

Partial Absorption and “Virtual” Traps

E. Ben-Naim,¹ S. Redner,¹ and G. H. Weiss²

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The spatial probability distribution associated with diffusion and attenuation in partially absorbing media is studied. An equivalence is established between a system with free diffusion for $x > 0$ and partial absorption for $x < 0$, and a semi-infinite system ($x > 0$) with a radiation boundary condition at $x = 0$. By exploiting this equivalence, it is shown that the effect of a partially absorbing medium in the long-time limit is equivalent to that of a perfect, “virtual” trap whose size is smaller than the original absorbing medium. For short times, however, there is substantial penetration of diffusing particles into the absorber. The virtual trap approach is readily generalized to higher dimensions. This allows one to obtain the density profile of diffusing particles around a partially absorbing spherical trap. An unusual crossover between short-time penetration and long-time trapping occurs in two dimensions; the size of the virtual trap is exponentially small in the case of weak absorption, corresponding to an absorption time which is exponentially large.

KEY WORDS: Partial absorption; virtual trap; radiation boundary condition.

1. INTRODUCTION

The physical basis of Brownian motion in translationally invariant media is well understood, and models based on this type of transport have been applied to the interpretation of an enormous variety of physical phenomena. There is likewise a large literature on Brownian motion in the presence of absorbing boundaries. Perfectly absorbing boundaries are known to change the properties of Brownian motion in ways that are largely understood. However, for many practical applications, the trapping medium is *partially absorbing*, as in the attenuation and multiple scattering

¹ Center for Polymer Studies and Department of Physics, Boston University, Boston, Massachusetts 02215.

² PSL, DCRT, National Institutes of Health, Bethesda, Maryland 20205.

of light in biological media, in heat conduction processes, and in colloidal suspensions. For example, recent studies of photon migration in a turbid medium suggest the validity of Brownian motion as the description of photon transport, as well as Beer's law of absorption.^(1,2) The analysis of scattered laser light in biological tissue suggests, for example, the importance of determining the maximum penetration depth of a Brownian particle in a partially absorbing medium. Another useful parameter for interpreting experimental data is the time required for a diffusing particle to reach an absorbing surface at a given distance from the interface of the laser beam into the sample. Some aspects of this problem have been addressed for models in which the sample is a semi-infinite, partially absorbing medium.⁽¹⁻⁴⁾

These situations motivate us to consider a theoretical analysis of the penetration of a Brownian particle in absorbing media. We are interested in developing a quantitative approach to describe how the probability distribution of the diffusing particles is influenced by partial absorption. For a one-dimensional composite that consists of an absorbing medium for $x < 0$ and a nonabsorbing medium for $x > 0$, we will show that a continuum description can be given either by separate equations for the two media, or by a diffusion equation in the nonabsorbing medium with a radiation boundary condition at the interface. As a consequence, we will show that the concentration of particles inside the partially absorbing medium decays rather modestly in time, as $t^{-1/2}$, leading to a concentration at the interface which also decays as $t^{-1/2}$. The equivalence between the two descriptions is the basis for a physical construction in which a partially absorbing medium can be replaced by an equivalent perfectly absorbing medium of a smaller spatial extent, that is, a perfect "virtual" trap. This analogy can be easily extended to higher dimensions, both for steady-state and time-dependent problems, and provides a simple way to quantify the effects of partial absorption.

In Section 2 we first determine the probability distribution for a one-dimensional composite system, which is described by a diffusion equation for $x > 0$ and a diffusion-absorption equation for $x < 0$. These results are exploited to obtain the time dependence of the maximal penetration of particles into the absorbing medium. In Section 3 we show that for sufficiently weak absorption, an intermediate-time regime exists, where the distance of the closest particle to the absorbing medium grows as $t^{1/2}$, before the asymptotic $t^{1/4}$ growth sets in. An equivalence between the solution of the composite system and that for diffusion in the half-space $x > 0$ with a radiation boundary condition at $x = 0$ is derived in Section 4. This result is the basis for the correspondence between the partially absorbing medium in the range $x \leq 0$ and a virtual perfect trap located at a position $r_T < 0$. In

Section 5 this virtual trap correspondence is extended to higher dimensions for both steady-state and time-dependent situations. As the strength of the partially absorbing trap decreases, the radius of the virtual trap vanishes, with a dependence that is strongly dimension dependent. Furthermore, in two dimensions there is an exponentially long time regime of negligible absorption before the virtual trap "turns on," in the limit of weak trapping.

