

## Self-segregation in chemical reactions, diffusion in a catalytic environment and an ideal polymer near a defect

P K DATTA and A M JAYANNAVAR

Institute of Physics, Sachivalaya Marg, Bhubaneswar 751 005, India

MS received 11 October 1991; revised 4 December 1991

**Abstract.** We study a family of equivalent continuum models in one dimension. All these models map onto a single equation and include simple chemical reactions, diffusion in presence of a trap or a source and an ideal polymer chain near an attractive or repulsive site. We have obtained analytical results for the survival probability, total growth rate, statistical properties of nearest-neighbour distribution between a trap and unreacted particle and mean-squared displacement of the polymer chain. Our results are compared with the known asymptotic results in the theory of discrete random walks on a lattice in presence of a defect.

**Keywords.** Diffusion; survival probability; nearest-neighbour density distribution; partial trap; self-segregation.

PACS Nos 82-20; 05-40; 02-50

### 1. Introduction

The subject of random walks in presence of defects has been extensively studied over several years and is now a classical subject by itself (Haus and Kehr 1987; Havlin and ben-Avraham 1987; Weiss and Rubin 1983). Most of the earlier studies were restricted to defects which being immobile traps (quenched defects). The motivations were the study of various reactions in physical, chemical as well as in biological sciences. Some of the examples include the migration of optical excitations (excitons) in solids which terminate upon reaching a trapping site (in this case the energy of excitons is dissipated or converted into other form of energy at the trapping site), diffusion-controlled reactions, dielectric relaxation, chemical binding of interstitial hydrogen in metals by impurities etc (Havlin and ben-Avraham 1987). A relatively good understanding of the survival probability or the rate at which the random walkers decay in such a media has now emerged (Balagurov and Vaks 1975; Grassberger and Procaccia 1982; Donsker and Varadhan 1979). It should also be noted that most of the analytical results are obtained in asymptotic (time) domain. Several extensions of the above mentioned phenomena are being studied extensively, namely, motions on fractal media (Webman 1984), interaction effects (Bunde *et al* 1985, 1986) and quantum effects (Parris 1989; Jayannavar 1991b). Very recently (Jayannavar 1991b) it has been explicitly shown that the well-known results on the asymptotic average survival probability (ASP) are difficult to observe in real physical situations. This is due to the fact that the ASP is a non-self averaging quantity i.e., the fluctuations dominate the mean value in asymptotic domain. Now we hope that

the study of the fluctuation effects in the ensemble of macroscopically identical samples will emerge. One can also treat the defects as catalytic sources of diffusing particles (random walkers) (ben-Avraham *et al* 1989; Redner and Kang 1984; Valsakumar and Murthy 1990; Jayannavar and Köhler 1990). This problem is equally relevant to the production of neutrons and population dynamics (Ebeling *et al* 1984).

In this paper we study the motion of diffusing particles in the presence of a single defect in one dimension. We exploit the analogy to various other fields. We have obtained explicit results for the survival probability, total growth rate, statistical properties of nearest-neighbour distance at a trap and mean-squared displacement of the polymer near the attractive site. All these quantities will be defined in the sections to follow. Several studies exist on the problems of discrete random walks on one-dimensional lattice in the presence of single defect (trap or source) (Weiss and Rubin 1983; Weiss 1981; Redner and Kang 1984; ben-Avraham *et al* 1989); however, some of the analytical results can be obtained only in the asymptotic (time) domain. Basically we have studied a continuum version of these problems and obtained some exact results, valid for all time ( $t$ ). We recover the known asymptotic results in the appropriate limit. Within a continuum description, the particle density obeys the reaction-diffusion equation (ben-Avraham *et al* 1989; Jayannavar and Köhler 1990),

$$\frac{\partial P(x, t)}{\partial t} = D \frac{\partial^2 P(x, t)}{\partial x^2} + V \delta(x) P(x, t), \quad (1)$$

where  $P(x, t)$  is the particle density,  $D$  is the diffusion constant. The defect is located at the origin ( $x = 0$ ) and represents a source or a trap respectively, when  $V \geq 0$ . The trapping reaction  $A + B \rightarrow B$  is one of the simplest models for the diffusion-controlled reactions in physical, chemical and biological sciences (Taitelbaum *et al* 1990). We consider a system of mobile identical particles ( $A$  type) diffusing in one dimension in the presence of an imperfect static trap ( $B$ ). Partial reaction takes place when  $A$  particles come in contact with  $B$  particles ( $V$  is proportional to local reaction rate). This can also be thought of as a reaction between activated  $A$  chemical species, which arrive at the trap (catalyst), get deactivated and converted into some other chemical species. It is now well known that due to the reaction, self-organization takes place among the diffusing particles. This self organization can be expressed in terms of a depletion zone for  $A$  particles formed around the trap leading to self-segregation. A measure of such self-organization can be characterized in terms of statistical properties of the distance from the trap to nearest unreacted  $A$  particles (Weiss *et al* 1989) which will be studied in §(3.2). The gradual development of correlations among the reacting particles leads to a dramatic deviation in the global reaction kinetics as compared to the earlier traditional studies in physical chemistry (Smoluchowski 1917). Another measure of the self-segregation is referred to as  $\theta$ -distance, i.e. a distance from the trap to a point where the concentration of  $A$ 's is equal to a given fraction  $\theta$  of its bulk value (Havlin *et al* 1990; Taitelbaum 1991).

Equation (1) can also be interpreted as an unnormalized probability density of an ideal polymer of length  $l$  ( $\equiv t$ ) in the presence of a single attractive or repulsive impurity (Nattermann and Renz 1989), respectively, when  $V \geq 0$ . In §§(3.3) and (4.2) we calculate the mean-squared end-to-end distance (MSEED) of a polymer in the presence of repulsive and attractive impurity, respectively, given that initially one end of the polymer is fixed on the defect site (Majumdar 1990; ben-Avraham *et al* 1989).

