Diffusion-limited reaction in the presence of n traps

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We solve the problem of a one-dimensional array of n imperfect traps. These traps are physically represented by small regions of space (in the one-dimensional version we discuss here these traps are represented by small sections of the x axis) with a smaller diffusion constant than that outside them. Small physical particles of one kind diffuse outside and through these small sections. In this work we investigate the changes of the particles density incurred by the presence of these traps. We also check how this density behaves when the density of traps becomes very large.

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I. INTRODUCTION

The problem of diffusion in the presence of traps has been studied by many authors (see, for example, [1,2,5–8]). These studies concern the effect of one, a few, or an infinite number of traps arranged along the whole spatial space. One can, however, imagine materials with a *high density* of traps (such as a highly doped semiconductors, or a dense system of plasma traps) [9]. Moreover, models for which the range of trapping is infinite, such as a classical analog of the Kronig-Penney model [10,11], may not be physically realistic. In principle, one should study models for which the extent of the region of trapping is bounded. In this paper, I use the transfer matrix method [10,12], in analogy to the quantum case [10–12], to study the diffusion of a flow of particles in a material with a large number of traps in a bounded region. This method is well adapted to a system of (imperfect) traps for which the effect of trapping is determined by boundary conditions [5].

Since the identical particles diffusing through the n traps system [6–8] are not exposed to any external force the equation that seems most appropriate to describe their density state is the homogenous diffusion equation [4]. This equation is taken to hold not only outside the n traps, but also in the small sections representing the traps. The diffusion constant of the traps denoted here by D_i (assumed to be all identical) must be smaller than the one outside them denoted by D_e. Since each trap has some small width it has also two sides; a front side through which the particles enter into it, and a back side out of which the particles leave (if they are not absorbed inside). The imperfect nature of the n traps must be given by the appropriate boundary conditions, and since each trap has two sides we have $2n$ boundary conditions.

In [2], a similar system of lattice sites are traversed by a random walker (at the end of [2] a one-dimensional random walk was numerically discussed) in the presence of a trap. The formalism used in [2] refers to the time variable as continuous [3], and to the space variable as discrete, and discusses how the presence of a trap influences the known probabilities of the random walker. In the work reported here the diffusion of the particles outside and inside the traps is discussed by using the homogenous diffusion equation with the appropriate boundary conditions at the traps, and we check both theoretically and numerically how the presence of the traps influences the density of the particles. Since our formalism uses the diffusion equation the space variable as well as the time variable are both continuous.

In Sec. II we show by using the continuity of both the function representing the particle density and its first space derivative at the $2n$ trap boundaries that we obtain a matrix equation of the form $x_n = Tx_0$, where T is a transfer matrix [10–12] that is composed of a product of n two-dimensional matrices, and x_n is a two-dimensional vector that denotes the imperfect and ideal trap components of the density function of the diffusing particles at the right hand side of the dense system. x_0 is the corresponding vector that denotes the same components at the left hand side of this system. We show that when the number of traps, arranged along the finite section alloted for them, becomes very large the particle density at the end of the n trap system is the same as the density at the beginning of this system. That is, the survival probability of these particles tends to unity in the limit, and in spite of very large number of traps. We have corroborated the analytical results obtained from the transfer matrix method by using directly the $4n \times 4n$ matrix for the solution of the relevant system of equations. We show by the last method that when the total width of the traps and the total interval among them grow the survival probability of the particles passing through the dense system tends to unity. The same result is obtained also if we apply the constraint of a fixed total length of the system and increase the total interval among the traps (thereby decreasing the total width of them).

II. THE TRANSFER MATRIX METHOD FOR THE IMPERFECT TRAP DIFFUSION-LIMITED REACTION

The physical problem we want to solve is the diffusion-limited reaction in the presence of n traps. We discuss here the one-dimensional version of this problem. That is, in a finite section of the x axis we have an array of n traps arranged in an ordered manner. These traps are assumed to be static and the physical particles diffuse between and through them. We consider each trap to have a finite width through which the particles diffuse. We denote the total width of all the n traps by a, so that the width of each one is a/n. We also denote the total width of all the separating intervals between the traps by b. It is obvious that the number of intervals between the traps is $n-1$, but assuming that the first trap begins at the point $x=b/n$ we obtain that the number of the separating intervals between the point $x=0$ and the nth trap is n, so the width of each such interval is b/n. Thus, we see that the entire section in which the n traps are situated has a finite length of $(a+b)$. We discuss here the imperfect traps version of this trapping problem in which the particles colliding with these traps are not instantaneously annihilated.

The appropriate one-dimensional initial and boundary value problem is the following:

$$\begin{gathered}\rho_t = D\rho_{xx}, \quad t>0, \quad 0<x\leqslant(a+b),\\ \rho(x,0)=\rho_0+f(x), \quad 0<x\leqslant(a+b), \\ \rho(x_i,t)=\frac{1}{k}\left.\frac{d\rho(x,t)}{dx}\right|_{x=x_i}, \quad t>0, \quad 1\leqslant i\leqslant 2n,\end{gathered} \tag{1}$$

where $\rho(x,t)$ is the density of the diffusing particles, ρ_t and ρ_{xx} are the first partial derivative with respect to time and the second partial derivative with respect to x respectively. The first equation is the homogenous one-dimensional diffusion equation and D is the diffusion constant. The second equation is the initial condition that we assume to depend on x through $f(x)$, and also on a constant term denoted by ρ_0. The third equation is the boundary value condition at the place of the ith trap and implies that we have here an imperfect trap. This third equation must be satisfied at all the places of all the n traps, and since each trap has two faces we have actually $2n$ boundary conditions. According to the conventional diffusion theory [4] the problem (1) can be reduced to the following two problems

$$\begin{gathered}\rho_t = D\rho_{xx}, \quad t>0, \quad 0<x\leqslant(a+b),\\ \rho(x,0)=f(x), \quad 0<x\leqslant(a+b), \\ \rho(x_i,t)=0, \quad t>0, \quad 1\leqslant i\leqslant 2n.\end{gathered} \tag{2}$$

$$\begin{gathered}\rho_t = D\rho_{xx}, \quad t>0, \quad 0<x\leqslant(a+b),\\ \rho(x,0)=\rho_0 \quad 0<x\leqslant(a+b), \\ \rho(x_i,t)=\frac{1}{k}\left.\frac{d\rho(x,t)}{dx}\right|_{x=x_i}, \quad t>0, \quad 1\leqslant i\leqslant 2n.\end{gathered} \tag{3}$$

