Survival probability with random-force-dominated dynamics in the presence of traps

D. Arora, D. P. Bhatia, and M. A. Prasad

Radiological Physics Division, Bhabha Atomic Research Center, Trombay, Bombay 400 085, India (Received 10 January 1994)

We consider a second-order process driven by Langevin dynamics without damping. Using the method of bounds, we show that in a one-dimensional system having a uniform distribution of traps, the asymptotic value of the average survival probability goes as $\exp(-ct^{0.6})$.

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INTRODUCTION

Recently [1-3] there has been some interest in the dynamics of particles moving in the field of a random force. In such systems particles execute random motion under the effect of a Gaussian random force, which is assumed to have δ correlation in time (white noise). The underlying dynamics is the Langevin type given by the second-order process

$$m\ddot{x} = f(t) , \qquad (1)$$

where f(t) is the random force satisfying

$$\langle f(t) \rangle = 0$$
, (2a)

and

$$\langle f(t)f(t')\rangle = C\delta(t-t')$$
. (2b)

Equation (1) is a zero damping $(\gamma \rightarrow 0)$ limiting case of the Langevin equation

$$m\ddot{x} + \gamma \dot{x} = f(t) . (3)$$

There is, however, some controversy regarding the survival probability of particles undergoing such random motion in the presence of stationary traps uniformly distributed in a one-dimensional system. Using numerical simulations and scaling arguments, Araujo *et al.* [1] have found an asymptotic relation for the survival probability $\langle S(t) \rangle \sim \exp(-ct^{0.6})$, whereas Heinrichs [2], using an analytical approach, obtained $\langle S(t) \rangle \sim \exp(-c't)$.

In this paper, using the method of bounds, we show that the survival probability $\langle S(t \to \infty) \rangle$ satisfies the inequalities

$$C_1 \le -\frac{\ln\langle S(t)\rangle}{t^{0.6}} \le C_2 , \qquad (4)$$

where C_1 and C_2 are constants, independent of time. This agrees with the asymptotic behavior obtained by Araujo *et al.* and is different from that obtained by Heinrichs. We believe that the boundary conditions used by Heinrichs for perfect absorbers situated at $x = \pm \xi$, i.e.,

$$P'(\pm \xi, t) = 0 \tag{5}$$

[where P'(x,t) is the marginal probability distribution at x] are in error. The proper boundary conditions to be used are

$$P(\xi, v, t) = 0$$
, $v < 0$
 $P(-\xi, v, t) = 0$, $v > 0$ (6)

[where P(x, v, t) is the joint probability distribution at x].

We were, however, unable to solve this problem using these boundary conditions. Therefore, we obtained lower and upper bounds to the survival probability. Before describing the method used to obtain the bounds, we give a brief derivation of the equation satisfied by the probability density function of a particle following the dynamics given by Eq. (1).

At any time t, let P(x,v,t) be the probability density of a particle with velocity v being found at x. We consider the dynamics given by Eq. (1) as the limit of a process defined as follows. The particle is subjected to random accelerations a_j 's which are constant over a time interval $(j-1)\Delta t - j\Delta t$. The a_j 's are identically distributed independent random variables obtained from a Gaussian distribution $p(a_j)$.

$$p(a_j) = \left[\frac{\Delta t}{2\lambda \pi}\right]^{1/2} \exp(-a_j^2 \Delta t / \lambda) . \tag{7}$$

Therefore we can write

$$P(x,v,t) = \prod_{J=1}^{M} \int p(a_j) da_j \delta \left[x - \sum_{J} a_j (\Delta t)^2 (M-j) \right]$$

$$\times \delta \left[v - \sum_{J} a_j \Delta t \right].$$
 (8)

M denotes the total number of kicks undergone by the particle up to time t ($=M\Delta t$). Taking the double Fourier transform of P(x, v, t),

$$\widetilde{P}(k_1, k_2, t) = \int \int P(x, v, t) \exp(ik_1 x + ik_2 v) dx \ dv \ .$$

$$(9)$$

Using Eq. (8) we obtain

$$\widetilde{P}(k_1, k_2, t) = \exp[-(\lambda \Delta t/4) \{ k_1^2 M^3 \Delta t^2 / 3 + k_2^2 M + k_1 k_2 M^2 \Delta t \}]. \quad (10)$$

Using $M\Delta t = t$ we get

$$\tilde{P}(k_1, k_2, t) = \exp[-(\lambda \Delta t/4)\{(k_2 + k_1 t/2)^2 + k_1^2 t^2/12\}].$$
 (11)