2. DIFFUSION-ABSORPTION EQUATION

Consider a one-dimensional medium which is partially absorbing for $x < 0$, with a finite absorption rate q , and nonabsorbing for $x > 0$ (Fig. 1). The time evolution of the density outside the absorber obeys the diffusion equation, while the density inside obeys a diffusion-absorption equation:

$$\begin{aligned} \frac{\partial c(x, t)}{\partial t} &= D \frac{\partial^2 c(x, t)}{\partial x^2} - qc(x, t), & x < 0 \\ \frac{\partial c(x, t)}{\partial t} &= D \frac{\partial^2 c(x, t)}{\partial x^2}, & x > 0 \end{aligned} \tag{1}$$

where D is the diffusion coefficient. At the origin, the concentration and the flux ($-D \partial c / \partial x$) must be continuous. Once the initial condition is specified, one can then solve for basic quantities, such as the concentration at the interface, and the total number of particles inside the absorber, $S_-(t) = \int_{-\infty}^0 c(x, t) dx$. This latter quantity is obtained by spatial integration of the first line of Eq. (1) to yield

$$\frac{\partial S_-(t)}{\partial t} = D \left. \frac{\partial c(x, t)}{\partial x} \right|_{x=0} - qS_-(t) \tag{2}$$

This reflects the decrease in $S_-(t)$ because of absorption, and its increase because of flux entering at $x = 0$. We now present the solution to Eq. (1) for two simple initial conditions, although the analysis can be carried out for an arbitrary initial condition.

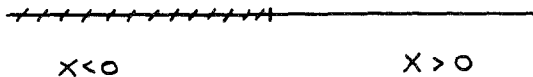


Fig. 1. The basic geometry in one dimension in which the region $x < 0$ absorbs at a rate q .

2.1. Uniform Initial Density for $x > 0$

For $c(x, t = 0) = c_0 H(x)$, with $H(x)$ the Heaviside step function, we first introduce the Laplace transform, $c(x, s) = \int_0^\infty c(x, t) \exp(-st) dt$, to reduce Eq. (1) to the ordinary differential equations

$$\begin{aligned} D \frac{\partial^2 c(x, s)}{\partial x^2} - (s + q) c(x, s) &= 0, & x < 0 \\ D \frac{\partial^2 c(x, s)}{\partial x^2} - s c(x, s) &= -c_0, & x > 0 \end{aligned} \quad (3)$$

subject to continuity of both $c(x, s)$ and its spatial derivative at the origin. The solution in Laplace space is

$$c(x, s) = \begin{cases} \frac{c_0}{s} \left\{ \frac{1}{1 + \alpha(s)} \exp \left[x \left(\frac{s + q}{D} \right)^{1/2} \right] \right\}, & x < 0 \\ \frac{c_0}{s} \left\{ 1 - \frac{1}{1 + \alpha^{-1}(s)} \exp \left[-x \left(\frac{s}{D} \right)^{1/2} \right] \right\}, & x > 0 \end{cases} \quad (4)$$

where $\alpha(s) = [(s + q)/s]^{1/2}$.

We are primarily interested in extracting quantities which characterize the penetration of particles into the absorber, such as the concentration at the interface, $c(x = 0, s) = c_0/s[1 + \alpha(s)]$, and the number of particles inside the absorber $S_-(s) = c_0[D/(s + q)]^{1/2}/s[1 + \alpha(s)]$. Inverting the above Laplace transforms yields the behavior of these two quantities in the time domain,⁽⁵⁾

$$c(x = 0, t) = \frac{c_0}{2} \left[I_0 \left(\frac{t}{2t_q} \right) + I_1 \left(\frac{t}{2t_q} \right) \right] \exp \left(-\frac{t}{2t_q} \right) \quad (5)$$

$$S_-(t) = c_0 l_q \left(\frac{1}{\pi t/t_q} \right)^{1/2} \left[1 - \exp \left(-\frac{t}{t_q} \right) \right] \quad (6)$$

where $I_n(x)$ is the n th-order modified Bessel function. Here we have introduced dimensionless variables by introducing the characteristic absorption time and the typical distance that a particle travels in the absorber before absorption

$$t_q = 1/q \quad \text{and} \quad l_q = (D/q)^{1/2} [= (Dt_q)^{1/2}] \quad (7)$$

Interestingly, the concentration at the origin is independent of D . In contrast, the behavior of $S_-(t)$ does depend on D , since the flux entering the absorber at a fixed time depends on D .

