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First-passage times for the Uhlenbeck–Ornstein process

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Abstract. A numerical solution is obtained for the Laplace-transformed backward Kramers equation, from which the mean first-passage time may be obtained. The main difficulties are associated with (*a*) the parabolic nature of the time-development operator and (*b*) the existence of a double structure in the solution near the absorbing barrier. Both of these difficulties are resolved by computational methods derived from boundary layer theory. The reliability of the method is assessed by comparing its results with an earlier analytic solution for the case of a uniform force field. We also present the results for a harmonic force field, for which no analytic solution is yet known.

1. Introduction

The Langevin equation of a massive Brownian particle, in suitable units [1], is

$$\ddot{x}+\dot{x}-F(x)=G(t) \tag{1.1}$$

where $F(x)$ is the force field and $G(t)$ is the derivative of a Wiener process. The corresponding Fokker–Planck equation has been called the Kramers equation [2] and is

$$\frac{\partial W}{\partial t}=\frac{\partial^2 W}{\partial u^2}-u\frac{\partial W}{\partial x}+\frac{\partial}{\partial u}[(u-F(x))W] \qquad u=\dot{x}. \tag{1.2}$$

Wang and Uhlenbeck [2] posed the problem of calculating the first-passage times for this process. This may be done by solving for $W(x, u; t)$ with certain finiteness conditions for large x and u, together with the boundary condition

$$W(0, u; t)=0 \qquad u>0. \tag{1.3}$$

We showed, however, in an earlier paper [1] that the Laplace transform of the first-passage time density, with initial values $x=y$, $u=v$, provides the more amenable boundary-value problem

$$\frac{\partial^2\Phi}{\partial v^2}+v\frac{\partial\Phi}{\partial y}-[v-F(y)]\frac{\partial\Phi}{\partial v}-p\Phi=0 \tag{1.4}$$

$$\Phi(0, v)=1 \qquad v<0. \tag{1.5}$$

Here p is the Laplace transform variable corresponding to t, so that the mean first-passage time is obtained by differentiating Φ at $p=0$. It may be noted that the time-development operator in (1.4) is the formal adjoint of that in (1.2). This is because W satisfies the backward Fokker–Planck or Kolmogorov [3] equation with the initial values as the dependent variables and the first-passage time density is obtained by integrating $uW(0, u; t)$ over negative values of u.

This latter boundary-value problem has been solved analytically [1] for the case of a uniform force field, $F(x)=-2\alpha$. It is no easy matter to extend the method to other force fields, but we find that it is possible to use certain analytic properties of the solution near $y=0$ in order to generate a numerical integration procedure. This procedure is described in the next section and we have been able to test its reliability by comparing its results with our analytic solution. We have also used the procedure with the harmonic force field $F(x)=-\omega^2(x+a)$. This would be relevant, for example, if we wanted to know the waiting time for an electrical tuned circuit to reach some specified final state from a given initial state.

Previous numerical approaches are considerably less reliable, as may be seen by comparison with our analytic solution. Essentially two methods have been tried. One of them [4] is a variational method based on a truncated eigenfunction expansion. The problem with this method is that, although we have good reason [5] to believe that the eigenfunctions have the necessary property of half-range completeness, the convergence is extremely slow [1, 4]. The second method is to return to the Langevin equations and use a computer simulation of the white noise on the right-hand side. As may be seen by consulting the figures of this paper [6], only modest accuracy is obtained from a large number of runs with different realisations of the noise. In addition, these authors did not know the asymptotic behaviour of the first-passage time density for large t and had to make certain guesses.

2. Numerical method of solution

In this section we consider a numerical solution to the following class of problem:

$$\frac{\partial^2\Phi}{\partial v^2}-f(y,v)\frac{\partial\Phi}{\partial v}+v\frac{\partial\Phi}{\partial y}-p\Phi=0 \qquad (2.1)$$

where $y>0$, $-\infty<v<\infty$, p is some constant and we assume $f(y,v)$ is a regular function of v and y $(y\geqslant 0)$. We suppose that the boundary condition to be applied to (2.1) is that

$$\Phi(0,v)=1 \qquad v<0 \text{ only} \qquad (2.2)$$

with $\Phi(0,v)$, $(v>0)$ remaining unspecified. We also suppose that

$$\Phi_v\to 0 \qquad \text{as } v\to\infty \qquad (2.3)$$

and

$$\Phi\to 0 \qquad \text{as } y\to\infty. \qquad (2.4)$$

We shall insist that Φ and Φ_v are (everywhere) continuous in $y>0$ (in particular along $v=0$).

