

# On the diffusion-influenced reversible trapping problem in one dimension

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(Received 19 January 2000; accepted 22 February 2000)

The exact Green function for a particle moving between two static reversible traps in one dimension is obtained for the continuous diffusion model. From this function, we derive the exact expressions of various survival probabilities, which are the key elements in devising the efficient Brownian dynamics algorithm. An exact expression of the mean survival probability is also obtained for the periodic distribution of reversible traps both for the crossing-allowed and crossing-forbidden cases. For the random distribution of reversible traps, the exact mean survival probability is obtained only for the crossing-forbidden case and its long time behavior is compared with that of the crossing-allowed case. We find, in this case, that not only the long time asymptotic relaxation behavior but also the equilibrium concentration itself can be changed from the classical results due to the fluctuation effect of the trap density. © 2000 American Institute of Physics. [S0021-9606(00)50719-3]

## I. INTRODUCTION

The trapping problem, where one single particle diffuses among many static traps, has been the subject of extensive theoretical and experimental studies.<sup>1-14</sup> The trapping process has been usually treated *irreversibly* whether the traps are perfect (infinitely deep) or imperfect (partially absorbing). Although the exact solutions were found only in one dimension (1D) for the trapping problem, the exact asymptotic behavior of the survival probability is known to be  $\sim \exp[-\text{const} \cdot t^{d/(d+2)}]$  in  $d$  dimensions. The slower decay compared with that of the classical kinetics,  $\sim \exp(-\text{const} \cdot t)$ , results from the existence of rare but large trap-free regions where the particle lifetime is extremely long. Thus the above result manifests the fluctuation effect of the trap density.

Our purpose in this paper is to investigate the effect of the *reversibility* on the trapping problem in 1D for the continuous diffusion model. The exact Green function for a particle between two static traps is obtained first. From this function, various probabilities are exactly derived for an initially unbound or bound state.

Some time ago, Edelman and Agmon developed an efficient Brownian dynamics simulation algorithm based on the exact Green function in 1D.<sup>15</sup> An extension of this method to three dimensions with spherical symmetry has been realized quite recently by Kim *et al.*<sup>16</sup> This simulation method is proven to be superior to the conventional lattice-based random walk method because the former allows much larger time steps and, thereby, the long time reaction dynamics can be investigated rather efficiently, especially for the reversible system. However, the above simulation technique has been restricted only to the target problem in which a fixed particle is surrounded by mobile reacting partners. Therefore, rigorous tests of various theories on diffusion-

influenced reactions against the above Brownian dynamics simulation could have been performed only for the target problem. With the exact Green function obtained in this paper, the above Brownian dynamics simulation can now be extended to the system with any type of mobility in 1D.

For the reversible trapping problem in 1D, in which many static traps are distributed along the line, we consider the periodic and random distributions. A moving particle is either forbidden or allowed to cross the traps for each type of trap distribution. Then the mean survival probabilities of the particle are obtained exactly for the periodic trap distribution for the crossing-forbidden and crossing-allowed cases, respectively. In fact, these are found to be the same. For the random trap distribution, we obtain the exact mean survival probability only for the crossing-forbidden case. For the crossing-allowed case, only the long time behavior was reported and the comparison is made between two cases only at long times. We will show that the fluctuation effect in the reversible trapping problem for the crossing-forbidden random trap distribution can change not only the long time asymptotic behavior but also the equilibrium concentration itself.

## II. EXACT SOLUTIONS FOR A PARTICLE MOVING BETWEEN TWO STATIC TRAPS

Consider a particle diffusing on a line of length  $L$ , connecting two reversible static traps at both ends. When the particle encounters a trap, it is trapped instantaneously with the intrinsic rate constant  $k_a$ . The dissociation from the trap can occur with the rate constant  $k_d$ . The “Green function”  $p(x, t|x_0)$  is the probability that the particle is located at  $x$  at time  $t$  given that it was at  $x_0$  at  $t=0$ . Its time evolution is governed by the following diffusion equation:

$$\frac{\partial p(x, t|x_0)}{\partial t} = D \frac{\partial^2 p(x, t|x_0)}{\partial x^2}, \quad (1)$$