For short times, $t \ll t_q$, absorption is negligible, and one recovers purely diffusive behavior, namely $S_-(t) \sim c_0(Dt/\pi)^{1/2}$ and $c(x, t) \cong c_0/2$. In this "diffusion-controlled" time regime, therefore, the absorption term in the diffusion-absorption equation can be neglected. In the long-time limit, we use⁽⁵⁾

$$I_n(z) \cong \frac{e^z}{(2\pi z)^{1/2}} \left(1 - \frac{n-1}{8z} + \dots \right), \quad z \gg 1 \tag{8}$$

to obtain

$$c(x=0, t) \sim \frac{c_0}{(\pi t/t_q)^{1/2}}, \quad t \gg t_q \tag{9}$$

Comparison with Eq. (6) shows that the concentration at the origin and the number of particles inside the absorber are proportional to each other in the long-time limit,

$$c(x=0, t) \sim \frac{1}{l_q} S_-(t), \quad t \gg t_q \tag{10}$$

Since $S_-(t) \sim t^{-1/2}$, the time derivative will be a subdominant contribution in Eq. (2). Neglecting this term and using Eq. (6) gives

$$D \frac{\partial c(x, t)}{\partial x} \Big|_{x=0} \sim q S_-(t) \sim \frac{Dc_0}{(\pi Dt)^{1/2}} \tag{11}$$

i.e., the flux is the same as that entering a perfect trap. There also is a depletion zone (the extent over which the concentration is spatially varying) which is of the order of $(Dt)^{1/2}$. In the long-time regime, therefore, the solution to Eq. (1) is essentially determined by the absorption term, since the time derivative in the diffusion-absorption equation is negligible. Thus the solution can be characterized as being "absorption controlled."

A useful way to characterize the penetration of particles into the absorber is to monitor the time dependence of the average position of the particles which are in the absorbing medium, $\langle l(t) \rangle \equiv -\int_{-\infty}^0 xc(x, t) dx/S_-(t)$. From the first line of Eq. (4), the Laplace transform of the numerator of $\langle l(t) \rangle$ is $Dc_0/s(s+q)[1+\alpha(s)]$. Laplace inversion gives

$$S_-(t)\langle l(t) \rangle = c_0 l_q^2 [I_0(t/2t_q) \exp(-t/2t_q) - \exp(-t/t_q)] \tag{12}$$

The penetration depth thus has the asymptotic behaviors

$$\langle l(t) \rangle \cong \begin{cases} (\pi Dt)^{1/2}, & t \ll t_q \\ l_q, & t \gg t_q \end{cases} \tag{13}$$

The short-time behavior merely recovers the behavior of freely diffusing particles. On the other hand, the long-time behavior can be understood in a simple way by applying a quasistatic approximation to the diffusion-absorption equation. This involves neglecting the time derivative term in this equation, and then solving subject to the time-dependent boundary condition $c(0, t) = c_0(t_q/\pi t)^{1/2}$ [Eq. (9)]. Inside the absorber, this yields

$$c(x, t) \sim \frac{c_0}{(\pi t/t_q)^{1/2}} \exp\left(\frac{x}{l_q}\right), \quad x < 0 \quad (14)$$

which immediately gives the above long-time behavior of $\langle l(t) \rangle$.

2.2. Single-Particle Initial Condition

For the complementary problem where one particle is initially at the origin, $c(x, t=0) = \delta(x)$, the solution to Eq. (1) in Laplace space is

$$c(x, s) = \begin{cases} \frac{1}{(Ds)^{1/2}} \frac{1}{1 + \alpha(s)} \exp\left[x \left(\frac{s+q}{D}\right)^{1/2}\right], & x < 0 \\ \frac{1}{(Ds)^{1/2}} \frac{1}{1 + \alpha(s)} \exp\left[-x \left(\frac{s}{D}\right)^{1/2}\right], & x > 0 \end{cases} \quad (15)$$

