FRACTIONAL EXPONENTIAL DECAY IN THE CAPTURE OF LIGANDS BY RANDOMLY DISTRIBUTED TRAPS IN ONE DIMENSION

bernard j. geurts and frederik w. wiegel
center for theoretical physics,
twente university,
op. box 217,
enschede 7500 ae,
the netherlands

in many biophysical and biochemical experiments one observes the decay of some ligand population by an appropriate system of traps. we analyse this decay for a one-dimensional system of randomly distributed traps, and show that one can distinguish three different regimes. the decay starts with a fractional exponential of the form \( \exp\left[-\left(t/t_0\right)^{1/2}\right] \), which changes into a fractional exponential of the form \( \exp\left[-\left(t/t_1\right)^{1/3}\right] \) for long times, which in its turn changes into a pure exponential time dependence, i.e. \( \exp\left[-t/t_2\right] \) for very long times. with these three regimes, we associate three time scales, related to the average trap density and the diffusion constant characterizing the motion of the ligands.

1. introduction. in many biophysical and biochemical experiments one observes the decay of some ligand population due to capture by an appropriate system of traps. in this paper we consider the decay of an initially homogeneous ligand population due to capture by a one-dimensional system of randomly distributed ideal point traps. as an example, one may think of the diffusion of a number of repressors along a dna-molecule, followed by their binding to the corresponding operators. the advantage of studying this problem in a strictly one-dimensional geometry is that most questions can be answered analytically.

it will be shown that for such a system, the average ligand decay starts with a square root exponential, i.e. \( \exp\left[-\left(t/t_0\right)^{1/2}\right] \), which turns into a decay of fractional exponential type for long times, i.e. \( \exp\left[-\left(t/t_1\right)^{1/3}\right] \). this behaviour in turn approaches a decay which is of the pure exponential type, i.e. \( \exp\left[-t/t_2\right] \), for very long times. fractional exponential decay types occur in the relaxation of a great variety of complex systems (ngai and wright, 1984). of course, this kinetic behaviour is completely different from the pure exponential decay which is usually assumed in the interpretation of such processes.

in section 2 we calculate the time dependence of the number of ligands for a special realization of the system, and show that it can be written as the sum of pure exponential decays. in section 3 the average ligand decay for long systems
is determined. The decay is characterized by a square root exponential for short times, by another fractional exponential for long times and by a pure exponential for very long times. Some concluding remarks are collected in Section 4.

2. Ligand Decay for a Special Realization of the System. Consider a system of \( M \) ideal point traps, randomly distributed on a line segment of length \( L \). On this line segment we place \( N_0 > M \) ligands which are assumed to diffuse along the line. For convenience we assume that the initial ligand distribution is homogeneous. A special realization of the system has traps at \( 0 \leq x_1 \leq x_2 \leq \cdots \leq x_M \leq L \). The endpoints \( x_0 = 0 \), and \( x_{M+1} = L \) will be treated as traps as well. Since the system is supposed to be large, boundary effects can be neglected and it is only for convenience that the endpoints are treated as traps.

The ligands are assumed to diffuse along the line; their motion is characterized by a diffusion constant \( D \). Essential for this system is that a ligand which initially \((t = 0)\) is found located between two traps, will remain there, until it is captured by one of them. Hence, the system decomposes into a large number of small subsystems consisting of a certain number of ligands and two traps at the endpoints, say at \( x_j \) and \( x_{j+1} \).

Let \( c_j \) denote the number density of ligands in the \( j \)th subsystem. One obtains, after introducing the new variable

\[
s = x - \frac{x_j + x_{j+1}}{2},
\]

the diffusion equation for the evolution of \( c_j(s, t) \),

\[
\frac{\partial c_j(s, t)}{\partial t} = D \frac{\partial^2 c_j(s, t)}{\partial s^2},
\]

with boundary conditions

\[
c_j(-\frac{1}{2}l_j, t) = c_j(\frac{1}{2}l_j, t) = 0
\]

where \( l_j = x_{j+1} - x_j \). Initially, the distribution of ligands is assumed to be homogeneous,

\[
c_j(s, 0) = \frac{N_0}{L}
\]

for \(-\frac{1}{2}l_j < s < \frac{1}{2}l_j\). The long-time behaviour of the decay of ligands, which will be derived below, is independent of the precise form of the initial distribution. The homogeneous initial situation is assumed only for convenience. It is straightforward to show that the solution of (2)–(4), is given by

\[
c_j(s, t) = \frac{4N_0}{\pi L} \sum_{k=1}^{\infty} \frac{(-1)^k+1}{(2k-1)} \cos \left( \frac{(2k-1)\pi s}{l_j} \right) \exp \left[ -\left( \frac{2k-1}{l_j} \right)^2 \pi^2 D t \right].
\]