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Taking the inverse transform gives

$$P(x,v,t) = (1/t^2) \exp[-\alpha_1 v^2/t - \alpha_2 (v + \alpha x/t)^2/t].$$
(12)

This equation satisfies the differential equation (3.27) of Masoliver [3]. Defining the transformation $y = v + \alpha x / t$ and $\phi(y,v,t) = tP(x,v,t)$, we get

$$\phi(y, v, t) \sim (\alpha_3/t) \exp[-\alpha_2 y^2/t - \alpha_1 v^2/t]$$
, (13)

which satisfies the partial differential equation

$$\frac{\partial \phi}{\partial t} = \beta_1 \frac{\partial^2 \phi}{\partial v^2} + \beta_2 \frac{\partial^2 \phi}{\partial v^2} \ . \tag{14}$$

Although Eq. (14) is derived for a particle starting at x = 0 with velocity v = 0 it is easy to see that this equation still holds for $x = x_0$ and $v = v_0$, with v and y replaced by V and Y, respectively, where

$$V = v - v_0 , \qquad (15a)$$

$$X = x - v_0 t - x_0$$
, (15b)

and

$$Y = V + \alpha X/t = v - v_0 + \alpha x/t - v_0 - \alpha x_0/t$$

= $y - y_0$, (16)

where

$$y_0 = (1+\alpha)v_0 + \alpha x_0/t$$
.

A particle starting at $x = x_0$ and $v = v_0$, therefore, satisfies the following equation:

$$\frac{\partial \phi}{\partial t} = \beta_1 \frac{\partial^2 \phi}{\partial Y^2} + \beta_2 \frac{\partial^2 \phi}{\partial Y^2} \ . \tag{17}$$

We now describe the methods used to obtain the lower and upper bounds.

LOWER BOUND

Consider a particle in a trap-free region of length 2L with traps at $x=\pm L$. The quantity of interest is the survival probability of the particle after a large time t_0 . To obtain the lower bound to this we divide time t_0 into N intervals of time τ , such that $N\tau=t_0$. We require the following two conditions to be met.

- (i) During each interval τ , the particle should not go out of (-L, +L) and $(-v_1, +v_1)$.
- (ii) At the end of τ it should be found in $(-v_0, v_0)$ and $(-x_0, x_0)$.

For the present, x_0 , v_0 , and v_1 are arbitrary. Conditions on these quantities will be imposed later.

We first consider the survival during a specific time interval [say, $i\tau \le t \le (i+1)\tau$]. At the beginning of this interval (i.e., at $t=i\tau$) the particle may be anywhere between $-x_0$ and $+x_0$ with a velocity between $-v_0$ and $+v_0$. Clearly the worst case (i.e., the lowest survival probability) will be if we take the initial position at x_0 (or $-x_0$) and initial velocity as v_0 (or $-v_0$).

Because of condition (1) the following restrictions are imposed on the transformed variables V and Y. During the time interval $i\tau \le t \le (i+1)\tau$ the transformed velocity V satisfies the inequalities

$$-v_1 - v_0 \le V \le v_1 - v_0 . \tag{18}$$

The condition on Y is more complicated since it depends on both v and t. At a transformed velocity V at time t, we have the inequalities

$$v - \alpha L / t - (1 + \alpha) v_0 - \alpha x_0 / t \le Y \le v + \alpha L / t - (1 + \alpha) v_0 - \alpha x_0 / t . \tag{19}$$

It is not possible to solve Eq. (17) with the boundary conditions imposed by the inequalities (18) and (19). However, since our interest here is in obtaining a lower bound, we make the following simplifications. First, we take $v_0 \ll v_1$ and $x_0 \ll L$, but still $v_1/v_0 = O(1)$ and $L/x_0 = O(1)$. Also, we define

$$v_1 - v_0 = \gamma v_1 \tag{20a}$$

$$\alpha(L - x_0) = \eta L , \qquad (20b)$$

and

$$v_1 + (1 + \alpha)v_0 = \eta v_1 . {(20c)}$$

We now impose the boundary condition that $\phi(Y, V, t) = 0$ at the rectangle (assuming that $L/\tau > v_1$) delineated by

$$-\gamma v_1 \le V \le \gamma v_1 , \qquad (21a)$$

$$-Y_1 \le Y \le Y_1 , \qquad (21b)$$

where

$$Y_1 = \eta(L/\tau - v_1)$$
 (21c)