Furthermore, when the potential term in (1), i.e.,  $V\delta(x)$ , is replaced by  $iV(x)$ , where  $i$  is the imaginary quantity and  $V(x)$  being random, the problem reduces to that of spin depolarization of a diffusing particle in an environment with random magnetic fields (Jayannavar and Köhler 1990). The replacement of the potential by a random space-time dependent potential  $V(x, t)$  coupled with some additional transformations maps the eq. (1) onto the fluctuations on growing interfaces, randomly stirred flows, directed polymer in random media and interface problems in the two dimensional Ising spin system, etc. (Kardar *et al* 1986; Medina *et al* 1989).

## 2. Mathematical method

One can readily notice that (1) is similar to the quantum problem of a single particle moving in a delta-function potential (Jayannavar and Köhler 1990). In particular, if we replace time  $t$  by the imaginary time  $(-it)$ ,  $1/2m$  by  $D$ , and  $V\delta(x)$  by  $-V\delta(x)$  in Schrödinger equation ( $\hbar = 1$ ) we get (1). Using this identification one can immediately write down the eigenfunctions and eigenvalues of (1) from the known results in quantum problems (Postma 1984; Blinder 1988). Due to the basic symmetry in the problem one can readily write down the eigenfunctions as symmetric (even)  $\Phi_S$  and antisymmetric (odd)  $\Phi_A$  functions. For negative  $V$ ,

$$\Phi_A(x) = \frac{\sin(kx)}{\sqrt{2\pi}} \quad (2a)$$

$$\Phi_S(x) = \frac{1}{\sqrt{2\pi} \left(1 + \frac{V^2}{k^2 D^2}\right)^{1/2}} \left[ \cos(kx) + \frac{|V|}{kD} \sin(k|x|) \right]. \quad (2b)$$

Eigenvalues associated with  $\Phi_A(x)$  and  $\Phi_S(x)$  are  $E(k) = k^2 D$ . If  $V$  is positive

$$\Phi_A(x) = \frac{\sin(kx)}{\sqrt{2\pi}}. \quad (3a)$$

$$\Phi_S(x) = \frac{1}{\sqrt{2\pi} \left(1 + \frac{V^2}{k^2 D^2}\right)^{1/2}} \left[ \cos(kx) - \frac{V}{kD} \sin(k|x|) \right] \quad (3b)$$

$$\Phi_B(x) = \sqrt{\alpha} \exp(-\alpha|x|). \quad (3c)$$

Eigenvalues associated with solutions (3a) and (3b) are  $E(k) = k^2 D$  and the eigenvalue associated with the bound state solution  $\Phi_B(x)$  is given by  $E_B = -\frac{1}{4}(V^2/D)$  and  $\alpha = (V/2D)$ . In the literature such solutions can be found in the discrete version of quantum problems e.g., the one-dimensional tight-binding Hamiltonian in the presence of a single defect (Bílek and Skála 1986). If the initial condition for particle density  $P(x, t=0)$  is given, then the general solution for (1) can be written down explicitly as,

$$P(x, t) = \sum_i C_i \Phi_i(x) \exp(-E_i t) \quad (4)$$

where  $C_i = \int_{-\infty}^{\infty} P(x, t=0) \Phi_i(x) dx$ ,  $\Phi_i(x)$ 's are the complete set of eigenfunctions.

### 3. Solutions when the defect site is a partial trap ( $V < 0$ )

In this section we explicitly use the eigenfunctions (2a) and (2b) to calculate various physical quantities.

#### 3.1 Survival probability of diffusing particles

The survival probability of diffusing particles is defined as  $P_s(t) = \int_{-\infty}^{\infty} P(x, t) dx$ . It is clear from (1) that  $P_s(t)$  is not a conserved quantity and it can be interpreted as the probability for a diffusing particle to survive until time  $t$  without being trapped. In principle this quantity can be related to the global reaction rate. One way to define the reaction rate is that after calculating  $P_s(t)$  we rewrite it in a differential form namely  $dP_s(t)/dt = -\lambda(t)P_s(t)$ , where  $\lambda(t)$  defines the time-dependent reaction rate. However, this definition is not unique. For simplicity we consider a diffusing particle to be at the origin at time  $t = 0$ , i.e.,  $P(x, t = 0) = \delta(x)$ . Now using the known eigen-solutions and eq. (4), we obtain a closed form solution for the survival probability as

$$P_s(t) = \exp(V^2 t/D) \operatorname{erfc}(V\sqrt{t/D}) \quad (5)$$

where  $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$  and  $\operatorname{erf}(x) = 2/\sqrt{\pi} \int_0^x \exp(-y^2) dy$ .

This result is exact and valid for all time  $t$ . In figure 1 we have plotted  $P_s(t)$  as a function of  $t(V^2/D)$ . In the small time domain ( $t < D/V^2$ ),  $P_s(t) \sim 1 - 2V\sqrt{t/\pi D}$  and in the asymptotic domain ( $t \rightarrow \infty$ ) it is given by

$$P_s(t) \sim \frac{1}{V} \sqrt{\frac{D}{\pi t}} \left[ 1 - \frac{D}{2V^2 t} \right].$$