The problem associated with the set (2) represents the diffusion-limited reaction in the presence of n ideal traps as can be seen from the third equation of the set (2), and the problem associated with the set (3) represents the diffusion-limited reaction in the presence of n imperfect traps as can be seen from the third equation of the set (3). As seen from the sets (2) and (3) the original imperfect trap problem from the set (1) has been decomposed into two problems, one of which is the ideal trap problem. The solution of the general problem from the set (1) is [4]

$$\rho(x,t)=A\rho_1(x,t)+B\rho_2(x,t), \tag{4}$$

where $\rho_1(x,t)$ is the solution of the ideal trap problem represented by the set (2), and $\rho_2(x,t)$ is the solution of the imperfect trap problem from the set (3). The $\rho_1(x,t)$, found from the separation of variables method [4], that satisfies the boundary and initial value conditions of the set (2) [for, as is necessary to satisfy the first and third conditions of the set (2), $f(x)=\sin(\pi x/x_i)$] is

$$\rho_1(x,t)=\sin\left(\frac{\pi x}{x_i}\right)e^{-(tD\pi^2/x_i^2)}. \tag{5}$$

The $\rho_2(x,t)$ that satisfies the initial and boundary conditions of the set (3) is given by [5]

$$\rho_2(x,t)=\rho_0\left[\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)+\exp(k^2Dt+kx)\times\operatorname{erfc}\left(k\sqrt{Dt}+\frac{x}{2\sqrt{Dt}}\right)\right]. \tag{6}$$

The erf is the error function defined as $\operatorname{erf}(x)=(2/\sqrt{\pi})\int_0^x e^{-u^2}du$, and the erfc is the complementary error function defined as $\operatorname{erfc}(x)=1-\operatorname{erf}(x)=(2/\sqrt{\pi})\int_x^\infty e^{-u^2}du$. Now, since the n traps are imperfect and have a finite width a/n the particles arriving at their places diffuse through them in a finite time. Thus, these particles, while inside these traps, must satisfies a similar diffusion equation as that satisfied outside them. The diffusion constant D_i inside the traps must be smaller from the one D_e outside them. Thus, the density inside the traps is given by Eq. (4) except for a different diffusion constant. Also, we assume that the density $\rho(x,t)$ from Eq. (4) and its rate of change with respect to x are continuous along the section $(a+b)$. That is, we can equate at all the $2n$ points (where all the n traps begin and end), the $\rho(x,t)$ and $d\rho(x,t)/dx$ outside each trap to the $\rho(x,t)$ and $d\rho(x,t)/dx$ inside it. This is the basis for the transfer matrix method used here. We begin by performing these comparisons at the two points b/n and $(a+b)/n$, where the first trap begins and ends, and obtain the following four equations:

$$\begin{aligned}&A\rho_0\left[\operatorname{erf}\left(\frac{b}{2n\sqrt{D_et}}\right)+\exp\left(k^2D_et+\frac{kb}{n}\right)\operatorname{erfc}\left(k\sqrt{D_et}+\frac{b}{2n\sqrt{D_et}}\right)\right]\\ &=C\rho_0\left[\operatorname{erf}\left(\frac{b}{2n\sqrt{D_it}}\right)+\exp\left(k^2D_it+\frac{kb}{n}\right)\operatorname{erfc}\left(k\sqrt{D_it}+\frac{b}{2n\sqrt{D_it}}\right)\right],\end{aligned} \tag{7}$$

$$A\rho_0 k \exp\left(k^2 D_e t + \frac{kb}{n}\right)\mathrm{erfc}\left(k\sqrt{D_e t} + \frac{b}{2n\sqrt{D_e t}}\right) + B\frac{n\pi}{b}\exp\left[-\left(\frac{n\pi}{b}\right)^2 tD_e\right]$$
$$= C\rho_0 k \exp\left(k^2 D_i t + \frac{kb}{n}\right)\mathrm{erfc}\left(k\sqrt{D_i t} + \frac{b}{2n\sqrt{D_i t}}\right) + D\frac{n\pi}{b}\exp\left[-\left(\frac{n\pi}{b}\right)^2 tD_i\right], \tag{8}$$

$$C\rho_0\left[\mathrm{erf}\left(\frac{(a+b)}{2n\sqrt{D_i t}}\right) + \exp\left(k^2 D_i t + \frac{k(a+b)}{n}\right)\mathrm{erfc}\left(k\sqrt{D_i t} + \frac{(a+b)}{2n\sqrt{D_i t}}\right)\right]$$
$$= E\rho_0\left[\mathrm{erf}\left(\frac{(a+b)}{2n\sqrt{D_e t}}\right) + \exp\left(k^2 D_e t + \frac{k(a+b)}{n}\right)\mathrm{erfc}\left(k\sqrt{D_e t} + \frac{(a+b)}{2n\sqrt{D_e t}}\right)\right], \tag{9}$$

$$C\rho_0 k \exp\left(k^2 D_i t + \frac{k(a+b)}{n}\right)\mathrm{erfc}\left(k\sqrt{D_i t} + \frac{(a+b)}{2n\sqrt{D_i t}}\right) + D\frac{n\pi}{(a+b)}\exp\left[-\left(\frac{n\pi}{(a+b)}\right)^2 tD_i\right]$$
$$= E\rho_0 k \exp\left(k^2 D_e t + \frac{k(a+b)}{n}\right)\mathrm{erfc}\left(k\sqrt{D_e t} + \frac{(a+b)}{2n\sqrt{D_e t}}\right) + F\frac{n\pi}{(a+b)}\exp\left[-\left(\frac{n\pi}{(a+b)}\right)^2 tD_e\right]. \tag{10}$$

