9), Eq. (S11) satisfies the radiation boundary condition when $\lambda=\kappa$. Eq. (S11) coincides with the solution found via other methods in Refs. [11, 12].

FIRST-PASSAGE PROBABILITY DISTRIBUTION

Here we present the first-passage probability distribution to x_c for a Brownian particle in the presence of a permeable interface at x_b, where $x_c>x_0>x_b$ or $x_b>x_0>x_c$. Using Eq. (10) of the main text we find,

$$\widetilde{\mathcal{F}}(x_c,\epsilon|x_0)=\frac{\left[\sqrt{D\epsilon}+2\kappa\right]e^{-|x_c-x_0|\sqrt{\frac{\epsilon}{D}}}+\sqrt{D\epsilon}e^{-|x_c+x_0-2x_b|\sqrt{\frac{\epsilon}{D}}}}{\sqrt{D\epsilon}\left[1+e^{-2|x_c-x_b|\sqrt{\frac{\epsilon}{D}}}\right]+2\kappa}. \tag{S12}$$

Eq. (S12) has the same asymptotic form as the barrier free case, $\mathcal{F}(x_c,t|x_0) \approx |x_c - x_0|/\sqrt{4\pi D t^3}$, showing that for long times the presence of a permeable interface has no impact on the FPP probability when it is not between x_0 and x_c. Note that Eq. (11) of the main text and Eq. (S12) can also be obtained by using Eq. (S4) in the renewal relation,

$$\widetilde{\mathcal{F}}(x_c,\epsilon|x_0) = \frac{\widetilde{P}(x_c,\epsilon|x_0)}{\widetilde{P}(x_c,\epsilon|x_c)}. \tag{S13}$$

MEAN FIRST-PASSAGE TIME

We start from the ordinary differential equation for the MFPT, $\tau(x_0)$, Eq. (13) in the main text, where we consider $x_r < x_b < x_c$. Due to the appearance of the derivative of the Dirac delta function we solve for when $x_0 \neq x_b$,

$$\tau(x_0) = \begin{cases} -\dfrac{x_0^2}{2D} + c_1 x_0 + c_2, \;\; x_r \leq x_0 < x_b, \\ -\dfrac{x_0^2}{2D} + c_3 x_0 + c_4, \;\; x_b < x_0 \leq x_c, \end{cases} \tag{S14}$$

where the constants, c_1, c_2, c_3, c_4 are to be determined. Using the boundary conditions, $\tau(x_c) = \tau'(x_r) = 0$, we find $c_1 = x_r/D$ and $c_4 = x_c^2/2D - c_3 x_c$. To determine the other two constants we must find two more conditions on the solution. By integrating over the inhomogeneity in Eq. (13)

$$\lim_{\varepsilon\to 0}\int_{x_b-\varepsilon}^{x_b+\varepsilon} dx_0 \left[\tau''(x_0) - \frac{D}{\kappa}\delta'(x_0 - x_b)\tau'(x_b) + \frac{1}{D}\right] = 0, \tag{S15}$$

we find $\tau'(x_b^+) = \tau'(x_b^-)$, since $\int_{x_b-\varepsilon}^{x_b+\varepsilon} dx_0 \delta'(x_0 - x_b) = 0$. Then a double integration over the inhomogeneity,

$$\lim_{\varepsilon\to 0}\int_{x_b-\varepsilon}^{x_b+\varepsilon} dx_0 \int dx_0 \left[\tau''(x_0) - \frac{D}{\kappa}\delta'(x_0 - x_b)\tau'(x_b) + \frac{1}{D}\right] = 0, \tag{S16}$$

leads to the condition $\tau(x_b^+) - \tau(x_b^-) = D\tau'(x_b)/\kappa$. By using Eq. (S14) to satisfy these two conditions, we find the remaining two constants to be $c_3 = x_r/D$ and $c_2 = (x_c^2 - 2x_r x_c)/2D + (x_b - x_r)/\kappa$. Performing the same procedure as above but for $x_c < x_b < x_r$, we obtain Eq. (14) of the main text.

Note the same expression for $\tau(x_0)$ can be obtained by finding the first-passage probability distribution to x_c when there is a permeable interface at x_b and a reflecting boundary at x_r, $\mathcal{F}_{x_r}(x_c,t|x_0)$. $\widetilde{\mathcal{F}}_{x_r}(x_c,\epsilon|x_0)$ is found by using Eq. (S13) where $\widetilde{P}(x,\epsilon|x_0)$ is found via Eq. (4) in the main text, except by replacing $\widetilde{G}_0(x,\epsilon|x_0)$ by $\widetilde{G}_0(x,\epsilon|x_0) + \widetilde{G}_0(x,\epsilon|2x_r - x_0)$. Then $\tau(x_0)$ is found by,

$$\tau(x_0) = -\lim_{\epsilon\to 0}\frac{\partial}{\partial\epsilon}\widetilde{\mathcal{F}}_{x_r}(x_c,\epsilon|x_0). \tag{S17}$$

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