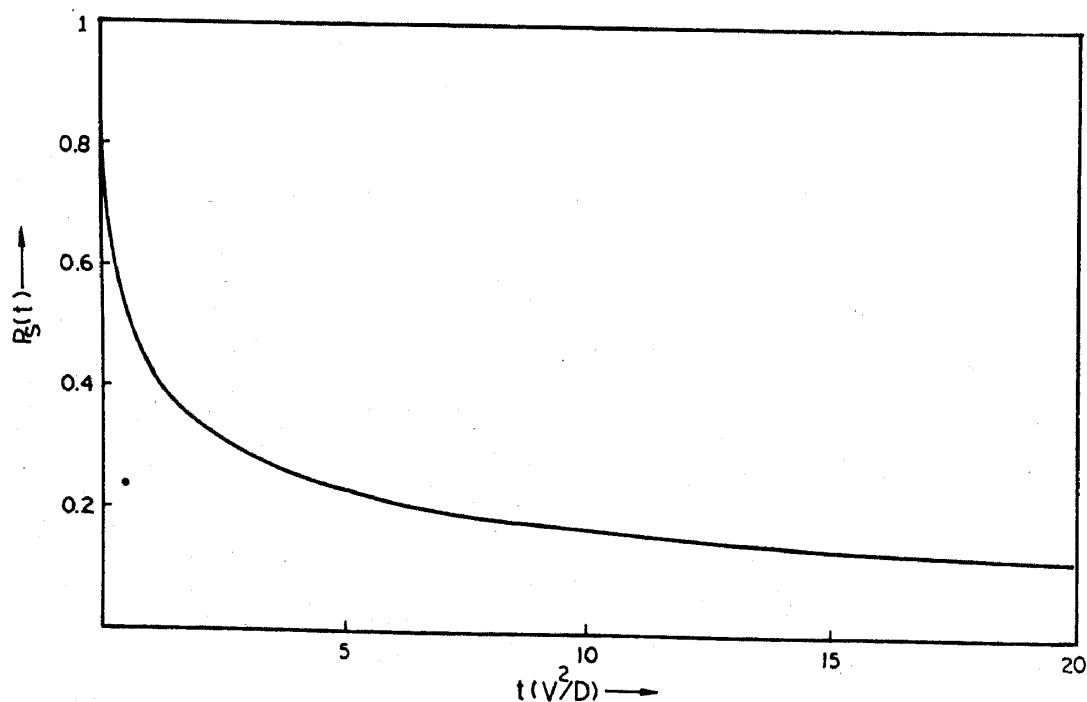


Figure 1. Plot for the survival probability  $P_s(t)$  as a function of rescaled time  $tV^2/D$ .

This asymptotic dependence ( $t^{-1/2}$ ) agrees with the result obtained by ben-Avraham *et al* (1989) and this is a special feature of one-dimensional system, where random walk is recurrent.

### 3.2 Statistical properties of the nearest-neighbour distance at a single imperfect trap

In the previous studies on one-dimensional problem, the trap is treated as either perfect (Weiss *et al* 1989) or imperfect with radiation boundary condition (Taitelbaum *et al* 1990). In the perfect trap, diffusing particles arriving at the trap site are absorbed instantaneously, whereas in the imperfect trap with the radiation boundary condition, a partial absorption takes place at the trap site, rest being reflected by the trap. It should be noted that in both cases a diffusing particle on one side of the trap never crosses to the other side of the trap. In our treatment we remove such a restriction, i.e., diffusing particles impinging on a trap can partially get absorbed and partially move away to either side of the trap. Such a situation is relevant to several physical systems, say for example the motion of excitons (energy transport) or other elementary excitations in molecular aggregates in the presence of quenched impurities which act like traps. However, we show that our exact results are equivalent to those obtained by using the radiation boundary condition, only when initial particles are uniformly distributed throughout the space ( $-\infty$  to  $+\infty$ ) with an appropriate *redefinition* of coefficients. This equivalence is a coincidence. For a particular choice of initial condition, namely  $P(x, t=0) = \delta(x - x_0)$ , one gets

$$P(x, t|x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-k^2 t D) \left[ \sin(kx) \sin(kx_0) + \frac{\{\cos(kx) + (V/kD)\sin(k|x|)\} \{\cos(kx_0) + (V/kD)\sin(k|x_0|)\}}{1 + (V^2/k^2 D^2)} \right] dk. \quad (6)$$

Integrals in the above expression can be evaluated exactly, but the final result for  $P(x, t|x_0)$  is too long to reproduce here.

Now given an expression for  $P(x, t|x_0)$  we can study the statistical properties of the nearest-neighbour distance. Following the analysis of Weiss *et al* (1989), let  $Q(L, t)$  be the probability that the nearest-neighbour particle is located at a distance  $\geq L$  from the origin. This distribution function is given by

$$Q(L, t) = \exp \left[ -c \int_0^L dx \int_{-\infty}^{\infty} P(x, t|x_0) dx \right], \quad (7)$$

where  $c$  is the initial constant density of the diffusing particles. We have assumed that initially the particles are distributed uniformly throughout the space, i.e., from  $-\infty$  to  $+\infty$  and we are considering the *one-sided* distribution function only. The one-sided probability density function (PDF) of the nearest-neighbour distance from the trap is given by  $f(L, t) = -(\partial Q / \partial L)$ . The double integral in (7) can be readily evaluated using (6), leading to the result

$$Q(L, t) = \exp \left[ -c \left\{ \text{Lerf} \left( \frac{L}{2\sqrt{Dt}} \right) - 2 \left( \frac{Dt}{\pi} \right)^{1/2} (1 - \exp(-L^2/4Dt)) \right\} \right]$$

$$\begin{aligned}
& + \frac{D}{V} \left[ \exp(-L^2/4Dt) \exp(V\sqrt{t/D} + (L/2\sqrt{Dt}))^2 \right. \\
& \quad \left. \operatorname{erfc} \left[ V \left( \frac{t}{D} \right)^{1/2} + \frac{L}{2\sqrt{Dt}} \right] - \exp(V^2 t/D) \operatorname{erfc} \left[ V \left( \frac{t}{D} \right)^{1/2} \right] \right. \\
& \quad \left. + \operatorname{erf} \left( \frac{L}{2\sqrt{Dt}} \right) \right] \Bigg\}. \quad (8)
\end{aligned}$$

Differentiating (8) with respect to  $L$  one can evaluate  $f(L, t)$ . Equation (8) is our exact result and it coincides with the result obtained by Taitelbaum *et al* (1990), if we *redefine* our  $(V/D)$  by  $\kappa$ . In Taitelbaum *et al* (1990),  $\kappa$  is a measure of the reaction strength and appears as a constant in the radiation boundary condition. Equivalence of our result to that by Taitelbaum *et al* (1990) is somewhat accidental, given that our expression of  $P(x, t|x_0)$  is completely different and does not obey the radiation boundary condition. Moreover, imposition of the radiation boundary condition prevents particle communication from one side of the trap to the other, whereas in our treatment such a restriction does not exist. The similarity of our result to that by Taitelbaum *et al* (1990) can be understood as follows. Since in our treatment, initially, particles are uniformly distributed throughout the space, the solution of  $P(x, t)$  is symmetric for all time. When the particles arrive at the trap from the right hand side, some of them are partially absorbed while the remaining particles symmetrically diffuse away to either side of the trap. The same thing is true for particles coming from the left hand side. Now due to the symmetry one can think that particles arriving at the trap from the right are partially absorbed while the rest are reflected back. This is because the number of particles (or flux) which are transmitted to the left are exactly compensated by the transmitted particles (flux) arriving at the trap from the opposite side. Hence, on this physical ground we expect the results to be similar, but with *redefined* coefficients.