Solving Eqs. (7)–(8) for the coefficients C and D in terms of A and B we obtain

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{bmatrix} \dfrac{\alpha\left(D_e, \frac{b}{n}, t\right)}{\alpha\left(D_i, \frac{b}{n}, t\right)} & 0 \\ \dfrac{\xi\left(D_e, \frac{b}{n}, t\right)}{\eta\left(D_i, \frac{b}{n}, t\right)} - \dfrac{\alpha\left(D_e, \frac{b}{n}, t\right)\xi\left(D_i, \frac{b}{n}, t\right)}{\alpha\left(D_i, \frac{b}{n}, t\right)\eta\left(D_i, \frac{b}{n}, t\right)} & \dfrac{\eta\left(D_e, \frac{b}{n}, t\right)}{\eta\left(D_i, \frac{b}{n}, t\right)} \end{bmatrix} \begin{pmatrix} A \\ B \end{pmatrix}, \tag{11}$$

where α, ξ, and η are given by (we write these expression for D_e and $x = b/n$)

$$\alpha\left(D_e, \frac{b}{n}, t\right) = \mathrm{erf}\left(\frac{b}{2n\sqrt{D_e t}}\right) + \exp\left[k^2 D_e t + \frac{kb}{n}\right]\mathrm{erfc}\left[k\sqrt{D_e t} + \frac{b}{2n\sqrt{D_e t}}\right], \tag{12}$$

$$\xi\left(D_e, \frac{b}{n}, t\right) = k\exp\left[k^2 D_e t + \frac{kb}{n}\right]\mathrm{erfc}\left(k\sqrt{D_e t} + \frac{b}{2n\sqrt{D_e t}}\right), \tag{13}$$

$$\eta\left(D_e, \frac{b}{n}, t\right) = -\frac{n\pi}{b}e^{-(n\pi/b)^2 D_e t}. \tag{14}$$

Then we find the coefficients of the density function between the first and second trap as functions of the coefficients of the density function inside the first trap at the point $x = (a+b)/n$. This dependence is given by Eqs. (9) and (10) from which we obtain

$$\begin{pmatrix} E \\ F \end{pmatrix} = \begin{bmatrix} \dfrac{\alpha(D_i, a+b/n, t)}{\alpha(D_e, a+b/n, t)} & 0 \\ \dfrac{\xi(D_i, a+b/n, t)}{\eta(D_e, a+b/n, t)} - \dfrac{\alpha[D_i, (a+b)/n, t]\xi[D_e, (a+b)/n, t]}{\alpha[D_e, (a+b)/n, t]\eta[D_e, (a+b)/n, t]} & \dfrac{\eta[D_i, (a+b)/n, t]}{\eta[D_e, (a+b)/n, t]} \end{bmatrix} \begin{pmatrix} C \\ D \end{pmatrix}. \tag{15}$$

Substituting in the last equation for $\binom{C}{D}$ from Eq. (11) we obtain

$$\begin{pmatrix} E \\ F \end{pmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{pmatrix} A \\ B \end{pmatrix}. \tag{16}$$

T_{11}, T_{12}, T_{21}, and T_{22} are given by the following expressions

$$T_{11} = \frac{\alpha\left(D_e, \frac{b}{n}, t\right) \alpha[D_i, (a+b)/n, t]}{\alpha\left(D_i, \frac{b}{n}, t\right) \alpha[D_e, (a+b)/n, t]}, \tag{17}$$

$$T_{12} = 0, \tag{18}$$

$$\begin{aligned} T_{21} = \rho_0 \Bigg\{ & \frac{\eta[D_i, (a+b)/n, t]}{\eta\left(D_e, \frac{(a+b)}{n}, t\right)} \left[\frac{\xi(D_e, b/n, t)}{\eta(D_i, b/n, t)} \right. \\ & \left. - \frac{\alpha(D_e, b/n, t)\, \xi(D_i, b/n, t)}{\alpha(D_i, b/n, t)\, \eta(D_i, b/n, t)} \right] \Bigg\} \\ & + \frac{\alpha(D_e, b/n, t)}{\alpha\left(D_i, \frac{b}{n}, t\right)} \left\{ \frac{\xi[D_i, (a+b)/n, t]}{\eta[D_e, (a+b)/n, t]} \right. \\ & \left. - \frac{\alpha[D_i, (a+b)/n, t]\, \xi[D_e, (a+b)/n, t]}{\alpha[D_e, (a+b)/n, t]\, \eta[D_e, (a+b)/n, t]} \right\}, \end{aligned} \tag{19}$$

$$T_{22} = \frac{\eta[D_e, b/n, t]\, \eta[D_i, (a+b)/n, t]}{\eta[D_i, b/n, t]\, \eta[D_e, (a+b)/n, t]}. \tag{20}$$

Equation (16) expresses the coefficients of the density function at the right hand side of the first trap as functions of the coefficients of the density function at the left hand side of this trap. We can repeat the same procedure for all the other traps and obtain the following equation that expresses the coefficients of the density function at the right hand side of the n traps array as functions of the coefficients of the density function at the left hand side of the first trap (since these matrices differ from one another only by the values of x we write them in the following equation as functions of x only)

$$\begin{aligned} \begin{pmatrix} A_{2n+1} \\ B_{2n+1} \end{pmatrix} = & T(a+b) T\left[\frac{(n-1)(a+b)}{n} \right] \\ & \times T\left[\frac{(n-2)(a+b)}{n} \right] \cdots T\left[\frac{2(a+b)}{n} \right] \\ & \times T\left(\frac{a+b}{n} \right) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \end{aligned} \tag{21}$$

Each T from the last equation is a 2×2 matrix that is the same as Eq. (16) except for the diffent values of x. We can see from Eqs. (11)–(21) that in the absence of traps when $D_i = D_e$ we have for each T from Eq. (21) $T_{11} = T_{22} = 1$, $T_{12} = T_{21} = 0$. That is, each one of these n matrices become the two-dimensional unity matrix, so that from Eq (21) we obtain the expected result

$$\begin{pmatrix} A_{2n+1} \\ B_{2n+1} \end{pmatrix} = \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \quad D_i = D_e. \tag{22}$$

The equality from Eq. (22) of the two components of the particles density at the point $x = a+b$ to those at the point $x = b/n$ means that, actually, we have $b = 0$. That is, when there are no traps there are also no intervals between them, and the whole section along the x axis has only one diffusion constant D_e or D_i. Thus, the densities at the two ends of this section are equal.