Perhaps the most important (and novel) feature of this system is that (2.1) is parabolic, with the propagation of information being in the direction of increasing y for $v<0$, but in the direction of decreasing y for $v>0$. Any numerical scheme must then possess the correct zone of dependence. The second point to note is that the system takes on a singular (double) structure for small y and details of this are given in the appendix. We may expect that any accurate numerical treatment of (2.1) must take this double/singular structure into account.

These two difficulties are not uncommonly encountered in the context of viscous flow theory, in particular in certain laminar boundary layer problems. This class of flow is generally governed by a parabolic differential system and double structures to the flow often occur, particularly when discontinuities in boundary conditions are encountered [7]. The second difficulty, of varying zones of dependence, arises if the boundary layer reverses in direction. Consequently, we may draw from our experience in boundary layer techniques, when treating equations of this form. Indeed, (2.1) possesses two simplifying features over boundary layer flows. Firstly, the system is linear and, secondly, we know *a priori* the appropriate zones of dependence, two features not usually present in the aforementioned fluid mechanics situations.

Since (2.1) is parabolic in character, it is amenable to numerical marching techniques. However, in order that information is propagated in the appropriate direction, we must march in the positive y direction for $v<0$, whilst for $v>0$ the marching process must be in the direction of decreasing y. Further we must ensure that these two solutions match along $v=0$.

For $y\leqslant 1$, we build in the double structure (which was seen to occur for small y) into our numerical scheme.

We write

$$\Phi-1=\xi^{1/2}F(\xi,\eta) \tag{2.5}$$

where η and ξ are defined by (A7), which then yields the following equations:

$$G_\eta-f_1(\xi,\eta)\xi G+\tfrac{1}{6}\eta F-\tfrac{1}{3}\eta^2 G+\tfrac{1}{3}\eta\xi F_\xi-p\xi^2F-p\xi^{3/2}=0 \tag{2.6}$$

$$G=F_\eta. \tag{2.7}$$

$$F(0,\eta)=C\exp\left(\frac{\eta^3}{18}\right)\left[\frac{\eta}{12^{1/3}}\mathrm{Ai}\left(\frac{\eta^2}{12^{2/3}}\right)-\mathrm{Ai}'\left(\frac{\eta^2}{12^{2/3}}\right)\right] \tag{2.8}$$

where C is a constant (to be determined globally—see the appendix), which is initially guessed, as is the distribution $\Phi_v(y,0)$. Finally $f_1(\xi,\eta)=f(\xi^3,\xi\eta)$.

Note that G and F are strictly not regular functions of ξ, due to the inhomogeneous term, but this singularity is only $O(\xi^{3/2})$ and as such did not appear to create any numerical difficulties. We then solve (2.6) in the region $0>\eta>-\eta_\infty$ (where η_∞ is suitably large), corresponding to $0>v>-\eta_\infty\xi$.

For $-\eta_\infty\xi>v>-(v_\infty+\eta_\infty\xi)$ (where v_∞ is suitable large), we solve the 'outer' problem, namely

$$\Psi_{\bar v}-f_2(\xi,\bar v)\Psi+\tfrac{1}{3}v\xi^{-2}(\Phi_\xi+\eta_\infty\Psi)-p\Phi=0 \tag{2.9}$$

with

$$\Psi(\xi,\bar v)=\Phi_{\bar v}(\xi,\bar v) \tag{2.10}$$

and

$$\bar v=v+\eta_\infty\xi \tag{2.11}$$

where $f_2(\xi,\bar v)=f(\xi^3,\bar v-\eta_\infty\xi)$ and so we solve (2.9) and (2.10) for $0>\bar v>-v_\infty$. Here we have used a transformed velocity coordinate and so our domain of solution in (y,v) space increases somewhat as ξ increases.