Thus the survival probability, $S(t) = \int_{-\infty}^{\infty} c(x, t) dx$, equals

$$S(t) = I_0(t/2t_q) \exp(-t/2t_q) \sim (t_q/\pi t)^{1/2}, \quad t/t_q \rightarrow \infty \quad (16)$$

while the survival probability in the absorbing medium is

$$S_-(t) = \frac{1}{2}[I_0(t/2t_q) - I_1(t/2t_q)] \exp(-t/2t_q) \\ \sim [1/(2\sqrt{\pi})](t_q/t)^{3/2}, \quad t/t_q \rightarrow \infty \quad (17)$$

These quantities are independent of the diffusion coefficient, in contrast to the corresponding behavior for the uniform initial condition. By applying standard Bessel function identities, it follows that $\dot{S}(t) = -qS_-(t)$, i.e., the loss of particles is simply related to the concentration in the absorbing medium, as required by integration of Eq. (1) over all space. Similarly, the density at the origin is

$$c(x=0, t) = \frac{t_q}{(4\pi Dt^3)^{1/2}} \left[1 - \exp\left(-\frac{t}{t_q}\right) \right] \quad (18)$$

For short times, this density is diffusion controlled [$\sim (4\pi Dt)^{-1/2}$], while for later times $c(0, t)$ approaches the value $S_-(t)/l_q$. Other properties such

as the concentration profile inside the absorber and the average penetration are similar to those obtained in the many-particle case.

Analogous results can be obtained within a discrete random walk formulation, where absorption is described by a random walk which is annihilated with probability $0 \leq p \leq 1$ when it lands on an absorbing site. The dominant contribution to the survival probability at the n th step arises from walks which remain in the region $x > 0$ up to this time, and the latter have a probability which is proportional to $n^{-1/2}$. Similarly, the survival probability inside the absorber is dominated by walks which enter the absorbing region for the first time at the n th step, which have a probability proportional to $\sim n^{-3/2}$. Formally, the full probability distribution in the composite can be found in terms of $P_n(x, r)$, the probability that an n -step random walk at position x has visited the region $x < 0$ exactly r times.^(6,7)

3. THE NEAREST-NEIGHBOR DISTANCE

One useful way to quantify the distribution of diffusing particles near a trap is through the position of the nearest particle to the trap, x_m ,⁽⁸⁻¹¹⁾ which may be defined by

$$\int_0^{x_m} c(x, t) dx = 1$$

In one dimension with a perfect absorber at the origin, $x_m \propto (Dt/c_0^2)^{1/4}$. For a sufficiently weak trap, however, we shall demonstrate that there is an intermediate-time regime where the closest distance grows as $t^{1/2}$.

From our previous results for the concentration at the origin and its first derivative, the behavior of the concentration near the origin is

$$c(x, t) \sim \frac{c_0}{(\pi t/t_q)^{1/2}} + \frac{c_0}{(\pi Dt)^{1/2}} x, \quad t \gg t_q \quad (19)$$

Using this form for the concentration, we obtain for x_m

$$x_m \cong l_q \{ [1 + 2(\pi t/t_0)^{1/2}]^{1/2} - 1 \} \quad (20)$$

with $t_0 = Dc_0^2/q^2$. Equation (20) is valid for $t \gg t_q = 1/q$, and thus $\theta = t_0/t_q = Dc_0^2/q$, which is a dimensionless measure of the strength of the absorber, is a relevant parameter. For a sufficiently weak absorber, $\theta \gg 1$, and the limiting behaviors of Eq. (20) are

$$x_m \sim \begin{cases} (\pi t/t_q c_0^2)^{1/2}, & t_q \ll t \ll t_0 \\ (4\pi Dt/c_0^2)^{1/4}, & t_0 \ll t \end{cases} \quad (21)$$

The different limiting behaviors arise from the two terms in Eq. (19); the constant term dominates at early times, while the linear term dominates at later times. Note that the intermediate-time behavior depends on the absorption rate, while the long-time behavior depends essentially on the diffusion coefficient. For $\theta < 1$, there is no intermediate-time regime, and the asymptotic behavior of a perfect trap is recovered. The physical meaning of t_0 can be seen from the expression for the total number of particles in the absorber [Eq. (6)]. Namely, for $t \gg t_q$, $S_-(t) \sim (t/\pi t_0)^{1/2}$, so that t_0 gives the time at which the total number of particles in the absorber falls below unity.