It should also be remembered that in the limit of  $V \rightarrow +\infty$  we obtain the result for a perfect trap (Weiss *et al* 1989) and for  $V \rightarrow 0$  we recover the result for no trap. In the case of the problem with radiation boundary condition (Taitelbaum *et al* 1990),  $\kappa \rightarrow 0$  implies that the trap becomes a reflector. If initially particles are distributed throughout the space with no trap or a perfect reflector, then the probability density does not evolve in time and hence we obtain the same result,  $Q(L, t) = \exp(-cL)$ . Using similar analysis (Weiss *et al* 1989) the PDF for the nearest-neighbour particle of the trap is given as

$$\begin{aligned}
f(L, t) = c \left[ \exp \left( \frac{V^2 t}{D} + \frac{VL}{D} \right) \operatorname{erfc} \left( V \left( \frac{t}{D} \right)^{1/2} + \frac{L}{2\sqrt{Dt}} \right) \right. \\
\left. + \operatorname{erf} \left( \frac{L}{2\sqrt{Dt}} \right) \right] Q(L, t). \quad (9)
\end{aligned}$$

For small time as  $t \rightarrow 0$ ,  $Q(L, t)$  behaves like  $\exp(-cL)$  as expected. For  $V(t/D)^{1/2} \gg 1$  and  $Dt \gg L^2$ , the function  $Q(L, t)$  takes a Gaussian form with a peak at  $L = -D/V$ ,

$$Q(L, t) \sim \exp \left[ -\frac{c}{2\sqrt{\pi Dt}} \left\{ \left( L + \frac{D}{V} \right)^2 - \left( \frac{D}{V} \right)^2 \right\} \right]. \quad (10)$$

Consequently in the same limit one can write down an expression for  $f(L, t)$  as

$$f(L, t) \sim \frac{c}{\sqrt{\pi Dt}} \left( L + \frac{D}{V} \right) Q(L, t). \quad (11)$$

From (11) the asymptotic value of the average distance  $\langle L(t) \rangle$  from the trap to the nearest-neighbour untrapped particle is found to be

$$\langle L(t) \rangle \sim \frac{\pi^{3/4} (Dt)^{1/4}}{\sqrt{2c}} \exp \left[ \frac{cD^{3/2}}{2V^2 \sqrt{\pi t}} \right] \operatorname{erfc} \left[ \frac{\sqrt{cD^{3/4}}}{\sqrt{2} V (\pi t)^{1/4}} \right], \quad (12)$$

which asymptotically approaches the value  $(Dt)^{1/4}/\sqrt{c}$ , independent of the strength  $V$  of the trap. The reaction rate is directly related to the particle flux at the trap

$$J(t) = -2cD \int_0^\infty \frac{\partial P}{\partial x} \Big|_{x=0} dx_0$$

and is given by

$$J(t) = -cV \exp(V^2 t/D) \operatorname{erfc}(V\sqrt{t/D}), \quad (13)$$

which follows the asymptotic behaviour,  $J(t) \sim -c\sqrt{D/\pi t}$  indicating the anomalous (fractional power dependence on  $t$ ) reaction rate. In figure 2 we have plotted  $f(L, t)$  as a function of  $L(V/D)$ , for  $c = 0.25$ ,  $(V/D) = 1$  and for various values of  $Dt$ . In figure 3 we have plotted  $f(L, t)$  as a function of  $(L/2\sqrt{Dt})$ , for  $Dt = 500$ ,  $c = 0.25$  and for various values of  $V/D$ . In the large time domain  $f(L, t)$  is a time dependent skewed Gaussian function. The large distance (from the trap) form of this function goes over