We make a second-order difference approximation to (2.6), (2.7), (2.9) and (2.10) with $\Delta\xi$, $\Delta\eta$, Δv denoting the grid sizes in the ξ, η, $\bar{v}$ directions respectively. This yields the following equations:

$$\begin{aligned}
&(2\Delta\eta)^{-1}[G(\xi,\eta)-G(\xi,\eta-\Delta\eta)-G(\xi-\Delta\xi,\eta-\Delta\eta)+G(\xi-\Delta\xi,\eta)]\\
&\quad -\tfrac{1}{4}f_1(\xi-\tfrac{1}{2}\Delta\xi,\eta-\tfrac{1}{2}\Delta\eta)(\xi-\tfrac{1}{2}\Delta\xi)[G(\xi,\eta)+G(\xi,\eta-\Delta\eta)\\
&\quad +G(\xi-\Delta\xi,\eta-\Delta\eta)+G(\xi-\Delta\xi,\eta)]\\
&\quad +\tfrac{1}{24}(\eta-\tfrac{1}{2}\Delta\eta)[F(\xi,\eta)+F(\xi-\Delta\xi,\eta)+F(\xi,\eta-\Delta\eta)\\
&\quad +F(\xi-\Delta\xi,\eta-\Delta\eta)]\\
&\quad -\tfrac{1}{12}(\eta-\tfrac{1}{2}\Delta\eta)^2[G(\xi,\eta)+G(\xi,\eta-\Delta\eta)+G(\xi-\Delta\xi,\eta)\\
&\quad +G(\xi-\Delta\xi,\eta-\Delta\eta)]\\
&\quad +\tfrac{1}{6}(\Delta\xi)^{-1}(\eta-\tfrac{1}{2}\Delta\eta)(\xi-\tfrac{1}{2}\Delta\xi)[F(\xi,\eta)-F(\xi-\Delta\xi,\eta)\\
&\quad +F(\xi,\eta-\Delta\eta)-F(\xi-\Delta\xi,\eta-\Delta\eta)]\\
&\quad -\tfrac{1}{4}p(\xi-\tfrac{1}{2}\Delta\xi)^2[F(\xi,\eta)+F(\xi-\Delta\xi,\eta)+F(\xi,\eta-\Delta\eta)\\
&\quad +F(\xi-\Delta\xi,\eta-\Delta\eta)]-p(\xi-\tfrac{1}{2}\Delta\xi)^{3/2}=0
\end{aligned} \qquad (2.12)$$

$$\tfrac{1}{2}[G(\xi,\eta)+G(\xi,\eta-\Delta\eta)]=(\Delta\eta)^{-1}[F(\xi,\eta)-F(\xi,\eta-\Delta\eta)] \qquad (2.13)$$

$$\begin{aligned}
&(2\Delta v)^{-1}[\Psi(\xi,\bar{v})-\Psi(\xi,\bar{v}-\Delta v)+\Psi(\xi-\Delta\xi,\bar{v})-\Psi(\xi-\Delta\xi,\bar{v}-\Delta v)]\\
&\quad -\tfrac{1}{4}f_2(\xi-\tfrac{1}{2}\Delta\xi,\bar{v}-\tfrac{1}{2}\Delta v)[\Psi(\xi,\bar{v})+\Psi(\xi-\Delta\xi,\bar{v})\\
&\quad +\Psi(\xi,\bar{v}-\Delta v)+\Psi(\xi-\Delta\xi,\bar{v}-\Delta v)]\\
&\quad +\tfrac{1}{6}[\bar{v}-\tfrac{1}{2}\Delta v-\eta_\infty(\xi-\tfrac{1}{2}\Delta\xi)](\xi-\tfrac{1}{2}\Delta\xi)^{-2}\{(\Delta\xi)^{-1}[\Phi(\xi,\bar{v})\\
&\quad -\Phi(\xi-\Delta\xi,\bar{v})+\Phi(\xi,\bar{v}-\Delta v)-\Phi(\xi-\Delta\xi,\bar{v}-\Delta v)]\\
&\quad +\tfrac{1}{2}\eta_\infty[\Psi(\xi,\bar{v})+\Psi(\xi,\bar{v}-\Delta v)\\
&\quad +\Psi(\xi-\Delta\xi,\bar{v})+\Psi(\xi-\Delta\xi,\bar{v}-\Delta v)]\}\\
&\quad -\tfrac{1}{4}p[\Phi(\xi,\bar{v})+\Phi(\xi-\Delta\xi,\bar{v})+\Phi(\xi,\bar{v}-\Delta v)\\
&\quad +\Phi(\xi-\Delta\xi,\bar{v}-\Delta v)]=0
\end{aligned} \qquad (2.14)$$

$$\tfrac{1}{2}[\Psi(\xi,\bar{v})+\Psi(\xi,\bar{v}-\Delta v)]=(\Delta v)^{-1}[\Phi(\xi,\bar{v})-\Phi(\xi,\bar{v}-\Delta v)]. \qquad (2.15)$$

(2.12) represents an approximation to (2.6) at the point $(\xi-\frac{1}{2}\Delta\xi, \eta-\frac{1}{2}\Delta\eta)$, (2.13) an approximation to (2.7) at the point $(\xi, \eta-\frac{1}{2}\Delta\eta)$, (2.14) an approximation to (2.9) at the point $(\xi-\frac{1}{2}\Delta\xi, \bar{v}-\frac{1}{2}\Delta v)$ and (2.15) an approximation to (2.10) at the point $(\xi, \bar{v}-\frac{1}{2}\Delta v)$.