4. EQUIVALENCE TO THE RADIATION BOUNDARY CONDITION

We now establish an equivalence between the partially absorbing one-dimensional composite and the free medium for $x > 0$ with a radiation boundary condition at $x = 0$. Such a boundary condition arises naturally in heat conduction between two media when the heat transfer is proportional to the temperature difference. As we shall see, this equivalence provides a useful tool for describing the physical manifestations of the partially absorbing medium.

Combining Eqs. (10) and (11), which are valid at long times, immediately gives the radiation boundary condition⁽¹²⁾

$$D \left. \frac{\partial c(x, t)}{\partial x} \right|_{x=0} = (Dq)^{1/2} c(x, t) \Big|_{x=0} \quad (22)$$

Equation (22) reduces to an absorbing boundary condition for $q = \infty$ and to a reflecting boundary condition for $q = 0$. However, for $q = 0$, the long-time limit $t \gg t_q$ is never reached, and Eq. (22) does not hold for this case.

To appreciate the consequences of the above equivalence, we solve the diffusion equation

$$\frac{\partial c(x, t)}{\partial t} = D \frac{\partial^2 c(x, t)}{\partial x^2}, \quad x > 0 \quad (23)$$

with the radiation boundary condition of Eq. (22) and the initial condition $c(x, t=0) = c_0 H(x)$. In Laplace space, the solution is

$$c(x, s) = \frac{c_0}{s} \left\{ 1 - \frac{1}{1 + \beta(s)} \exp \left[- \left(\frac{s}{D} \right)^{1/2} x \right] \right\} \quad (24)$$

where $\beta(s) = (st_q)^{1/2}$, while the solution in the time domain is

$$c(x, t) = c_0 \operatorname{erf} \left(\frac{x}{(4Dt)^{1/2}} \right) + c_0 \left[\exp \left(\frac{x}{l_q} + \frac{t}{t_q} \right) \operatorname{erfc} \left(\frac{x}{(4Dt)^{1/2}} + \left(\frac{t}{t_q} \right)^{1/2} \right) \right] \quad (25)$$

with the notations of Eq. (7). In the long-time limit, the behavior given by the solution to the diffusion-absorption equation is recovered. For example, the concentration at the interface is

$$c(x=0, t) = c_0 \operatorname{erfc}((t/t_q)^{1/2}) \exp(t/t_q) \sim c_0 (t_q/\pi t)^{1/2}, \quad t \gg t_q \quad (26)$$

Similarly, the intermediate-time behavior for the distance of the nearest particle from the interface varies as $t^{1/2}$, provided that the trap is sufficiently weak ($\theta \gg 1$).

An essential aspect of the radiation boundary condition is that it provides, in conjunction with the image method, an alternative and useful way to quantify the effect of a partially absorbing medium. For the radiation boundary condition, the concentration profile given in Eq. (24), when evaluated at $t=0$ and for $x < 0$, leads to an initial distribution of "image" concentration

$$c_I(x) = c_0 [2 \exp(x/l_q) - 1], \quad x < 0 \quad (27)$$

This is a uniform distribution of antiparticles at concentration $-c_0$ and an exponentially decaying distribution of particles (Fig. 2a). The superposition of these two components gives rise to a change in sign of this initial image distribution at $x = -l_q \ln 2$. Owing to the equivalence between the solutions to the diffusion-absorption equation and to the diffusion equation with the radiation boundary condition, the effect of a partially absorbing medium is equivalent to a free medium with an initial distribution of images given in Eq. (27).

This equivalence motivates our introduction of the virtual trap, which is the position where the time-dependent concentration vanishes in the solution to the diffusion equation with the radiation boundary condition. Equating $c(r_T, t) = 0$ in Eq. (25) and keeping only the leading behavior for $t \gg t_q$ gives $r_T \sim -l_q$. Thus, the time-dependent solution to a perfect trap located at $-l_q$ provides an excellent approximation to the concentration obtained by imposing the radiation boundary condition (Fig. 2b). The position of this virtual trap is at the interface in the limit of a perfectly absorbing medium, and is infinitely far away in the no-absorption limit.