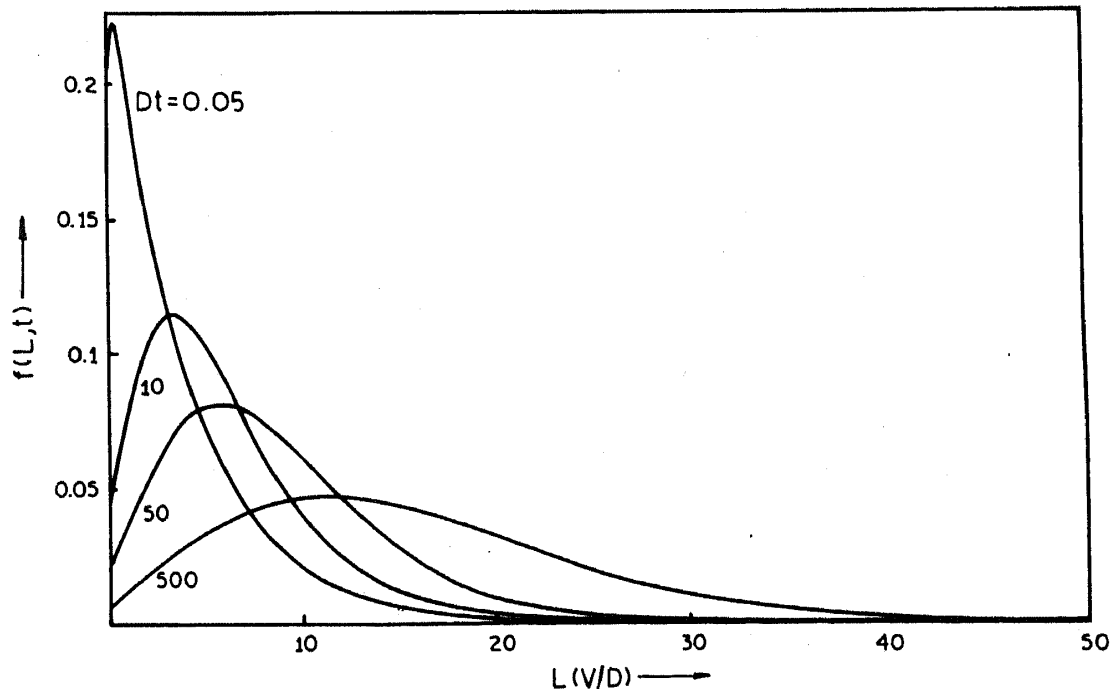


Figure 2. Plot for  $f(L, t)$  as a function of  $L(V/D)$  with parameters  $V/D = 1.0$ ,  $c = 0.25$  and for different values of  $Dt$ .

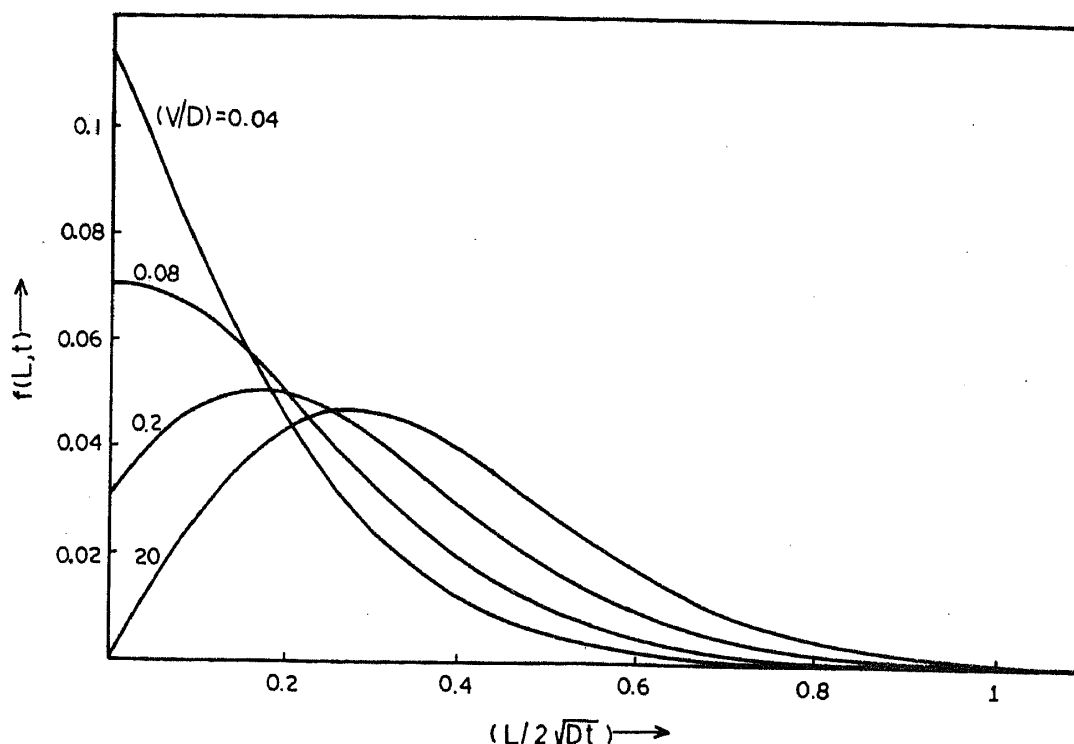


Figure 3. Plot for  $f(L, t)$  as a function of  $(L/2\sqrt{Dt})$  with parameters  $Dt = 500$  and  $c = 0.25$  and for different values of  $V/D$ .

to simple exponential. As mentioned earlier, our solution  $P(x, t|x_0)$  does not obey the radiation boundary condition. We have got totally different result for  $f(L, t)$  as compared to the problem with radiation boundary condition, when the initial distribution is non-uniform and asymmetric. However, as expected in the truly asymptotic domain, the results cross over to those obtained for a perfect trap for arbitrary initial distribution of particles. In the asymptotic regime results are independent of trap strength. This follows from the fact that random walk is a recurrent in one dimension i.e., if a walker (diffusing particle) comes in contact with a defect, it comes in contact infinite number of times and eventually absorbed.

### 3.3 Mean-squared end to end distance of a polymer in presence of a repulsive defect

As mentioned in the introduction, eq. (1) maps onto the polymer problem in the presence of a repulsive defect ( $V < 0$ ). More specifically  $P(x, t)$  should be interpreted as the restricted partition function of one dimensional ideal Gaussian polymer chain of length  $l (\equiv t)$ , the diffusion constant  $D$  being related to Kuhn's step length (Edwards and Muthukumar 1988; Nattermann and Renz 1989). We now assume that one end of the polymer is located on (attached to) the defect site, then MSEED is given by

$$\langle x^2(t) \rangle = \frac{\int_{-\infty}^{\infty} x^2 P(x, t) dx}{\int_{-\infty}^{\infty} P(x, t) dx}. \quad (14)$$

Finally  $t$  should be replaced by the total length  $l$  of the polymer. If we multiply (1)