We require a solution to (2.12)-(2.15) for $0>\eta>-\eta_\infty$ and $0>\bar{v}>-v_\infty$, with a match between the inner and outer solutions. This is achieved by setting

$$\xi^{1/2}F(\xi,-\eta_\infty)+1=\Phi(\xi,\bar{v}=0) \qquad (2.16)$$

$$\xi^{1/2}G(\xi,-\eta_\infty)=\Psi(\xi,\bar{v}=0). \qquad (2.17)$$

In order to close the system, we set

$$\Psi(\xi,\bar{v}=-v_\infty)=0 \qquad (2.18)$$

whilst $G(\xi, \eta=0)$ is set equal to the (previously) guessed value.

This general technique of splitting the governing equations into systems of first-order equations, which are then approximated using four mesh points was a technique originally used in fluid mechanics situations by Keller and Cebeci [8] and this method is particularly suitable when dealing with systems of equations involving double structures [9].

Notice that the error terms in our approximations to the differential equations are generally $O((\Delta\xi)^2+(\Delta\eta)^2)$ in the inner solution and $O((\Delta\xi)^2+(\Delta v)^2)$ in the outer solution.

The (algebraic) system we have to solve, along a line of constant ξ, is then of the form

$$\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b} \tag{2.19}$$

where

$$\boldsymbol{x}=\begin{bmatrix} F(\xi,0)\\ G(\xi,0)\\ F(\xi,-\Delta\eta)\\ G(\xi,-\Delta\eta)\\ \vdots\\ F(\xi,-\eta_\infty)\\ G(\xi,-\eta_\infty)\\ \Phi(\xi,0)\\ \Psi(\xi,0)\\ \vdots\\ \Phi(\xi,-v_\infty)\\ \Psi(\xi,-v_\infty)\end{bmatrix}. \tag{2.20}$$

$\boldsymbol{A}$ is a block diagonal matrix (with each block being just 4×2) and as such is amenable to Gaussian elimination techniques.

We solve for F, G, Φ, Ψ along lines of constant ξ, at $\xi=\Delta\xi$, $\xi=2\Delta\xi,\ldots,1-\Delta\xi$, $1(v<0)$. At $\xi=1+\Delta\xi$ we switch to the Φ, Ψ, y, v system, an operation that is particularly simple to perform if we have

$$\begin{aligned}\Delta v&=\eta_\infty\Delta\xi\\ \Delta\eta&=\Delta v\end{aligned} \tag{2.21}$$

since then mesh points from the double structure at $\xi=1$ correspond identically to mesh points for a single structure grid, with spacing Δv.

Notice that at $\xi=1$ we also have

$$\begin{aligned}1+F(1,\eta)&=\Phi(1,v=\eta)\\ G(1,\eta)&=\Psi(1,v=\eta).\end{aligned} \tag{2.22}$$

In the y, v coordinate system, the difference equations that we must solve are then

$$\begin{aligned}(2\Delta v)^{-1}&[\Psi(y,v)-\Psi(y,v-\Delta v)+\Psi(y-\Delta y,v)-\Psi(y-\Delta y,v-\Delta v)]\\ &-\tfrac{1}{4}f(y-\tfrac{1}{2}\Delta y,v-\tfrac{1}{2}\Delta v)[\Psi(y,v)+\Psi(y,v-\Delta v)\\ &+\Psi(y-\Delta y,v-\Delta v)+\Psi(y-\Delta y,v)]\\ &+(2\Delta y)^{-1}(v-\tfrac{1}{2}\Delta v)[\Phi(y,v)-\Phi(y-\Delta y,v)\\ &+\Phi(y,v-\Delta v)-\Phi(y-\Delta y,v-\Delta v)]\\ &-\tfrac{1}{4}p[\Phi(y,v)+\Phi(y-\Delta y,v)+\Phi(y-\Delta y,v-\Delta v)+\Phi(y,v-\Delta v)]\\ &=0\end{aligned} \tag{2.23}$$

$$\tfrac{1}{2}[\Psi(y,v)+\Psi(y,v-\Delta v)]=(\Delta v)^{-1}[\Phi(y,v)-\Phi(y,v-\Delta v)]. \tag{2.24}$$

We require to solve for Φ and Ψ for $0 \geq v \geq -2v_\infty$, $1+\Delta y \leq y \leq y_\infty$. (2.23) and (2.24) can then be solved (in a manner similar to that employed for $\xi \leq 1$), subject to $\Psi(y, -2v_\infty) = 0$, whilst $\Psi(y, 0)$ is set equal to the previously guessed value.