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where  $D$  is the diffusion constant of the particle. The appropriate initial and boundary conditions are given, respectively, by

$$p(x,0|x_0) = \delta(x-x_0), \tag{2}$$

$$D \frac{\partial p(x,t|x_0)}{\partial x} \Big|_{x=0} = k_a p(0,t|x_0) - k_d p(*_0,t|x_0), \tag{3a}$$

$$D \frac{\partial p(x,t|x_0)}{\partial x} \Big|_{x=L} = -k_a p(L,t|x_0) + k_d p(*_L,t|x_0), \tag{3b}$$

where  $\delta(x)$  is the Dirac delta function and  $p(*,t|x_0)$  is the binding probability that the particle is in the bound state ( $*$ ) at time  $t$  given that it was initially at  $x_0$ . The two bound states at  $x=0$  and  $L$  are designated as  $*_0$  and  $*_L$ , respectively. The evolution equations of  $p(*,t|x_0)$  are given by

$$\frac{\partial p(*_0,t|x_0)}{\partial t} = k_a p(0,t|x_0) - k_d p(*_0,t|x_0), \tag{4a}$$

$$\frac{\partial p(*_L,t|x_0)}{\partial t} = k_a p(L,t|x_0) - k_d p(*_L,t|x_0). \tag{4b}$$

It should be noted that Eqs. (1), (3), and (4) hold for any initial condition. If we use the Laplace transform,  $\tilde{f}(z) \equiv \int_0^\infty dt f(t) \exp(-zt)$ , the boundary conditions given in Eqs. (3) can be rewritten, with the help of Eqs. (4), as

$$D \frac{\partial \tilde{p}(x,z|x_0)}{\partial x} \Big|_{x=0} = X(q) q D \tilde{p}(0,z|x_0), \tag{5a}$$

$$D \frac{\partial \tilde{p}(x,z|x_0)}{\partial x} \Big|_{x=L} = -X(q) q D \tilde{p}(L,z|x_0), \tag{5b}$$

$$X(q) \equiv k_a q / (k_d + q^2 D), \tag{5c}$$

where  $q \equiv \sqrt{z/D}$ . The solution for an arbitrary initial distribution  $p^0(x_0)$  can be obtained from  $p(x,t|x_0)$  by the following relation:

$$p(x,t|p^0) = \frac{1}{L} \int_0^L dx_0 p(x,t|x_0) p^0(x_0). \tag{6}$$

We try the following form of the solution:<sup>17</sup>

$$\begin{aligned} \tilde{p}(x,z|x_0) &= \frac{1}{2Dq} \exp(-q|x-x_0|) \\ &+ A \exp(qx) + B \exp(-qx). \end{aligned} \tag{7}$$

Here  $A$  and  $B$  are to be chosen so as to satisfy the above initial and boundary conditions. One can readily obtain

$$A = \frac{1-X(q)}{2DqY(q,L)} [\cosh qx_0 + X(q) \sinh qx_0] \exp(-qL), \tag{8a}$$

$$B = \frac{1-X(q)}{1+X(q)} \left[ \frac{1}{2Dq} \exp(-qx_0) + A \right], \tag{8b}$$

$$Y(q,L) \equiv [1+X^2(q)] \sinh qL + 2X(q) \cosh qL. \tag{8c}$$

After some rearrangements, we find

$$\begin{aligned} \tilde{p}(x,z|x_0) &= \frac{1}{2DqY(q,L)} \{ [1+X^2(q)] \cosh q(L-|x_0-x|) \\ &+ 2X(q) \sinh q(L-|x_0-x|) \\ &+ [1-X^2(q)] \cosh q[L-(x_0+x)] \}. \end{aligned} \tag{9}$$

$p(x,t|x_0)$  can be obtained by the inversion theorem for the Laplace transformation technique<sup>17</sup> by summing up the infinitely many residues of  $qY(q,L)$  in Eq. (9):

$$\begin{aligned} p(x,t|x_0) &= \frac{1}{L+2K} + \sum_{n=1}^\infty \frac{2W(\beta_n,x)W(\beta_n,x_0)}{Z(\beta_n,L)} \\ &\times \exp(-D\alpha_n^2 t/L^2), \end{aligned} \tag{10a}$$