As pointed out earlier, the boundary condition $\phi(Y, V, t) = 0$ for all values of V is not correct, but we now show that use of this boundary condition [instead of the true one given by Eq. (6)] leads to a lower value of ϕ and therefore it may be used in the lower bound. For the process under consideration in which the particle gets a constant (random) acceleration during a period Δt , we have

$$P_1(x,v,k,\Omega,)$$

$$= P_1(x - v\Delta t - 0.5a_{k-1}\Delta t^2, v - a_{k-1}\Delta t, k - 1, \Omega),$$

where $k - t/\Delta t$ and $P_1(x, v, k, \Omega)$ is the value of P(x, v, t) [Eq. (12)] for the realization Ω .

It can be easily shown that by expanding P_1 in a Taylor series and averaging over a_k , we get Eq. (3.27) of Masoliver [3]. P_1 may be considered as the limit of the following equation where x and v have been discretized.

$$P_1(i,j,k,\Omega) = \sum_{i'=-N}^{N} \sum_{j'=-M}^{M} A_{i',j',i,j}(a_k) P_1(i,j,k-1,\Omega) \ ,$$

where $i=x/\Delta x$, $j=v/\Delta v$. The coefficients A depend on the type of interpolation used. It is possible to keep all the A's non-negative (for example, by using a linear interpolation formula). The true boundary condition may be incorporated by writing

$$A_{-N,j',i,j} = 0$$
 for all i,j and for $j' \ge 0$,

$$A_{N,j',i,j} = 0$$
 for all i,j and for $j' \le 0$.

Use of $\phi(Y, V, t) = 0$ implies use of the boundary condition

$$A_{\pm n,j',i,j} = 0$$
 for all i,j , and j' .

Since all P_1 's are positive, the use of the boundary condition $\phi = 0$ clearly leads to lower values of P_1 and hence to lower values of ϕ also. Therefore the use of this boundary condition is justified in obtaining a lower bound.

Note that the rectangle implied by the inequalities (21a) and (21b) is smaller than the parallelogram implied by the inequalities (18) and (19) at all times $[i\tau \le t \le (i+1)\tau]$. The probability of a particle being found in dV about V and dY about Y at the end of time τ with the above boundary conditions is

$$\begin{split} Q(V,Y,\tau) dV \, dY \sim & (dV \, dY/v_1 Y_1) \\ \times & \cos(\pi V/2 \gamma v_1) \cos(\pi Y/2 Y_1) \\ \times & \exp[-(\pi^2 \tau/\gamma^2 v_1^2) - (\pi^2 \tau/Y_1^2)] \; . \end{split}$$

By replacing V and Y in terms of v and x we get the probability $S(\tau,L)$ so that the particle at the end of time interval τ is found in $(-v_0,v_0)$ and $(-x_0,x_0)$ [without going out of (-L,L) and $(-v_1,v_1)$ during this interval]. This is given by

$$S(\tau, L) \ge \int_{-v_0}^{v_0} \int_{-x_0}^{x_0} (dx \ dv / \tau v_1 Y_1) \times \cos(\pi v / 2\gamma v_1) \cos(\pi Y / 2Y_1) \times \exp[-(\pi^2 \tau / \gamma^2 v_1^2) - (\pi^2 \tau / Y_1^2)] .$$
(23)

The above integral can be shown to be

$$\sim (1/A) \exp[(\pi^2 \tau / \gamma^2 v_1^2) - (\pi^2 \tau / Y_1^2)],$$
 (24)

where A is O(1) because we have chosen v_1/v_0 and L/x_0 both to be O(1).

So at $t = t_0$ after N steps of τ , the probability of survival $S(t_0, L)$ is given by

$$S(t_0, L) \ge [S(\tau, L)]^N$$

$$= \exp[(-\pi^2 t_0 / \gamma^2 v_1^2) - (\pi^2 t_0 / Y_1^2) - N \ln A].$$
(25)