Having swept the solution for $v<0$ out to y_∞ (and one finds $\Phi \to 0$ as $y \to \infty$, in agreement with (2.4)) in the manner described, we now have a $\Phi(y, 0)$ distribution. The next stage is to generate the solution for $v>0$, using this computed $\Phi(y, 0)$ distribution. The process is started at $y = y_\infty$, where we set

$$\Phi(y_\infty, v) = 0 \qquad v > 0 \tag{2.25}$$

and the solution in $v>0$ is marched back towards $y=1$, solving the modified form of (2.23) and (2.24) (with $-\Delta y$ replacing Δy). Along $v=0$ we set $\Phi(y, 0)$ equal to the value obtained from the sweep through $v<0$. For $\xi<1$ (i.e. $y<1$), we revert to the double structure and solve (2.12)-(2.15) (but with $-\Delta\xi$ and $-\eta_\infty$ replacing $\Delta\xi$ and η_∞), this time setting $G(0, \Delta\xi)$ equal to the value obtained from the sweep through $v<0$. The solution is continued up to $\xi = \Delta\xi$. Comparing the value of $F(0, \xi)$ with the differentiated form of (2.8) yields a new estimate for C. Note that this particular process involves an error of $O(\Delta\xi)$ larger than for the differential equation approximation, but was used in order to bypass possible computational difficulties in extending the solution up to $\xi = 0$. The process of sweeping through $v>0$ also produces a new set of estimates for $G(\xi, 0)$, $\Psi(y, 0)$, which we then employ when we repeat the entire procedure.

The overall iteration procedure was applied repeatedly, until the change in C fell below some prescribed tolerance level (typically 10^{-9}).

3. Results

The first class of problem treated was for

$$f(y, v) = v + 2\alpha \qquad \alpha = \text{constant} \tag{3.1}$$

corresponding to the system considered analytically in some detail in [1], from which we have 'exact' solutions to compare with our present numerical results. In particular, in [1] the quantity computed was the first-passage time, namely $\psi = -\Phi_p(p=0, v=0)$.

We generated this quantity by evaluating Φ for two (small) values of p, Δp and $2\Delta p$ say, noting that for $p=0$, $\alpha>0$,

$$\Phi \equiv 1 \text{ everywhere} \tag{3.2}$$

and using the approximation

$$\psi(p=0) = -(2\Delta p)^{-1}[4\Phi(\Delta p) - \Phi(2\Delta p) - 3] \tag{3.3}$$

where the error involved in making this assumption can be shown to be generally $O((\Delta p)^2)$.

In our computations, we chose two values of Δp, namely 0.006 25 and 0.0125. The computations were performed using three grids in order to gauge the effect of the various truncation errors. All grids were chosen with $\Delta\xi = 0.025$, $\Delta\eta = \Delta v = 0.256$, $v_\infty = \eta_\infty = 10.256$; grid A was chosen with $\Delta y = 0.25$, $y_\infty = 81$, grid B with $\Delta y = 0.5$, $y_\infty = 81$, and grid C with $\Delta y = 0.5$, $y_\infty = 161$.

Two values of α were taken, namely 1 and $\frac{1}{2}$, and the results for $\psi(y, v=0; \alpha)$ are shown in tables 1 and 2, respectively, together with the corresponding 'exact' results of [1].

Table 1. Comparison of 'exact' and computed $\psi(y, 0; 1)$.

		Grid A		Grid B		Grid C	
$y/2\alpha = y/2$	'Exact'	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$
0.5	1.401 134	1.4417	1.4171	1.4689	1.4284	1.4316	1.4105
1	2.053 077	2.0940	2.0694	2.1232	2.0816	2.0851	2.0637
1.5	2.629 684	2.6705	2.6454	2.6996	2.6576	2.6609	2.6394
2	3.173 490	3.2139	3.1883	3.2437	3.2006	3.2047	3.1822
2.5	3.699 995	3.7403	3.7135	3.7702	3.7261	3.7310	3.7073
3	4.216 537	4.2563	4.2288	4.2871	4.2412	4.2469	4.2225
4	5.233 827	5.2728	5.2421	5.3043	5.2550	5.2645	5.2334
5	6.241 086	6.2788	6.2439	6.3115	6.2572	6.2694	6.2374
10	11.246 86	11.2707	11.3486	11.3093	11.2062	11.2597	11.1832
15	16.246 57	16.3990	15.7399	16.2853	16.0787	16.2247	16.0512
20	21.246 57	21.1830	20.8359	20.5236	20.8591	21.1622	20.8245

Table 2. Comparison of 'exact' and computed $\psi(y, 0; \frac{1}{2})$.