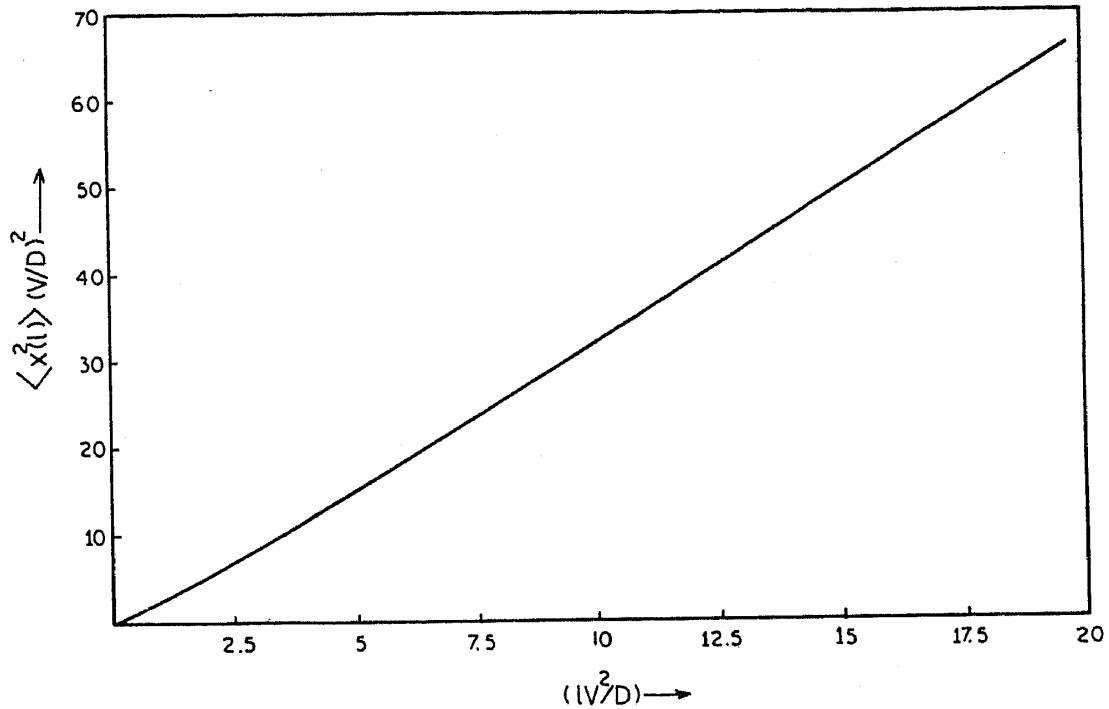


Figure 4. Plot for  $\langle x^2(l) \rangle (V/D)^2$  as a function of  $lV^2/D$ , in presence of a repulsive defect.

by  $x^2$  and integrate over space we get after some algebra,

$$\langle x^2(l) \rangle = \frac{2D \int_0^l P_s(l') dl'}{P_s(l)} = \frac{2D \int_0^l \exp(V^2 l'/D) \operatorname{erfc}(V \sqrt{l'/D}) dl'}{\exp(V^2 l/D) \operatorname{erfc}(V \sqrt{l/D})}. \quad (15)$$

In figure 4 we have plotted rescaled  $\langle x^2(l) \rangle$  as a function of rescaled length  $l$ . In the small length regime [ $l < (D/V^2)$ ], the above result takes the form  $\langle x^2(l) \rangle \sim 2Dl + 4Vl^{3/2}/3\sqrt{D/\pi}$ . In this domain the entropic term associated with the random walk (or the Gaussian polymer chain) dominates over the energy term. Asymptotically  $\langle x^2(l) \rangle \sim 4Dl$ . In the presence of a repulsive defect, polymer swells and asymptotically  $\langle x^2(l) \rangle$  scales linearly with the length  $l$  and is independent of the strength of potential  $V$ . However, the effective diffusion constant (coefficient in front of  $l$ ) is two times as compared to the result in the absence of a defect (ben-Avraham *et al* 1989). It should be mentioned that ideal Gaussian chain performs a random walk, but in the presence of a single defect, repeated visits to the defect site in one dimension induces a long range correlation in the random walk.

#### 4. Solutions when the defect site is a catalytic source ( $V > 0$ )

In this section we use the eigenfunctions (3a), (3b) and (3c) to calculate physical quantities.

##### 4.1 Particle growth in the presence of a single catalytic defect

In (1), positive  $V$  implies that each time a diffusing particle arrives at the defect site, more particles are created with a multiplication rate proportional to  $V$  (Redner and

Kang 1984; ben-Avraham *et al* 1989; Valsakumar and Murthy 1990). The newly created particles along with the others in the medium again create additional particles due to recurrence of random walkers in one dimension. This multiplication process continues as the time progresses. This phenomenon of a random multiplication has been studied (Redner and Kang 1984) for the case of discrete random walks on a lattice with a single catalytic source where the asymptotic result is obtained. In our treatment we assume for simplicity that initially at  $t = 0$ , there is a single diffusing particle on the defect site and we calculate the total growth of the particles (i.e. total number of particles) at a later time  $t$ . This quantity is given by  $P_g(t) = \int_{-\infty}^{\infty} P(x, t) dx$ . One can readily obtain  $P_g(t)$  in a closed form as

$$P_g(t) = 2\exp(V^2 t/4D) - \exp(V^2 t/D) \operatorname{erfc} \left[ V \left( \frac{t}{D} \right)^{1/2} \right]. \quad (16)$$

For initial or short time ( $t < t_c = D/V^2$ ),  $P_g(t)$  is given by  $\sim 1 + 2V(t/\pi D)^{1/2}$ , and for asymptotic time ( $t \rightarrow \infty$ ),  $P_g(t) \sim 2\exp(V^2 t/4D) - 1/V(D/\pi t)^{1/2}$ . As expected in the asymptotic domain, the growth law is purely exponential. The similar exponential behaviour has been obtained for the discrete random walk in the large time (number of steps =  $n$ ) domain,  $P_g(t)$  grows as  $\exp(\alpha n)$ . The coefficient  $\alpha$  is proportional to the bound state energy of a particle on a lattice with a single defect (Redner and Kang 1984). In figure 5 we have plotted  $P_g(t)$  as a function of  $t(V^2/D)$ .