$$W(\beta,x) = [\cosh \beta x + X(\beta) \sinh \beta x], \tag{10b}$$

$$Z(\beta,L) = \{L[1-X^2(\beta)] + 2dX(\beta)/d\beta\}, \tag{10c}$$

$$Y[\beta(\neq 0),L] = 0, \tag{10d}$$

where  $K \equiv k_a/k_d$  and  $\beta_n \equiv \alpha_n i/L$  ( $n=1,2,\dots$ ). Note that  $\beta_n$  and  $\alpha_n$  can be obtained by finding the roots of Eq. (10d). One can find easily that  $\lim_{n \rightarrow \infty} \alpha_n \sim n\pi$ . Although Eq. (10a) is not a closed form solution, its value can be easily calculated since the exponential factor,  $\exp(-D\alpha_n^2 t/L^2)$ , decays rapidly as  $\alpha_n$  becomes large. Note that the Green function given by Eqs. (10) can be reduced to obtain the solutions for the imperfect traps (finite  $k_a$  and  $k_d=0$ ), the perfect traps ( $k_a \rightarrow \infty$  and  $k_d=0$ ), and the reflecting boundaries ( $k_a=0$  and  $k_d=0$ ),<sup>17</sup> respectively. This can also be reduced to that of the reversible geminate reaction when  $L \rightarrow \infty$ .<sup>18</sup>

The survival probability for an initially unbound state to be remained unbound,  $S(t|x_0)$ , can be obtained by the direct integration of Eq. (10) over  $x$  to give

$$\begin{aligned} S(t|x_0) &= \frac{L}{L+2K} - \sum_{n=1}^\infty \frac{2X(\beta_n)W(\beta_n,x_0)}{\beta_n Z(\beta_n,L)} [1+H(\beta_n)] \\ &\times \exp(-D\alpha_n^2 t/L^2), \end{aligned} \tag{11}$$

where  $H(\beta) \equiv [1+X^2(\beta)]/[1-X^2(\beta)] \cosh \beta$ . The value of  $H(\beta)$  is either 1 or -1, since  $Y(\beta,L)=0$ . Note that  $S(t|x_0)$  has a maximum value at  $x_0=L/2$ .

The binding probabilities for the initially unbound state can be obtained from the Laplace inverted Eqs. (5) via Eq. (9) as follows:

$$\begin{aligned} p(*_0,t|x_0) &= \frac{K}{L+2K} + \sum_{n=1}^\infty \frac{2X(\beta_n)W(\beta_n,x_0)}{\beta_n Z(\beta_n,L)} \\ &\times \exp(-D\alpha_n^2 t/L^2), \end{aligned} \tag{12}$$

$$\begin{aligned} p(*_L,t|x_0) &= \frac{K}{L+2K} + \sum_{n=1}^\infty \frac{2X(\beta_n)W(\beta_n,x_0)H(\beta_n)}{\beta_n Z(\beta_n,L)} \\ &\times \exp(-D\alpha_n^2 t/L^2). \end{aligned} \tag{13}$$

One can readily verify from Eqs. (12) and (13) that the following symmetric relations hold:

$$p(*_0,t|L/2) = p(*_L,t|L/2), \tag{14}$$

$$p(*_0,t|0) = p(*_L,t|L), \tag{15}$$

$$p(*_0, t|L) = p(*_L, t|0). \quad (16)$$

The normalization condition,  $S(t|x_0) + p(*_0, t|x_0) + p(*_L, t|x_0) = 1$ , can also be obtained from Eqs. (11), (12), and (13).

The probability of finding the unbound particle at  $x$  at time  $t$  for the initially bound state can be obtained from Eqs. (12) and (13) by using the detailed balance condition,  $k_{ad}p(x, t|*) = k_{dp}(*, t|x)$ , as

$$p(x, t|*_0) = \frac{1}{L+2K} + \sum_{n=1}^{\infty} \frac{2X(\beta_n)W(\beta_n, x)}{K\beta_n Z(\beta_n, L)} \times \exp(-D\alpha_n^2 t/L^2), \quad (17)$$

$$p(x, t|*_L) = \frac{1}{L+2K} + \sum_{n=1}^{\infty} \frac{2X(\beta_n)W(\beta_n, x)H(\beta_n)}{K\beta_n Z(\beta_n, L)} \times \exp(-D\alpha_n^2 t/L^2). \quad (18)$$

The survival probability  $S(t|*_0$  or  $*_L)$  is the probability of finding the particle in the unbound state when it was initially in the bound state, either  $*_0$  or  $*_L$ , which can be obtained readily from Eq. (17) as

$$S(t|*_0) = \frac{L}{L+2K} - \sum_{n=1}^{\infty} \frac{2X^2(\beta_n)}{K\beta_n^2 Z(\beta_n, L)} [1 + H(\beta_n)] \times \exp(-D\alpha_n^2 t/L^2). \quad (19)$$

Note that  $S(t|*_L) = S(t|*_0)$  since  $H^2(\beta) = 1$ .