Now, we discuss the limit of very large n. In this case since the total section $a+b$, along which all this dense array of traps are arranged, is finite, the width of each such trap that is a/n, and the interval between each two neighboring traps that is b/n become both very small. Thus, as can be seen from Eqs. (12)–(14), we have in this case

$$\begin{aligned} \lim_{n\to\infty} \alpha\left(D_e, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \alpha\left(D_e, \frac{d(a+b)}{n}, t\right), \\ \lim_{n\to\infty} \alpha\left(D_i, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \alpha\left(D_i, \frac{d(a+b)}{n}, t\right), \\ \lim_{n\to\infty} \xi\left(D_e, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \xi\left(D_e, \frac{d(a+b)}{n}, t\right), \\ \lim_{n\to\infty} \xi\left(D_i, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \xi\left(D_i, \frac{d(a+b)}{n}, t\right), \\ \lim_{n\to\infty} \eta\left(D_e, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \eta\left(D_e, \frac{d(a+b)}{n}, t\right), \\ \lim_{n\to\infty} \eta\left(D_i, \frac{(d-1)a+db}{n}, t\right) &= \lim_{n\to\infty} \eta\left(D_i, \frac{d(a+b)}{n}, t\right), \end{aligned} \tag{23}$$

$$\begin{aligned} & \lim_{n\to\infty} \alpha\left(D_e, \frac{(n-c)a+[n-(c-1)]b}{n}, t\right) \\ & \quad = \lim_{n\to\infty} \alpha\left(D_e, \frac{[n-(c-1)](a+b)}{n}, t\right), \\ & \lim_{n\to\infty} \alpha\left(D_i, \frac{(n-c)a+[n-(c-1)]b}{n}, t\right) \\ & \quad = \lim_{n\to\infty} \alpha\left(D_i, \frac{[n-(c-1)](a+b)}{n}, t\right), \end{aligned}$$

$$\lim_{n\to\infty} \xi\left(D_e , \frac{(n-c)a+[n-(c-1)]b}{n} ,t\right)$$
$$= \lim_{n\to\infty} \xi\left(D_e , \frac{[n-(c-1)](a+b)}{n} ,t\right),$$

$$\lim_{n\to\infty} \xi\left(D_i , \frac{(n-c)a+[n-(c-1)]b}{n} ,t\right)$$
$$= \lim_{n\to\infty} \xi\left(D_i , \frac{[n-(c-1)](a+b)}{n} ,t\right),$$

$$\lim_{n\to\infty} \eta\left(D_e , \frac{(n-c)a+[n-(c-1)]b}{n} ,t\right)$$
$$= \lim_{n\to\infty} \eta\left(D_e , \frac{[n-(c-1)](a+b)}{n} ,t\right),$$

$$\lim_{n\to\infty} \eta\left(D_i , \frac{(n-c)a+[n-(c-1)]b}{n} ,t\right)$$
$$= \lim_{n\to\infty} \eta\left(D_i , \frac{[n-(c-1)](a+b)}{n} ,t\right),$$

where d and c are positive integers (for example, d receive the value of 1 for the first trap and c receives this value for the last trap). We must note that the first six equations of the set (23) are applied to the matrices that represent the traps that are close to the left hand side of the n traps system near the point $x=b/n$. The last six equations of the set (23) are applied to the matrices that represent the traps that are close to the right hand side of the n traps system near the point $x=a+b$. Using Eqs. (16)–(20) and the first six equations of the set (23) we can see that we have for each two dimensional matrix that represents a trap close to the point $x=b/n$ the following limits:

$$\lim_{n\to\infty} T_{11}=1, \tag{24}$$

$$\lim_{n\to\infty} T_{21}=0, \tag{25}$$

$$\lim_{n\to\infty} T_{22}= \lim_{n\to\infty} e^{-(n\pi)^2 t(D_e-Di)\{(2adb+2da^2-a^2)/[d(a+b)]^2[(d-1)a+db]^2\}}=0. \tag{26}$$

The last equation is obtained by using the inequality $D_e > D_i$. Equation (25) is obtained by a repeated application of l'Hôpital theorem [17]. That is, in the limit of $n\to\infty$ each of the two terms of Eq. (19) is a product of the kind $(\infty\cdot 0)$, so we use the l'Hôpital theorem [17] that yields a result of the same kind $(\infty\cdot 0)$. Thus, we have to apply repeatedly the same theorem until we obtain a finite result that turns out to be zero. We see, therefore, that each one of these matrices becomes, in the limit of very large n, a constant two-dimensional matrix the first column of it is composed of 1 and 0, and the second column is composed of zeroes,

$$\lim_{n\to\infty} T_n = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{27}$$

Also the product of any number of two dimensional matrices of the form (27) yields back again a matrix of the same form.