		Grid A		Grid B		Grid C	
$y/2\alpha = y$	'Exact'	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$	$\Delta p = 0.006\,25$	$\Delta p = 0.0125$
0.5	1.860 302	1.8694	1.8608	1.8737	1.8622	1.8648	1.8587
1	2.545 837	2.5666	2.5487	2.5815	2.5536	2.5576	2.5442
1.5	3.144 272	3.1656	3.1465	3.0463	3.1290	3.1318	3.1384
2	3.704 213	3.7253	3.7045	3.7419	3.7110	3.7178	3.7016
2.5	2.243 102	4.2634	4.2410	4.2050	4.2228	4.2292	4.2324
3	4.769 264	4.7891	4.7645	4.8053	4.7703	4.7811	4.7606
4	5.799 873	5.8178	5.7879	5.8341	5.7935	5.8097	5.7838
5	6.815 137	6.8307	6.7937	6.8471	6.7995	6.8222	6.7897
10	11.831 026	11.8238	11.3049	11.8459	11.7316	11.8151	11.7213
15	16.831 71	16.7788	16.5621	16.7981	16.5683	16.7695	16.5574
20	21.831 74	21.7031	21.2691	21.7242	21.3043	21.6935	21.2926

Generally the computations required 50–100 iterations in order to obtain the required convergence criterion, the actual number being dependent on the first estimate for C and also $\Phi_v(v=0)$, although there never appeared to be very much difficulty in obtaining convergence.

One difficulty encountered was that large values of y_∞ were required for adequate numerical accuracy. This problem arises from our need for small p (which we required in order to obtain estimates for the first-passage times). From (3.2) we see that $\Phi \to 1$ everywhere as $p \to 0$, and as a result our condition that $\Phi \to 0$ as $y \to \infty$ becomes increasingly difficult to implement at finite values of y (y_∞). Hence the need for these comparatively large values of y_∞.

For large y, the major contribution to the error in ψ appears to be our usage of (3.3). It can be shown that, as $y \to \infty$,

$$\psi \to \frac{y+v}{2\alpha} + c(\alpha) \tag{3.4}$$

where $c(\alpha)$ is independent of both y and v, depending solely on α. (3.4) then demands that we take smaller values of Δp for large values of y.

However, for the particular choice of parameters taken, tables 1 and 2 indicate that our results generally agree with the 'exact' results to within 1%, confirming our confidence in our scheme.

The next class of problem tackled was for

$$f(y, v) = v + \omega^2(y + a) \tag{3.5}$$

with ω constant. This models the situation involving a harmonic restoring force acting about $y = -a$. This particular class of problem is not amenable to the analytic techniques employed in [1] (which relied on performing a Laplace transform of (2.1) with respect to y) and hence it appears that a numerical approach is necessary. Our routine for treating (3.1) required only minimal modification for studying (3.5).

In all our computations we set $\omega^2 = 1$ and chose a number of values of a. The results for the first-passage times for $v = 0$, $\psi(y, v = 0)$, are shown in figure 1. All these results were obtained using grid C, with $\Delta p = 0.0125$. However, all these computations were checked by control calculations on grids A and B, and also with $\Delta p = 0.006\,25$, and were deemed to be accurate to within the accuracy of the figures. The $\psi(y \to \infty, v = 0)$ behaviour is quite different from the previous example (3.1) and is seen to be asymptotic to a constant value—in fact, the same value for all values of a (~ 2.4). From the point of view of our numerical scheme, this had a very beneficial effect, eliminating the difficulties we experienced in the previous example when employing (3.3) at large values of y. It may be noted that negative values of a differ substantially more from the $a = 0$ example than do the corresponding positive values of a.