The binding probability  $p(*, t|*)$  that the initially bound state remains bound by time  $t$  can be obtained from Eqs. (4) which hold also for the initially bound state. Accounting for different initial and final states, one can obtain

$$p(*_0, t|*_0) = p(*_L, t|*_L) = \frac{K}{L+2K} + \sum_{n=1}^{\infty} \frac{2X^2(\beta_n)}{K\beta_n^2 Z(\beta_n, L)} \times \exp(-D\alpha_n^2 t/L^2), \quad (20)$$

$$p(*_0, t|*_L) = p(*_L, t|*_0) = \frac{K}{L+2K} + \sum_{n=1}^{\infty} \frac{2X^2(\beta_n)H(\beta_n)}{K\beta_n^2 Z(\beta_n, L)} \times \exp(-D\alpha_n^2 t/L^2). \quad (21)$$

The normalization condition also holds for the initially unbound state.

The equilibrium expressions for the above probabilities can be readily obtained to give

$$\lim_{t \rightarrow \infty} p(x, t) \sim \frac{1}{L+2K}, \quad (22a)$$

$$\lim_{t \rightarrow \infty} p(*_0, t) = \lim_{t \rightarrow \infty} p(*_L, t) \sim \frac{K}{L+2K}, \quad (22b)$$

$$\lim_{t \rightarrow \infty} S(t) \sim \frac{L}{L+2K}. \quad (22c)$$

Since the equilibrium expressions are independent of the initial condition, we omit the initial condition in Eqs. (22). As shown by Eq. (22a), the distribution of the particle is uniformly distributed over the extended system length of  $L + 2K$  at equilibrium. The total concentration in the bound states at equilibrium is given by  $p(*_0, \infty) + p(*_L, \infty) = 2K/(L+2K)$ . Note that  $S(\infty) < 1$  for this system, while the ultimate fate of an isolated pair is always dissociation, namely,  $S(\infty) = 1$ .<sup>18</sup> This is explained by the fact that the particle cannot escape to infinity because of the traps at both ends.

With the above exact solutions, we are now equipped with all the key elements for developing the efficient Brownian dynamics algorithm for the reversible trapping problem. Since no direct interaction is assumed between two traps in the above analysis, we can apply the above exact results in developing the Brownian dynamics algorithm for the trapping problem without loss of accuracy.

This method can also be utilized to simulate the pseudo-first-order system in which both the particle and the traps are mobile. In most simulations, one particle moves or reacts while the remaining particles are fixed during one step. Therefore, the particle can move as in the trapping problem while the trajectory of mobile traps can be calculated as in the target problem.<sup>15</sup> It is well known that the mobility of the particle or the traps can affect the dynamics in the reversible system<sup>16</sup> as well as in the irreversible one.<sup>19</sup> However, the mobility effect has not been fully understood yet because no exact or reliable simulation results have been reported for systems with various mobility. We believe that the present results are useful to study the mobility effect for the pseudo-first-order system since the reliable simulation results can now be obtained for any type of mobility. This method removes not only the limitation of the mobility but also that of the concentration and thus applicable to the second-order system. The present results can be also applied to higher dimensional systems by moving particles along each of the Cartesian coordinates successively.<sup>20</sup> This method is useful for investigating reaction dynamics in the complex geometry frequently encountered in biological systems.

### III. THE REVERSIBLE TRAPPING PROBLEM

We now consider the reversible trapping problem in which many traps are distributed along the line. Unlike the perfect trapping problem in 1D, there can be the following two cases for the reversible system. When the dissociation reaction occurs, the particle bound to the trap can be released to the same or different direction from which it associates. However, for a usual chemical reaction, the particle tends to be bound to the trap and be released to the same direction unless the rotational diffusion of the ‘‘product’’ is so fast that the particle can ‘‘forget’’ the direction while it is in the bound state. Another case would be the recombination of charge carriers<sup>4</sup> for which the particle can be released from the trap randomly. The former case corresponds to the crossing-forbidden trapping problem (CFTP) while the latter can be regarded as the crossing-allowed trapping problem (CATP). The CFTP can be effectively reduced to the problem of a particle between two static traps considered above.