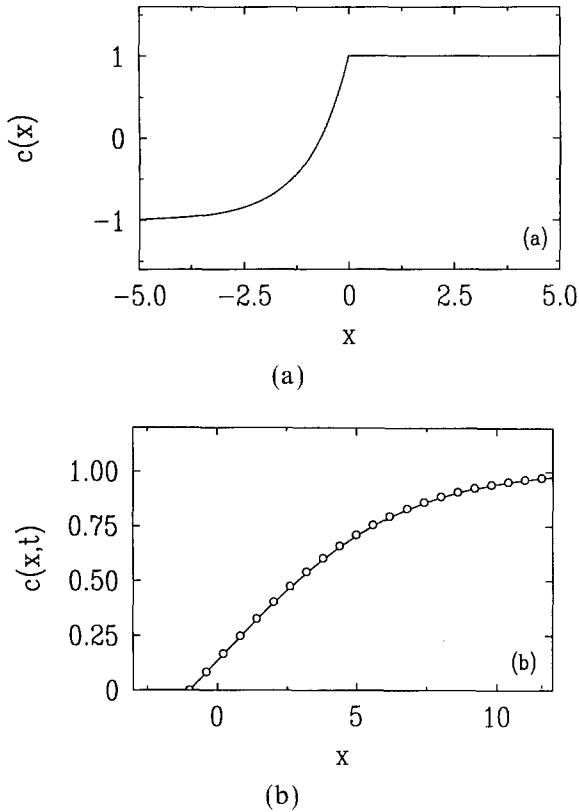


Fig. 2. Illustration of the virtual trap method. (a) For a radiation boundary condition, an initial uniform concentration of particles c_0 gives rise to an image distribution which consists of a uniform concentration c_0 of antiparticles and an exponential distribution of particles. This image distribution vanishes at $x = -l_q \ln 2$. (b) The time-dependent concentration in the case of the radiation boundary condition (solid) is well approximated by the concentration in the presence of a perfect virtual trap at $x = -l_q$, namely $c(x, t) = c_0 \operatorname{erf}((x + l_q)/(4Dt)^{1/2})$ (dots). For both plots $l_q = t_q = c_0 = 1$, and for (b) $t = 16$.

5. PARTIAL ABSORPTION IN HIGHER DIMENSIONS

The notion of a virtual trap can be readily extended to higher dimensions. In Section 5.1 we use the steady-state solution to the diffusion equation to find the location of the virtual trap for a radially symmetric geometry in arbitrary spatial dimension. An application to a time-dependent problem is presented in Section 5.2, where the virtual trap method is combined with the quasistatic approximation.

5.1. Steady-State Solution

To illustrate the utility of the virtual trap method, consider radially symmetric flow of particles (or heat) into an imperfect trap. The steady-state concentration exterior to an absorber of radius a obeys the d -dimensional Laplace equation

$$Dr^{1-d} \frac{\partial}{\partial r} r^{d-1} \frac{\partial c(r)}{\partial r} = 0, \quad r > a \quad (28)$$

with the radiation boundary condition

$$D \left. \frac{\partial c(r)}{\partial r} \right|_{r=a} = (Dq)^{1/2} c(r) |_{r=a} \quad (29)$$

This equation describes, for example, the flow of particles to the trap from a continuous source of particles at a large outer sphere (in order to reach a steady state in one and two dimensions the system must be finite in extent). We are primarily interested in the solution for $r > a$, where the density takes the following forms:

$$c(r) \propto \begin{cases} r - r_T, & r_T = a - l_q, & d = 1 \\ \ln(r/r_T), & r_T = a \exp(-l_q/a), & d = 2 \\ r_T^{-1} - r^{-1}, & r_T = a/(1 + l_q/a), & d = 3 \end{cases} \quad (30)$$

We interpret the point where the concentration vanishes as the location of the virtual trap. For $d=1$, this location agrees with the form suggested in the previous section. For strong absorption or for a very large trap, i.e., $l_q/a = (Dt_q)^{1/2}/a \ll 1$, the one-dimensional expression $r_T = a - l_q$ holds for any dimension. In the opposite limit of weak absorption, the position of the virtual trap is

$$r_T \cong \begin{cases} a \exp(-l_q/a), & d = 2 \\ a/(l_q/a), & d = 3 \end{cases} \quad l_q/a \gg 1 \quad (31)$$

Thus, as expected, the size of the virtual trap vanishes in the limit of weak absorption. The exponential behavior occurs only in two dimensions, so that there is a significant difference between the dependence of the virtual trap size on the rate q for two and three dimensions.