As for the matrices that represent traps close to the point $x=a+b$ we can see from the seventh and eighth equations of the set (23) that the element T_{11} of each matrix of this kind satisfies the same limit relation of Eq. (24). Figure 1 shows a three-dimensional graph of the element T_{11} as a function of the total width a of all the traps a, and the number n of them. The range of a is $1\leqslant a\leqslant 50$, and that of n is $1\leqslant n\leqslant 800$, b is $a/2$, $t=2$, and the other parameters D_e, D_i, and k are 0.5, 0.1, and 1 respectively. [These values illustrate the method and give results that should be qualitatively similar for a wide class of applications, for example, 0.5 cm^2/sec is the order of magnitude of the diffusion constant D at room temperature and atmospheric pressure (p. 337 in [13]).] It can be seen from this figure that for smaller values of n the element T_{11} receives values in the range $0.4\leqslant T_{11}\leqslant 2$, and the rate of change of T_{11} for these small n's is large compared to this rate for large values of n. As n grows the value of T_{11} tends to unity. But as seen from Fig. 1 the approach to unity is faster for small values of a than for the larger values. The reason for this is that when the total width a of the n traps is small, whereas, n itself is large then these n traps are densely arrayed along the finite section $a+b$. And as we have seen [see Eq. (24)] when we have a dense array (large density) of traps the element T_{11} tends to unity. When a becomes larger the n traps are not densely arrayed along the finite section $a+b$, and correspondingly the element T_{11} does not receives the exact value of 1. It can be seen that the element T_{22} of the matrices that represent traps near the point $x=a+b$ have the following limit

$$\lim_{n\to\infty} T_{22} = \lim_{n\to\infty} \exp\left[-(n^2\pi)^2 t(D_e - Di)\, \frac{(a^2+2b^2)(1-2c)+2ab(1+c)+2n(a^2+b^2-cb^2+ab)}{\{[n-(c-1)](a+b)\}^2\{(n-c)a+[n-(c-1)]b\}^2} \right] = 1.$$

It can be seen also that in the limit of $n\to\infty$ the element T_{21} of each matrix of the matrices that represent traps close to the point $x=a+b$ is zero as for the matrices that represent traps close to the point $x=b/n$ [see Eq. (25)]. This time we obtain the value of zero in the limit of $n\to\infty$ without having to use the l'Hôpital theorem as in the former case. That is, in this limit of $n\to\infty$ each of the matrices that represent traps close to the point $x=a+b$ becomes the two-dimensional unity matrix. Now, taking into account that the product of any number of two-dimensional unity matrices by a matrix of the form (27) results in a matrix of the same form as Eq. (27), we can write the limit (for very large n) of Eq. (21) using Eqs. (23)–(27) as

$$\lim_{n\to\infty}\begin{pmatrix} A_{2n+1} \\ B_{2n+1}\end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}\begin{pmatrix} A_1 \\ B_1\end{pmatrix}. \tag{28}$$

From the last equation we conclude that the imperfect trap component of the density remains at the point $x=a+b$ (the right hand side of the n trap system), at the same value it had at the point $x=b/n$ (the left hand side of the n trap system). That is, for this component {which is actually the only component of the density [see the original problem (1)]} the presence of a very large number of traps is the same as if not even a single trap is present. As for the ideal trap component we see from Eq. (28) that it vanishes at the point $x=a+b$.

In all the numerical computations done so far we have assigned to the coefficient k of the boundary value conditions of the imperfect traps problem the value of 1 [see the third equations of the sets (1) and (3)]. We can see from Eqs. (12) and (17) that when $k\to\infty$ and a, b, n, and t have finite values then the element T_{11} satisfies $|T_{11}|<1$. This is because the element T_{11} [see Eq. (17)] of each matrix T from Eq. (21) is composed of products and divisions by the expressions α from Eq. (12). The second term of α that involves the erfc is zero, in the limit of $k\to\infty$, by application of the l'Hôpital theorem. We remain in Eq. (17) with only products and divisions of the erf functions as seen from the following equation that is written for the first trap

$$\lim_{k\to\infty} T_{11} = \frac{\operatorname{erf}\left(\dfrac{b}{2n\sqrt{D_e t}}\right)\operatorname{erf}\left(\dfrac{a+b}{2n\sqrt{D_i t}}\right)}{\left[\operatorname{erf}\left(\dfrac{b}{2n\sqrt{D_i t}}\right)\operatorname{erf}\left(\dfrac{a+b}{2n\sqrt{D_e t}}\right)\right]}. \tag{29}$$

For finite a, b, n, and t each T_{11} from the last equation results in an outcome that is between 0 and 1, so that the nth order product of these T_{11}'s in Eq. (21) results in a small number if n is large. But we can see that when a and b become very large (for finite n and t) then the erf function tends to unity in this case [see Eq. (12)], and each element T_{11} of each matrix T from Eq. (21) tends to 1, so that the nth order product of Eq. (21) results in 1. That is, according to our discussion so far, the density at the point $x=a+b$ at the right hand side of the n trap system is the same as that at the left hand side of this system at the point $x=b/n$. We can show that we obtain the same result also when $n\to\infty$ or $t\to\infty$ or when both limits are satisfied. Figure 2 shows a three-dimensional graph of T_{11} in the limit of $k\to\infty$, that is, a graph of the T_{11} from Eq. (29) as a function of n and a. The range of n is $1\leq n\leq 150$, and that of a is $1\leq a\leq 200$. The values of the other parameters are: $D_e=0.5$, $D_i=0.1$, and t=2. It can be seen from the graph that the surface of T_{11} tends to unity for large n and small a, because in such a case the large number of traps are densely arrayed along the small section $a+b$. It can also be seen that when a begins to grow the value of T_{11} exceeds 1 even for large n. When n is small the surface of T_{11} tends to the value of unity as a becomes large as can be seen from Fig. 2. As seen from Eq. (29) we obtain the same situation if we replace n by t. That is, when $t\to\infty$ we obtain a value of unity for the T_{11} of Eq. (29), and with it a value of unity also for the infinite product from Eq. (21).