#### 4.2 Mean-squared end to end distance of a polymer in presence of a single attractive impurity

The analysis of this section is same as that of §(3.3). When  $V > 0$ , the defect acts as an attractive impurity (Majumdar 1990) for a Gaussian polymer chain. If one end of

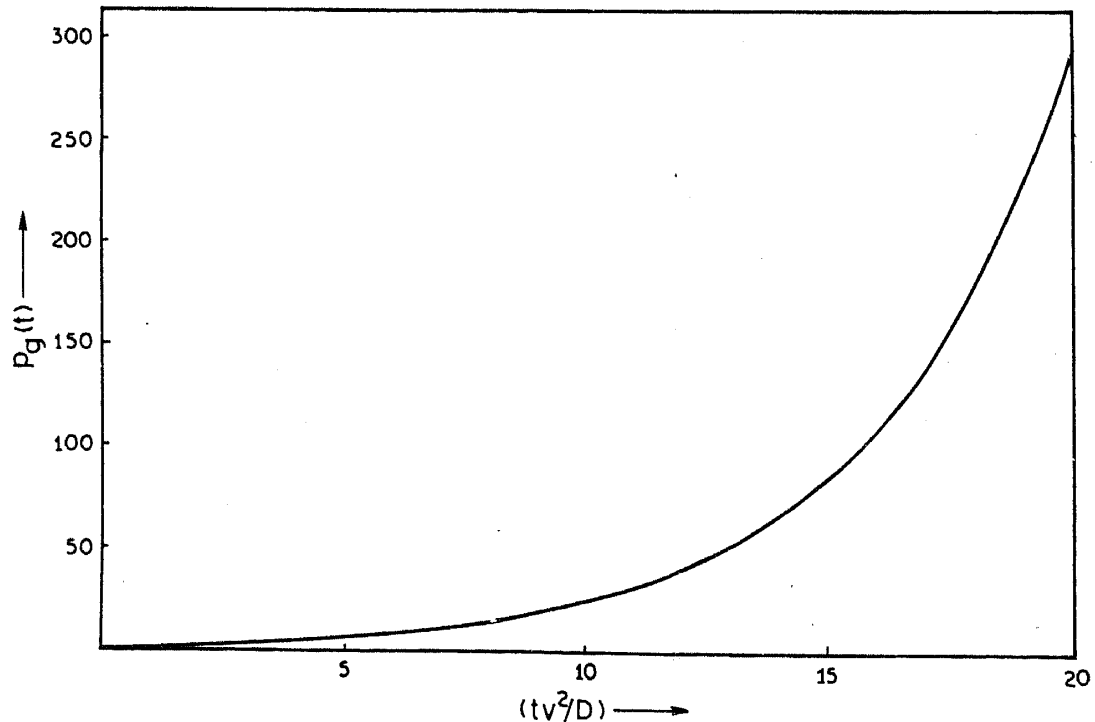


Figure 5. Plot for total growth of particles  $P_g(t)$  as a function of  $tV^2/D$ .

the chain is located at (attached to) the impurity site MSEED is given by

$$\begin{aligned}\langle x^2(l) \rangle &= \frac{2D \int_0^l P_g(l') dl'}{P_g(l)} \\ &= \frac{2D \int_0^l [2\exp(V^2 l'/4D) - \exp(V^2 l'/D) \operatorname{erfc}(V(l'/D)^{1/2})] dl'}{2\exp(V^2 l/4D) - \exp(V^2 l/D) \operatorname{erfc}(V(l/D)^{1/2})}.\end{aligned}\quad (17)$$

In the special case of  $l < D/V^2$ ,  $\langle x^2(l) \rangle \sim 2Dl - 4V(D/\pi)^{1/2} l^{3/2}$ , whereas in the large length regime  $\langle x^2(l) \rangle \sim 8(D/V)^2 - 2D^{3/2}/V(l/\pi)^{1/2} \exp(-V^2 l/4D)$ . Asymptotically the MSEED saturates exponentially to a constant value (ben-Avraham *et al* 1989) equal to  $8(D/V)^2$ . In figure 6 we have plotted rescaled  $\langle x^2(l) \rangle$  as a function of  $l(V^2/D)$ . It should be noted that in the asymptotic (large  $l$ ) domain the size of the polymer is related to the localization length (or size) of the eigenfunction of the lowest eigenvalue associated with Schrödinger equation. This analogy can be extended to a polymer in a quenched random potential. In this case the associated Schrödinger equation maps onto the well-known Anderson localization problem in condensed matter physics. Especially when the random potential is given by a white noise Gaussian form, the localization length approaches zero as we approach the lowest eigenvalue. In this case the size of the polymer collapses to zero or to a finite value when the potential is correlated in space (Nattermann and Renz 1989).

It should also be emphasized that the results obtained for mean squared displacement in § (3.3) and (4.2) are the same for a diffusing particle obeying nonlinear diffusion equation, namely

$$\frac{\partial P_1(x, t)}{\partial t} = D\nabla^2 P_1(x, t) + V\delta(x)P_1(x, t) - VP_1(x, t)P_1(x=0, t). \quad (18)$$