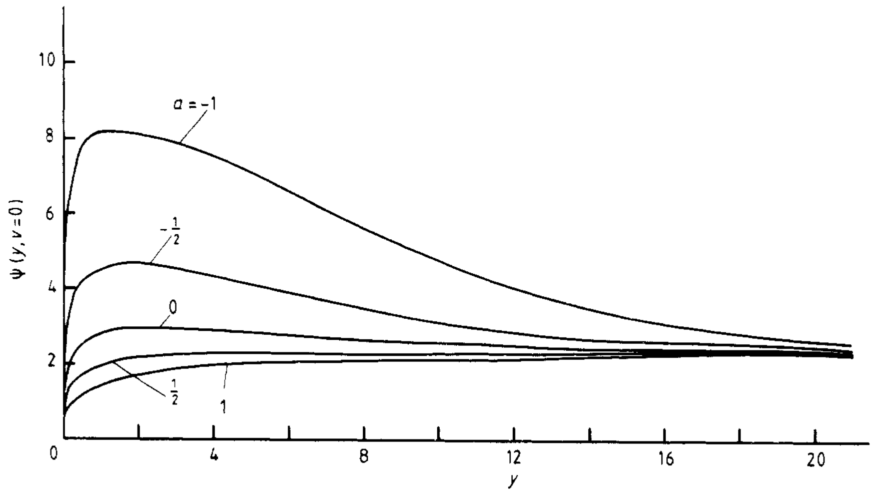

Figure 1. The first-passage time as a function of initial position (y) for a particle with initial velocity (v) = 0 in a harmonic potential well having equilibrium at $y = -a$.

Figure 2 shows the distribution of the recurrence times $\psi(y = 0, v > 0)$. In fact, because of the previously mentioned computational difficulties with extending the solution right back to $y = 0$ for $v > 0$, these profiles were obtained at $y = (\Delta\xi)^3 = O(10^{-5})$—within the accuracy of the graphs. The control computations which were carried out again indicated at least graphical accuracy.

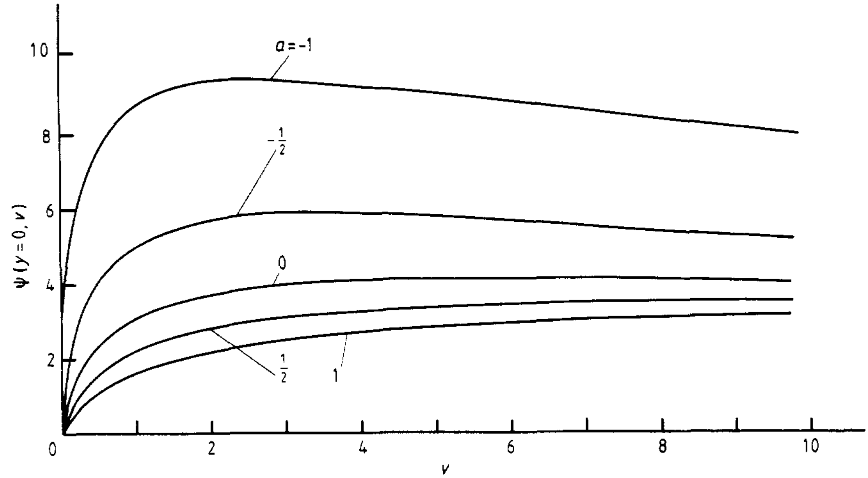

Figure 2. The recurrence time as a function of initial velocity for a particle moving in the same potential well as for figure 1.

The recurrence time distributions appear to be asymptotic to a constant value as $v \to \infty$ and this point is taken up in the following section. Further, as in the case of the $\psi(y, v=0)$ distributions, the negative a profiles differ considerably more from the $a=0$ example than do the positive a distributions. A fuller discussion of the physical implications of these results now follows.

4. Discussion

The asymptotic behaviour of $\psi(y, v)$ for large values of either argument, as depicted in figures 1 and 2, is explained by reference to the Langevin equation (1.1) with which we began, putting $F(x) = -x - a$. For either $v = 0$ and y large and positive, or $y = 0$ and v large and positive, we would expect to be able to disregard the noise term altogether. In that case the (deterministic) solution is, for $y = 0$,

$$x = a(e^{-t/2}\cos\tfrac{1}{2}t\sqrt{3} + 3^{-1/2}e^{-t/2}\sin\tfrac{1}{2}t\sqrt{3} - 1) + (2v/\sqrt{3})\,e^{-t/2}\sin\tfrac{1}{2}t\sqrt{3}. \tag{4.1}$$