5.2. Time-Dependent Solution

The determination of the location of the virtual trap for transient problems is based on solving the time-dependent diffusion equation with a

perfect trap at r_T given by Eq. (30), and considering this solution for $r \geq a$. Although the exact solution to this problem is straightforward, it is much simpler to solve the problem in the quasistatic approximation to find the asymptotic behavior of the concentration. In this approximation, the time derivative in the diffusion equation is neglected and the time dependence is introduced by imposing the appropriate moving boundary conditions⁽⁹⁾

$$c(r) |_{r=(4Dt)^{1/2}} = c_0 \quad \text{and} \quad c(r) |_{r=r_T} = 0 \quad (32)$$

These conditions reflect the fact that the depletion zone width is controlled by diffusion, and outside this zone the concentration is equal to its initial value c_0 . Solving Laplace's equation within the depletion zone, $a \leq r \leq \sqrt{4Dt}$, and according to the above boundary conditions, we obtain

$$c(r, t) = \begin{cases} c_0(r - r_T)/(4Dt)^{1/2}, & d = 1 \\ c_0 \{ \ln(r/r_T) / \ln[(4Dt)^{1/2}/r_T] \}, & d = 2 \\ c_0(r_T^{-1} - r^{-1}) / [r_T^{-1} - (4Dt)^{-1/2}], & d = 3 \end{cases} \quad (33)$$

The concentration at the interface $r = a$ can now be evaluated by using the expressions for r_T from Eq. (30),

$$c(a, t) = \begin{cases} c_0(t_q/t)^{1/2}, & d = 1 \\ c_0 / \{ (a/l_q) \ln[(4Dt)^{1/2}/a] + 1 \}, & d = 2 \\ c_0 / (1 + a/l_q), & d = 3 \end{cases} \quad (34)$$

The expression for $d = 1$ differs by a factor of $\sqrt{\pi}/2$ from the exact result, a by-product of the quasistatic approximation. For three dimensions, in contrast, the concentration reaches a constant value, since a steady state is ultimately reached. The strength of the trap does not affect the time necessary to reach a steady concentration. In the marginal case of two dimensions, on the other hand, the time for the concentration to become appreciably less than the initial concentration occurs when the two terms in the denominator of Eq. (34) are comparable. We define this as the "initiation" time of the trap,

$$\tau \equiv (a^2/D) \exp(2l_q/a), \quad l_q/a \gg 1 \quad (35)$$

In the weak absorption limit, τ is exponentially long, since the virtual trap is exponentially small. Amusingly, τ can be rewritten as $t_0 = (a^2/D)(a/r_T)^2$, i.e., the initiation time equals a diffusion time multiplied by the ratio of the areas of the imperfect trap to the perfect trap. The initiation time is

relevant in calculating the nearest neighbor distance, since for $t < \tau$, the nearest neighbor distance varies roughly as $c_0^{-1/2}$, and for $t \gg \tau$, the distance grows as $(\ln t)^{1/2}$.⁽⁹⁻¹¹⁾

6. SUMMARY

We investigated the properties of diffusion in the presence of an imperfect absorber. Our primary result is that the effect of a partial absorber is equivalent to a virtual, perfect trap whose spatial extent is smaller than the partially absorbing medium. By exploiting this analogy, we found the survival probability of a diffusing particle in the presence of a semi-infinite one-dimensional absorber to decay as $\sim t^{-1/2}$, just as in the case of a perfect trap. This result follows because the survival probability is dominated by particles in the nonabsorbing region ($x > 0$) that reach the edge of the trapping region for the first time at time t . It is this observation that accounts for the success of the virtual trap analogy in reproducing the principal features of the kinetics of the system. However, in the case of weak absorption, there is an intermediate-time regime where there is substantial penetration of particles into the absorbing medium. The temporal range for which this penetration occurs can be described as the time domain before the virtual trap turns on, in the virtual trap description.

For higher dimensions, the virtual trap size tends to zero if the absorber is weak. In two dimensions, this size decays exponentially and that gives rise to an exponentially large crossover time compared with a power-law dependence in one dimension. Although we used terminology appropriate for diffusing particles, the temperature obeys the same diffusion equation and thus this analogy is relevant to heat conduction problems as well. The virtual trap method is relatively versatile for treating more general geometries and may be applied to situations such as partial absorption of an anisotropic absorber.

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