We must note that when $k\to\infty$, in such a case the imperfect traps become ideal [see the third equations of the sets (1) and (3)], the situation obtained is still different from the ideal traps component of the density function as given by the set (2) and Eq. (5). This is because the ideal trap problem from the set (2) has an initial condition that is entirely different from the initial condition of the set (3). Thus, as seen from the set (2), we obtain a result of zero for the ideal trap component of the density at the point $x=a+b$, whereas we may obtain, as we see in Fig. 2, a result of unity for the ideal trap situation obtained from the imperfect problem [see the sets (1) and (3)] in the limit of infinite k.

All the results obtained so far by the transfer matrix method may be obtained also by considering the equivalent $4n\times 4n$ matrix method that deals with only one large matrix instead of the n two-dimensional matrices that compose the transfer matrix. Using this method we have, numerically computed and plotted the ratio (denoted by V) of the imperfect trap function coefficient at the point $x=a+b$ (at the right hand side of the n trap system) to that at the point $x=b/n$ (at the left hand side of this system) as a function of the total width a of the n trap system. Figure 3 shows the graphs of V for different values of the time t, as functions of the total width a of the n traps where we have assigned to n the value of $n=50$. The range of a is $46\leq a\leq 300$, and the seven curves shown are for the following values of the time: $t=1,6,11,16,21,26,31$. The correct chronological order of the curves shown in the figure is downward. That is, the upper curves in Fig. 2 are for the small t's, and the lower curves are for the large ones. Note that as t grows the corresponding

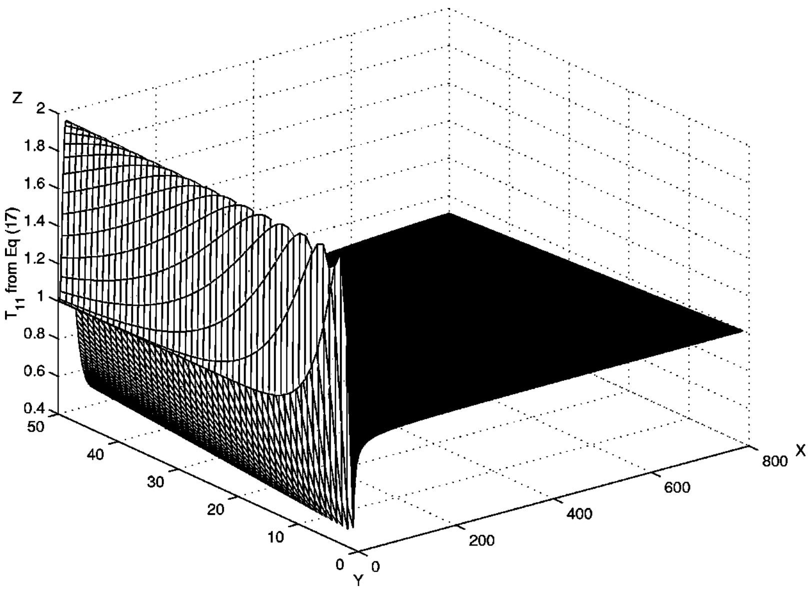

FIG. 1. The surface T_{11} as a function of the number of traps n and the total width a.

curves tend to give the value of $V=0.62$. When a becomes large V tends to unity for all values of t as can be seen from Fig. 3. Figure 4 shows that when a grows V tends to unity also for all values of the number of traps n. In Fig. 4 we see nine graphs of V as a function of a for nine different values of n. The range of a is $46 \leqslant a \leqslant 200$, and n has the values of 2, 8, 14, 20, 26, 32, 38, 44, and 50. t has the value equal to 2, and the other parameters D_e, D_i, k has the same values as in Fig. 3. It is seen from Fig. 4 that all the curves tend to the value of unity when a becomes large. The curves fit the different given values of n from above so that the upper curves correspond to the smaller values of n, and the lower ones correspond to the larger values. For small values of n the graph of V begins from a value close to 1, and as n grows the initial point of the corresponding curve tends to the value $V=0.8$ and continues from there to unity as a grows. The approach of V to 1 is faster when n is small than when n is large as can be seen from the figure. If we measure the ratio of the imperfect trap coefficient of the density *inside* the last trap to that at the left hand side of the trap system then we find similar results to those we found for the ratio V of the imperfect trap coefficient of the density *outside* and to the right of the last trap to this coefficient at the point $x=b/n$. Measuring the ratios of the ideal trap coefficient outside the traps or inside them to the imperfect trap coefficient at the point $x=b/n$ we find a very small result for all n and all a. This is expected since this component of the density function is absorbed completely at the sides of the traps. At $t=0$ we find that the value of V is unity for all values of n and a. We have obtained this result for $k=1$, $D_e=0.5$, $D_i=0.1$, and $b=a/2$. That is, at the initial time the densities at the two extreme sides of the trap system are equal. When t departs from zero this coefficient becomes smaller for the same values of n and a. That is, as time progresses the density after the n trap system becomes smaller than that before this system as expected from a physical point of view. We note that

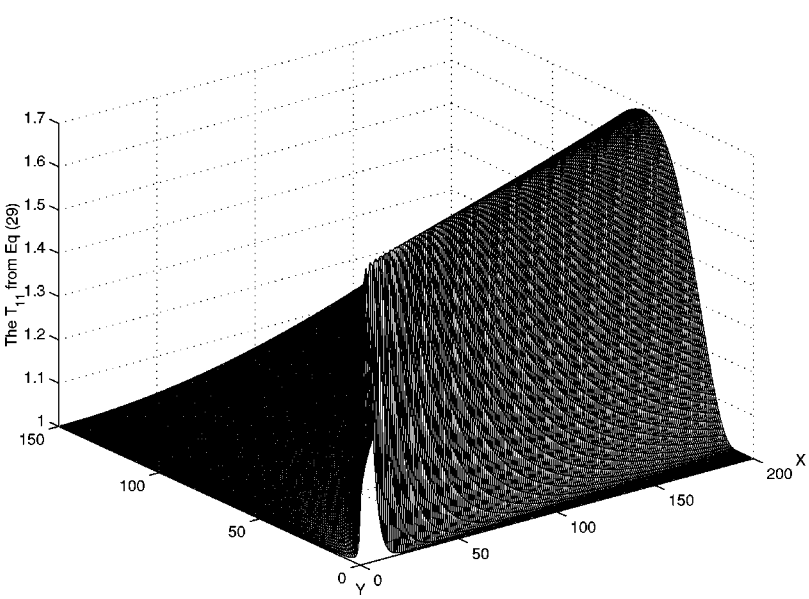

FIG. 2. The surface T_{11} as a function of the number of traps n and the total width a.