With the perfect traps, the CATP does not exist since the particle cannot jump over a trap without being affected by it. We expect that the difference between the CATP and the CFTP will decrease as the dimensionality of the system increases since the particle is less confined in the higher dimensions.

We first consider the survival probability  $Q(t)$  for an unbound particle when the initial distribution of the particle is uniform:

$$Q(t) = \frac{1}{L} \int_0^L dx_0 S(t|x_0) = \frac{L}{L+2K} + \sum_{n=1}^{\infty} \frac{4X^2(\beta_n)}{L\beta_n^2 Z(\beta_n, L)} [1 + H(\beta_n)] \times \exp(-D\alpha_n^2 t/L^2), \quad (23)$$

which shows the same asymptotic behavior as in Eq. (22c) since it is independent of the initial position. The mean survival probability  $\langle S(t) \rangle$  for an initially unbound particle averaged over all intertrap intervals for the CFTP can be calculated by<sup>8,13</sup>

$$\langle S(t) \rangle = \int_0^{\infty} dL Q(t) w(L), \quad (24)$$

where  $w(L)$  is the weight for an interval  $L$ . We consider two types of trap distributions: periodic and random.

### A. The periodic trap distribution

The mean survival probability for the periodic traps  $\langle S_p(t) \rangle$  in the CFTP can be easily obtained from Eq. (24) with the weight,  $w(L) = \delta(L - c^{-1})$ , as follows:

$$\langle S_p(t) \rangle = \frac{1}{1+2cK} - \sum_{n=1}^{\infty} \frac{4X^2(c\alpha_n i)}{c\alpha_n^2 Z(c\alpha_n i, c^{-1})} [1 + H(c\alpha_n i)] \times \exp(-\alpha_n^2 c^2 D t). \quad (25)$$

It should be noted that the CFTP is indistinguishable from the CATP due to the symmetry of the periodic traps and, therefore, Eq. (25) is the exact solution not only for the CFTP but also for the CATP over the whole time regime for the reversible periodic traps. As previously mentioned, we exclude the situation where the particle can jump over a trap. One can also verify that the equilibrium constant is given by

$$K_{\text{eq}} \equiv \frac{1 - \langle S_p(\infty) \rangle}{c \langle S_p(\infty) \rangle} = 2K. \quad (26)$$

In contrast to the two-trap problem considered in Sec. II, we have to count incoming fluxes of the particle from both sides of a trap for the many-trap problem. This is equivalent to replacing  $k_a$  by  $2k_a$  and, hence, the equilibrium constant becomes twice the usual expression of  $k_a/k_d$ .

For the irreversible perfect traps ( $k_a \rightarrow \infty$  and  $k_d = 0$ ) Eq. (25) reduces to<sup>13</sup>

$$\langle S_p(t) \rangle = \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp[-c^2(2n+1)^2 \pi^2 D t]. \quad (27)$$

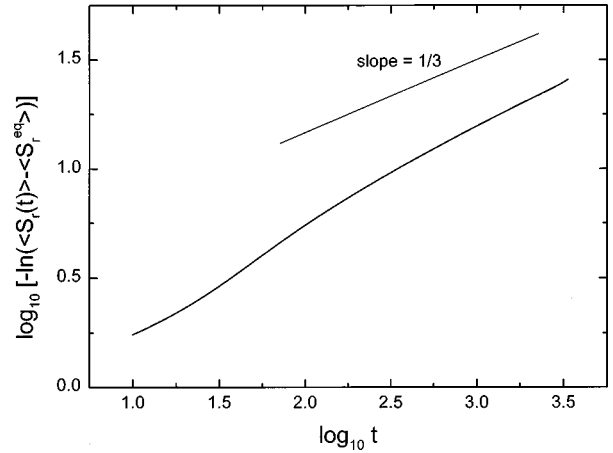


FIG. 1. The long time relaxation behavior of the concentration deviation,  $\langle S_r(t) \rangle - \langle S_r^{\text{eq}} \rangle$ , for the random CFTP. Note that the long time slope of 1/3 on a log-log scale is clearly shown in the figure.