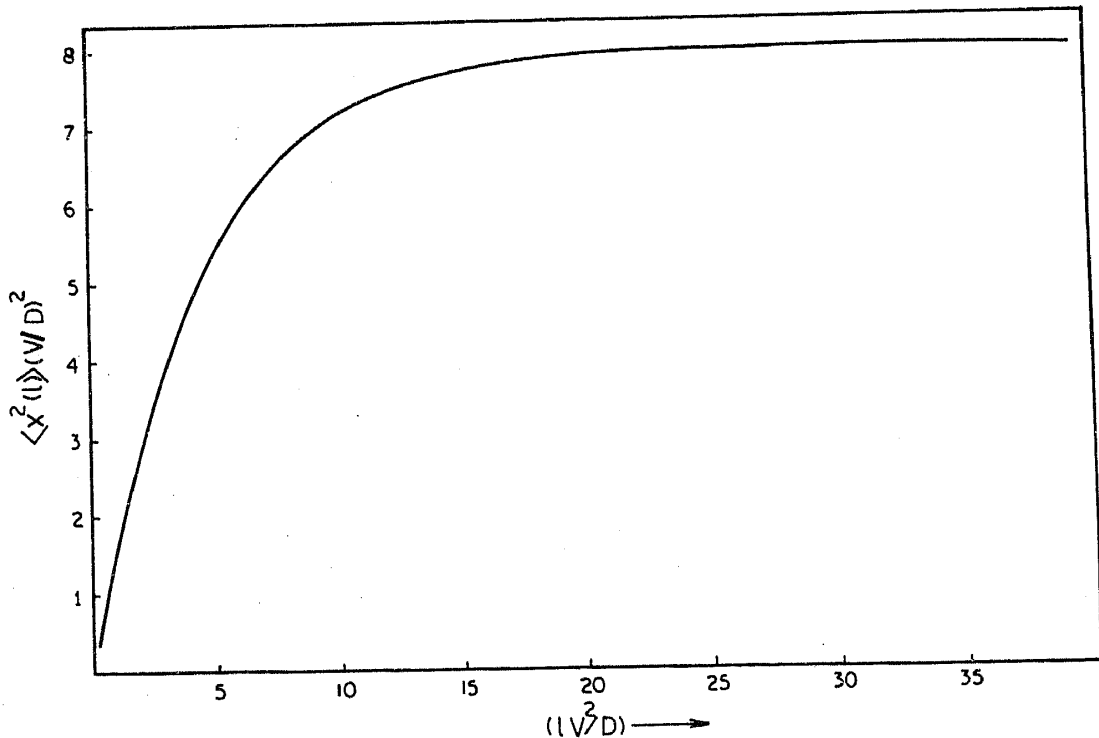


Figure 6. Plot for  $\langle x^2(l) \rangle (V/D)^2$  as a function of  $lV^2/D$  in presence of an attractive defect.

In above equation  $P_1(x, t)$  should be interpreted as a probability density of a particle to be at space point  $x$  and at time  $t$  and  $P_1(x, t)$  is a conserved quantity. This equation has been obtained by writing  $P_1(x, t) = P(x, t) / \int P(x, t) dx$  and using (1).

## 5. Conclusions

We have studied the dynamics of diffusion of particles in one-dimensional medium with a single trap and source. Various physical quantities have been evaluated explicitly using analogies to other areas of physics. In our treatment the defect is static i.e., immobile. The problem of treating a single mobile trap seems to be intractable at present. Only partial answers have been obtained (ben-Avraham and Weiss 1989; Szabo *et al* 1988). We hope that along the similar lines one can easily extend the results to higher dimensions and in the presence of randomly distributed traps. We have already obtained some preliminary results for survival probability and its fluctuations and mean squared displacement of polymers in a random medium both in one and higher dimensions. Work along the direction of understanding growing interfaces in random media and directed polymers in the presence of stochastic random potential is in progress.

## Acknowledgement

Authors thank S Suresh Rao and V S Uma Maheswari for computational help. One of us (AMJ) thank Dr Somendra M Bhattacharjee for useful discussions on various topics mentioned in this paper.

## References

- Balagurov B Ya and Vaks V G 1973 *Zh. Eksp. Theor. Fiz.* **65** 1939 (1974 *Sov. Phys. - JETP* **38** 968)
- ben-Avraham D, Redner S and Cheng Z 1989 *J. Stat. Phys.* **56** 437
- ben-Avraham D and Weiss G H 1989 *Phys. Rev.* **A39** 6436
- Bilek O and Skála L 1986 *Phys. Lett.* **A119** 300
- Blinder S M 1988 *Phys. Rev.* **A37** 973
- Bunde A, Havlin S, Nossal R and Stanley H E 1985 *Phys. Rev.* **B32** 3367
- Bunde A, Moseley L L, Stanley H E, ben-Avraham D and Havlin S 1986 *Phys. Rev.* **A34** 2575
- Donsker M D and Varadhan S R S 1979 *Commun. Pure Appl. Math.* **32** 721
- Ebeling W, Engel A, Esser B and Feistel R 1984 *J. Stat. Phys.* **37** 369
- Edwards S F and Muthukumar M 1988 *J. Chem. Phys.* **89** 2435
- Grassberger P and Procaccia I 1982 *J. Chem. Phys.* **77** 12
- Haus J W and Kehr K W 1987 *Phys. Rep.* **150** 263
- Havlin S and ben-Avraham D 1987 *Adv. Phys.* **36** 695
- Havlin S, Larralde H, Kopelman R and Weiss G H 1990 *Physica* **A169** 337
- Jayannavar A M and Köhler J 1990 *Phys. Rev.* **A41** 3391, and references therein
- Jayannavar A M 1991a *Solid State Commun.* **77** 457
- Jayannavar A M 1991b *Physica* **A179** 243
- Kardar K, Parisi G and Zhang Y C 1986 *Phys. Rev. Lett.* **56** 889
- Majumdar S N 1990 *Physica* **A169** 207
- Medina E, Hwa T, Kardar M and Zhang Y C 1989 *Phys. Rev.* **A39** 3053
- Nattermann T and Renz W 1989 *Phys. Rev.* **A40** 4675

- Parris P E 1989 *Phys. Rev.* **B40** 4928  
Postma B J 1984 *Am. J. Phys.* **52** 725  
Redner S and Kang K 1984 *Phys. Rev.* **A30** 3362  
Smoluchowski M V 1917 *Z. Phys. Chem.* **92** 129  
Szabo A, Zwanzig R and Agmon N 1988 *Phys. Rev. Lett.* **61** 2496  
Taitelbaum H, Kopelman R, Weiss G H and Havlin S 1990 *Phys. Rev.* **A41** 3116  
Taitelbaum H 1991 *Phys. Rev.* **A43** 6592  
Valsakumar M C and Murthy K P N 1990 *Pramana – J. Phys.* **35** 461  
Webman I 1984 *Phys. Rev. Lett.* **62** 357  
Weiss G H 1981 *J. Math. Phys.* **22** 562  
Weiss G H and Rubin R J 1983 *Adv. Chem. Phys.* **52** 363  
Weiss G H, Kopelman R and Havlin S 1989 *Phys. Rev.* **A39** 466, and references therein