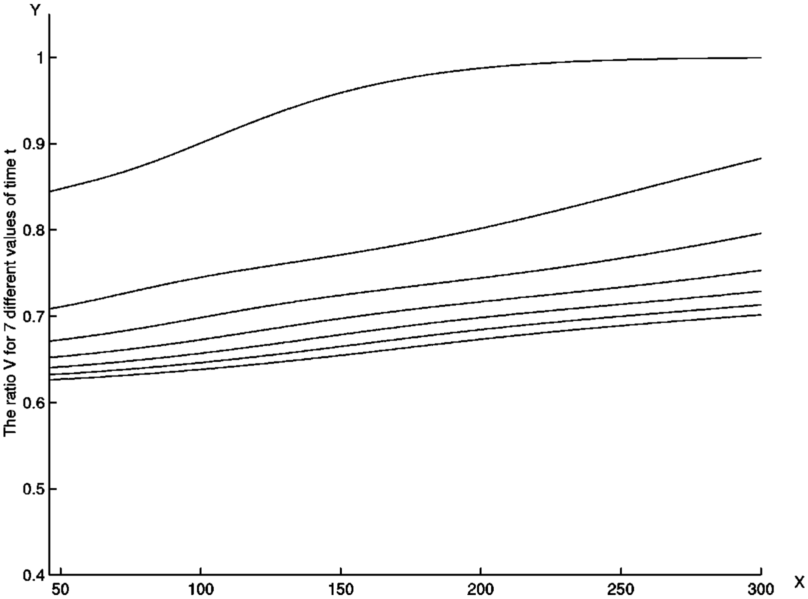

FIG. 3. The ratios V_n as functions of the total width a for seven different values of the time t.

the equality of $A_{2n+1}=A_0$ for very large a obtained from Figs. 3 and 4 is not the same as the identical equality (22) obtained for $b=0$ [see the discussion after Eq. (22)]. The reason is that a very large value of a in Figs. 3 and 4 does not entails an existence of only one diffusion constant along the entire section $a+b$ as we have obtained from Eq. (22). Note that in these figures we have all the time $b=a/2$, so when a becomes very large b also does so, and we have still the two diffusion constants D_e and D_i along the section $a+b$. Thus, it is entirely different from the $D_e=D_i$ case of Eq (22).

We must note that in all the analytical and numerical discussion so far the finite length of the system, we denote it by $L=a+b$, is not kept constant as, for example, in Figs. 3 and 4 that shows the ratios V's as functions of a, where $b=a/2$, so that when a increases, b and L also do so. That is, as turns out from these figures the ratios V's tend to 1 when the total width a and the total length L grow. If we impose the constraint of a strictly constant L, such that when a increases b must decrease in order to remain with a constant L, then we can express the total width a and total interval b in terms of the total length L and another parameter c that is a positive real number defined as $c=b/a$. That is, a and b can be written as

$$a=\frac{L}{1+c} \quad b=\frac{Lc}{1+c}. \tag{30}$$

From the last two relations we see that as c increases a decreases to the limit of zero, and b grows to the limit of L. In this case of a fixed total length L the ratio V depends on c and n in such a manner that for small n, V exceeds unity already at small values of c. As n increases V tends to the unity for larger values of c as can be seen from Fig. 5 that

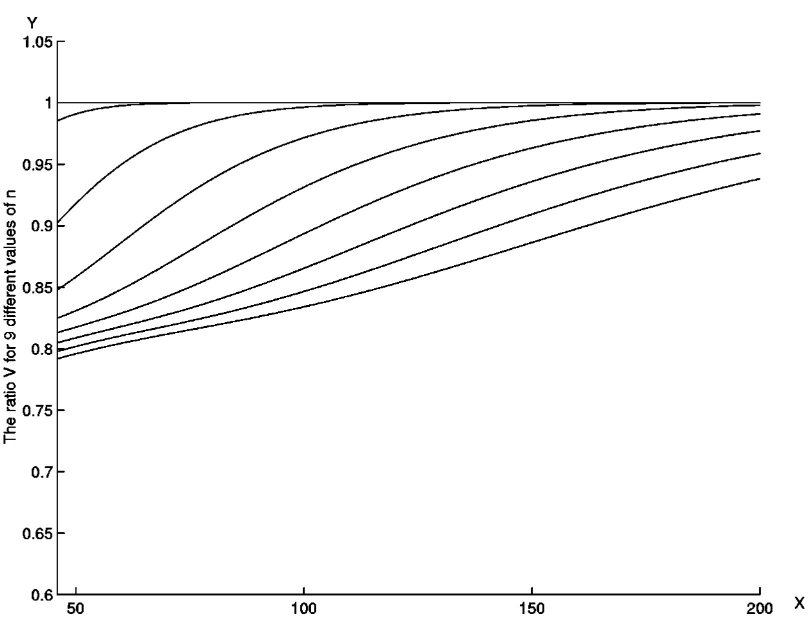

FIG. 4. The ratios V_n as functions of the total width a for nine different values of n.