Note that, for the periodic traps, the mean survival probability is governed by  $\exp(-t)$  for both reversible and irreversible cases at long times, namely, the same decay law as in the classical kinetics. This can be explained by the lack of fluctuation effect for the periodic traps. It is interesting that the mean survival probability of the trapping problem can decay *faster* than that of the irreversible target problem which shows the familiar  $\exp(-t^{1/2})$  long time behavior due to the fluctuation effect.

### B. The random trap distribution

The mean survival probability for the random traps  $\langle S_r(t) \rangle$  in the CFTP can be evaluated again from Eq. (24) with the well known weight,<sup>8,13</sup>  $w(L) = c^2 L \exp(-cL)$ , to give

$$\langle S_r(t) \rangle = \langle S_r^{\text{eq}} \rangle + \int_0^{\infty} dL \sum_{n=1}^{\infty} \frac{4c^2 X^2(\beta_n)}{\beta_n^2 Z(\beta_n, L)} [1 + H(\beta_n)] \times \exp[-(D\alpha_n^2 t/L^2) - cL], \quad (28)$$

where

$$\langle S_r^{\text{eq}} \rangle = \int_0^{\infty} dL \frac{c^2 L^2}{L+2K} \exp(-cL) = 1 - 2cK + (2cK)^2 \exp(2cK) E_1(2cK), \quad (29)$$

with  $E_1(z) \equiv \int_z^{\infty} dt e^{-t}/t$  the exponential integral.<sup>21</sup> Note that  $\langle S_r^{\text{eq}} \rangle \sim (cK)^{-1}$  for large  $cK$  and  $\langle S_r^{\text{eq}} \rangle \sim 1 - 2cK - (2cK)^2 \ln(2cK)$  for small  $cK$ . For the irreversible perfect traps, Eq. (28) reduces correctly to Eq. (11) of Ref. 13.

The long time asymptotic behavior of the second term of Eq. (28),  $\langle S_r(t) \rangle - \langle S_r^{\text{eq}} \rangle$ , which corresponds to the concentration deviation, becomes  $\sim \exp(-\text{const} \cdot t^{1/3})$  which can be obtained by the same technique used for the perfect traps. We also check this behavior numerically in Fig. 1. The figure clearly shows that the slope converges to 1/3 in the long time limit. We set the parameters as  $D = k_a = k_d = 1$  and  $c = 0.1$ . We find that summation over 16 terms ( $n = 16$ ) is enough for

our purpose and the numerical integration is performed over  $10^3$  points along  $L$  which is truncated at  $L = 100$  to obtain the converged result.

The CATP for the random traps has never been solved exactly. However, the long time asymptotic expressions have been reported.<sup>22,23</sup> The asymptotic result of the average survival probability for the random traps in 1D is given by<sup>23</sup>

$$\lim_{t \rightarrow \infty} \langle S_r(t) \rangle \sim \frac{1}{1 + cK_{\text{eq}}} + \frac{K_{\text{eq}}}{(1 + cK_{\text{eq}})^{3/2}} \frac{1}{\sqrt{\pi Dt}} \quad (\text{CATP}). \quad (30)$$

A comparison of Eq. (28) and Eq. (30) reveals that, for the random traps, the CFTP is different from the CATP not only in the asymptotic temporal behavior but also in the equilibrium concentration. By using the inequality relation,<sup>21</sup>  $e^x E_1(x) > (1+x)^{-1}$ , the equilibrium concentration in the CFTP is proven to be always higher than that of the CATP, namely,  $\langle S_r^{\text{eq}} \rangle > (1 + 2cK)^{-1}$ . On the other hand, the rate of approach to equilibrium for the CFTP is faster than that for the CATP, namely,  $\sim \exp(-\text{const} \cdot t^{1/3})$  vs  $\sim t^{-1/2}$ . This may be due to the fact that equilibration should be achieved independently in each of all intervals among traps for the CFTP while it should be done over the whole range for the CATP.

The equilibrium concentration of the CATP for the random traps is the same as that of the periodic traps and, therefore, it is also not affected by the fluctuation. It is well known that the fluctuation effect can change the asymptotic relaxation behavior.<sup>24-27</sup> For the target problem the initial fluctuation in the distribution of traps can disappear as the traps become mobile. For the CATP the fluctuation remains longer to make the approach to the equilibrium slower than that of the target problem. But the fluctuation disappears eventually since a particle can cross traps by reaction and the equilibrium concentration becomes the same as that of the target problem. On the other hand, the fluctuation does not disappear for the CFTP and its effect remains to be so large as to change not only the asymptotic behavior but also the equilibrium concentration. Here we have shown for the first time that the fluctuation effect can also change the equilibrium concentration itself.