To get the average survival probability we multiply $S(t_0,L)$ with $\exp(-2\omega L)dL$ (the probability to get a trap-free region of length 2L with traps at its boundaries at $x=\pm L$), and integrate over L from the limits $-\infty$ to $+\infty$. Here ω is the concentration of traps per unit length. Now maximizing over τ and v_1 and evaluating the integral over L by the method of steepest descent we get

$$\tau \sim t_0^{0.4}$$
 , $L \sim t_0^{0.6}$, $v_1 \sim t_0^{0.2}$,

and

$$\langle S(t_0) \rangle \ge \exp(-C_1 t_0^{0.6}) . \tag{26}$$

UPPER BOUND

As in the case of the lower bound, here also we divide the time t_0 into N equal intervals of duration τ each. We can easily obtain the probability $S(\tau,L)$ that a particle starting at x=0, v=0 at the beginning of each interval in an infinite medium without any absorbers will be within the interval $-L \le x \le L$ at the end of time τ . Clearly this probability will be greater than the probability of a particle starting at x=0, v=0 with absorbing boundaries at $x=\pm L$, since in the former case some particles would have gone out of the interval (-L,L) and come back.

$$S(\tau, L) \le \int_{-L}^{L} (1/\sqrt{2\pi d} \tau^{1.5}) \exp(-x^2/d\tau^3) dx$$
, (27)

where d is a constant of O(1). Defining

$$Z = L / \sqrt{d} \tau^{1.5}$$

and

(22)

$$E(Z) = 2 \int_0^Z (1/\sqrt{2\pi}) \exp(-x^2/2) dx$$
,

we get

$$S(\tau,L) \leq E(Z)$$
,

and after time $t_0 = N\tau$, we have the survival probability

$$S(t_0,L)=[E(Z)]^N$$
.

Averaging over L as before,

$$\langle S(t_0) \rangle \le \int [E(Z)]^N \exp(-2\omega L) dL$$

$$= \int \exp(N \ln E[Z] - 2\omega L) dL . \qquad (28)$$

We note that most of the contribution to the integral comes from values of L given by

$$[t_0 \exp(-Z^2/2)/E(Z)\sqrt{2\pi d} \tau^{2.5}] = \omega$$
 (29)

Now, minimizing over τ , we get

 $(t_0/\tau^2)\ln E(Z)$

$$+3[t_0/\tau E(Z)]\exp(-Z^2/2)L/\sqrt{2\pi d}\tau^{2.5}=0$$
, (30)

i.e.,

$$\ln[E(Z)] + 3\exp(-Z^2/2)Z/E(Z) = 0.$$
 (31)

The graphical solution of Eq. (31) gives

$$Z \sim 0.3 = O(1)$$
.

Therefore,

$$L/\tau^{1.5} = C$$
.

Substituting the value of Z in Eq. (29), we get

$$\tau \sim t_0^{0.4}$$
, $L \sim \tau^{1.5} \sim t_0^{0.6}$.

Substitution of these values of L and τ in Eq. (28) leads to the inequality

$$\langle S(t_0) \rangle \le \exp(-C_2 t_0^{0.6}) . \tag{32}$$

Note that we have proved the above inequality, assuming that the particle starts from x = 0, v = 0 at the beginning of every time interval. In actual practice, however, it has a probability distribution in x and v both. It is easy to show (as indicated below) that the assumption of x = 0, v = 0 is an overestimate.

First, for a particle starting at x' with initial velocity v' in an infinite medium, the probability distribution function at time t is given by

$$P(x,t/x',v') \sim (1/t^{1.5}) \exp[-(x-x'-v't)^2/t^3]$$
 (33)

The probability of finding the particle within (-L, +L) is therefore

$$= \int_{-v_0}^{v_0} \int_{-x_0}^{x_0} \int_{-L}^{L} \int_{-\infty}^{\infty} p(x', v', \tau) P(x, \tau/x', v') \times dx \ d\tau \ dv' dx', \qquad (34)$$

where $p(x',v',i\tau)dx'dv'$ is the probability that at time $i\tau$ the particle was in x' and dv' about v'. Because of the symmetry of the problem,

$$p(x',v',i\tau)dx'dv' = p(-x',-v',i\tau)dx'dv'.$$
 (35)

Using this as well as the inequality,

$$\int_{-a}^{a} \exp[-(z-\alpha)^{2}]dz + \int_{-a}^{a} \exp[-(z+\alpha)^{2}]dz$$

$$\leq 2 \int_{-a}^{a} \exp(-z^{2})dz , \quad (36)$$

we obtain the desired result, namely that the assumption of x'=0, v'=0 always gives an overestimate. Combining this result with the inequalities (26) and (32) we get the result for $t_0 \to \infty$,

$$C_1 \le -\frac{\ln \langle S(t_0) \rangle}{t_0^{0.6}} \le C_2 .$$

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