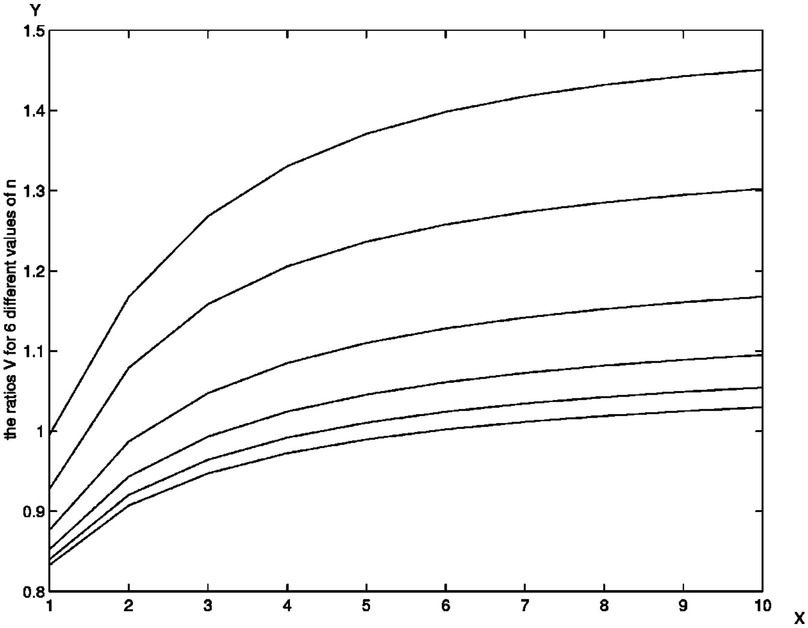

FIG. 5. The ratio V_n for a fixed total length of the system and for six different values of n.

shows the ratio V as a function of c in the range $1 \leqslant c \leqslant 10$ for a total system length of $L=60$, and for six different values of n: 20,40,60,80,100,120. The upper curves fit the lower values of n and vice versa. That is, the uppermost curve corresponds to $n=20$. The second curve from above is for $n=40$ and so on. Note that as n grows V tends to begin from the value of $V=0.83$. If we compare Fig. 5 with Fig. 3, which shows the ratios V's for the case in which the total length L *is not fixed* we see that for this case the ratio V tends to the unity only when both the total width a and the total interval b increases (note that in Fig. 3, $b=a/2$), whereas when the total length L *is fixed* the ratio V tends to the unity only when the total interval b increases and the total width a decreases. Thus, we see that the survival probability of the particles represented by the imperfect trap density tends to unity also for a fixed total length of the system when n and c increases.

We note that if the number of traps n is a power of 2, that is, $n=2^m$, then we can use a property of the transfer matrix mentioned in [12] in connection to the quantum system of n potential barriers. First, a pair of traps are combined in the manner of Eqs. (11)–(20) to produce a transfer matrix of these two traps. Then the same construction is repeated regarding the former transfer matrix as the new elementary building block. Continuing in the same manner we obtain at the level m the transfer matrix of 2^m identical traps. For instance, if $m=15$ then $n=2^{15}=32\,768$. That is, at the level 15 of the construction we build the transfer matrix of 32 768 identical traps. When n is not a power of 2 we can use the following binary representation of 2

$$n=c_m 2^m + c_{m-1} 2^{m-1} + \cdots + c_0 2^0,$$

in order to write Eq. (21) as

$$\begin{pmatrix} A_{2n+1} \\ B_{2n+1} \end{pmatrix} = [T(2^m)]^{c_m} [T(2^{m-1})]^{c_{m-1}} \cdots [T(2^0)]^{c_0} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{31}$$

In summary, we see that the survival probability of the particles represented by the imperfect trap component of the density tends to unity as the number of traps becomes a very large number if [14,15]. This situation in which the diffusing particles survive in spite of the very large number of traps surrounding them has been alluded in [16], and it was argued there that if the particles survive all these traps then they must have performed anomalous diffusion.

We note that we have found in the former section a result of unity for the survival probability of the imperfect trap component of the density also for very small times in addition to finding it for the case of very small widths of the traps (when their number n becomes very large). This reminds us of the Zeno effect that is conventionally believed to be a quantum phenomenon [18], although one of the first authors [19] that discuss this effect argued that it holds not only in the quantum regime, but also in the classical and macroscopic one, and that it may be the prime factor that stabilized many physical phenomena. This Zeno effect is thought to be a time effect [18], that is, the large repetitions of some measurement over a total finite time interval, where the time alloted for each separate measurement is correspondingly very small, preserves the initial state of the system. It has been argued [20,21] that this preservation may also be obtained through the space analog of this effect. That is, when the repetitions of this very large number of the same interaction is performed over space and not over time such that each interaction is confined in its specific space domain and when the very large number of these small domains are contained in a finite region of space. The result we have obtained in this section in which the density is preserved in the limit, and in spite of the large number of traps, may allude to a space

Zeno type effect that is responsible for the unit survival probability we have obtained in this section. A similar result has been obtained for the classical concentric billiard for which a Zeno type effect has been established [22].

III. CONCLUDING REMARKS

We have discussed the problem of a one-dimensional diffusion-limited reaction in the presence of n imperfect traps. The physical entity we have tried to determine is the density $\rho(x,t)$ of the identical particles that diffuse between and through the n traps. We have shown that the original problem may be decomposed into two secondary ones, one of which is the ideal trap problem, and the other is the imperfect trap problem. By using the continuities of the density function and its first space derivatives at the $2n$ boundaries of the n traps we have obtained a transfer matrix that enables us to discuss the dense system analytically. We have shown that when n becomes very large the density, after all the n traps are passed through, remains the same as it was at the left hand side of the first trap before these traps were traversed. That is, the density is preserved along the x axis in spite of the very large number of traps arrayed along the finite section $a+b$. It appears that this unit value for the survival probability of the traversing particles may be a manifestation of a space Zeno type effect. These results were corroborated numerically using the equivalent $4n\times 4n$ matrix from it we have obtained that when the total width a and the total interval b of the n traps increases the survival probability of the passing particles tends to 1. The same result was obtained also when the total length $a+b$ of the dense system is kept fixed, and the total interval b increases (in this case the total width a decreases).

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