We plot the ratio of the equilibrium concentration of the CFTP to that of the CATP for the random trap distribution in Fig. 2. For larger values of  $cK$ , the difference between the equilibrium concentrations becomes larger. This can be explained by the fact that the probability of finding the particle in the trap-free region for the CATP gets smaller than that of the CFTP because traps are crossing-allowed. Moreover, the probability gets even smaller for large values of  $cK$  since traps can be crossed more easily as the trap concentration becomes high and the trap-free region is reduced. However, this effect is smeared out when the trap concentration becomes very small and the ratio is reduced to 1. Note that the ratio reaches the limiting value of 2 as the value of  $cK$  gets very large which can be seen from the limiting expression  $\langle S_r^{\text{eq}} \rangle \sim (cK)^{-1}$  for large  $cK$ .

The long time asymptotic behavior of the average survival probabilities for the periodic and random trap distribu-

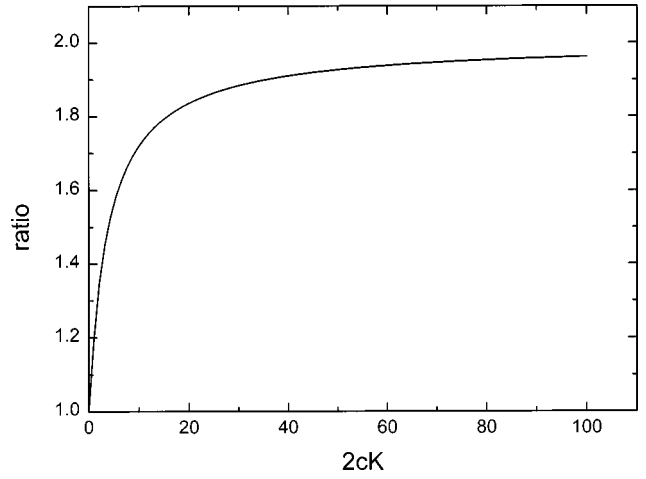


FIG. 2. The concentration dependence of the ratio of the equilibrium concentration of the CFTP to that of the CATP for the random trap distribution.

tions for the CFTP and the CATP are summarized as follows:

$$\lim_{t \rightarrow \infty} \langle S_p(t) \rangle \sim (1 + 2cK)^{-1} \sim \exp(-\text{const} \cdot t) \quad (\text{CFTP, CATP}), \quad (31)$$

$$\lim_{t \rightarrow \infty} \langle S_r(t) \rangle \sim (1 + 2cK)^{-1} \sim t^{-1/2} \quad (\text{CATP}), \quad (32)$$

$$\lim_{t \rightarrow \infty} \langle S_r(t) \rangle - \langle S_r^{\text{eq}} \rangle \sim \exp(-\text{const} \cdot t^{1/3}) \quad (\text{CFTP}). \quad (33)$$

Other interesting quantities such as the probability for returning to the origin can be exactly derived from the above results and the effect of a linear potential for the present system can also be exactly derived. These results will be reported elsewhere.

#### IV. CONCLUDING REMARKS

We have presented the exact survival and binding probabilities of one particle between two static reversible traps in 1D for the continuous diffusion model. These are the most general results that can be reduced to the previous other results. The limitations of the efficient Brownian dynamics simulation method on the mobility of particles can now be greatly removed by utilizing these solutions. Therefore, the present results serve not only to explain the experimental results but also to obtain the exact numerical results for many particle problems. We have also obtained the exact analytical result for the trapping problem in 1D for a periodic distribution of reversible traps for both the CFTP and the CATP. For a random distribution of reversible traps, the exact mean survival probability has been obtained only for the CFTP and its long time behavior has been compared with that of the CATP. From this comparison, it has been revealed that the fluctuation effect of the trap density changes not only the asymptotic relaxation behavior but also the equilibrium concentration itself.

## ACKNOWLEDGMENTS

This work was supported by a grant (1998-015-D00148) from the Basic Science Research Program, Ministry of Education and by the Korea Science and Engineering Foundation through the Center for Molecular Catalysis at Seoul National University. H.K. thanks the Ministry of Education for the Brain Korea 21 Fellowship.

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