For large v the particle returns to $x = 0$ after a time $t = (2\pi/\sqrt{3}) = 3.6276$ irrespective of a. This corresponds to the position of the asymptote in figure 2. We also see from this analysis why the asymptote is approached from below for $a > 0$ and from above for $a < 0$. Similarly, for $v = 0$, the deterministic solution is

$$x = a(e^{-t/2}\cos\tfrac{1}{2}t\sqrt{3} + 3^{-1/2}e^{-t/2}\sin\tfrac{1}{2}t\sqrt{3} - 1) + y(e^{-t/2}\cos\tfrac{1}{2}t\sqrt{3} + 3^{-1/2}e^{-t/2}\sin\tfrac{1}{2}t\sqrt{3}) \tag{4.2}$$

and for large y this gives a return time of $(4\pi/3\sqrt{3}) = 2.4184$, which corresponds to the asymptote of figure 1. Notice that this case (equivalent to $\omega^2 = 1$) is typical of an under-damped case; the critically or over-damped cases are, of course, rather different.

The shapes of the curves in figures 1 and 2 may be understood qualitatively by noting that the external harmonic force has its equilibrium position at $x = -a$. For positive a this is on the other side of the absorbing barrier. Hence the behaviour of the function $\psi(y, v)$ is qualitatively no different from that obtained for the uniform force field. If, however, a is negative, then there is a real potential well at $x=-a$, in which the particle may be trapped for a long time before it acquires, through thermal agitation, enough energy to jump back to the absorbing barrier. Such behaviour for $v=0$ will be most pronounced when $y=-a$, when it may be expected that the first-passage time will be the inverse of a Boltzmann factor, i.e. $\exp(\frac{1}{2}a^2)$ or, in dimensional units, $\exp[M\omega^2a^2/(2kT)]$. For very small y the thermal agitation is more important than the force field, so $\psi(y,0)$ tends to zero as y tends to zero, while for large y the deterministic force field dominates and we approach the asymptote discussed above. This gives us a set of curves as in figure 1. The behaviour of $\psi(0, v)$, as depicted in figure 2, is similar: for a particle released at $x=0$ the return time is short for small v and tends to the limit 3.6276 as v tends to infinity, while for a range of medium values it may become trapped with a return time of the order $\exp(\frac{1}{2}a^2)$.

Appendix. The singularity at $y=v=0$

We consider the equation

$$\Phi_{vv}-[v+2\alpha(y)]\Phi_v+v\Phi_y-p\Phi=0 \tag{A1}$$

where

$$\Phi(0+, v)=1 \qquad \text{for } v<0 \tag{A2}$$

and $\Phi(y, v)$ is required to be bounded for all v and y. We assume that near $y=0$

$$\alpha(y)=\alpha_0+\alpha_1y+\alpha_2y^2+\ldots. \tag{A3}$$

If we look for a power series expansion in y, so that

$$\Phi(y, v)=\sum_{n=0}^{\infty}F_n(v)y^n \tag{A4}$$

then we find, on equating coefficients, that

$$(n+1)vF_{n+1}=pF_n+(v+2\alpha_0)F'_n-F''_n+2\sum_{m=1}^{n}\alpha_mF'_{n-m}. \tag{A5}$$

The initial condition (A2) gives, when $v<0$,

$$F_0(v)=1$$

so that

$$F_1(v)=p/v$$
$$F_2(v)=[p(p-1)/2v^2]-\alpha_0p/v^3-p/v^4 \tag{A6}$$

and in general

$$F_n(v)=\sum_{m=3}^{3n-2}f_{mn}v^{-m}.$$

The expansion (A4) therefore fails as $v\to0-$, becoming non-uniform when $v=O(y^{1/3})$. This suggests that it should be regarded as an outer expansion and should be supplemented by an inner expansion in terms of the variables

$$\xi=y^{1/3} \qquad \eta=v/y^{1/3}. \tag{A7}$$

From (A6) we obtain the matching condition that

$$\Phi \sim 1 + p(\eta^{-1} - \eta^{-4} + \ldots)\xi^2 + \alpha_0 p(-\eta^3 + \ldots)\xi^3 + \ldots \tag{A8}$$

as $\eta \to -\infty$.

In terms of the inner variables (A7), we have

$$\Phi_{\eta\eta} - [\xi^2\eta + 2(\alpha_0\xi + \alpha_1\xi^4 + \ldots)]\Phi_\eta + \tfrac{1}{3}\eta(\xi\Phi_\xi - \eta\Phi_\eta) - p\xi^2\Phi = 0 \tag{A9}$$

and we seek an inner expansion in the form

$$\Phi = \sum_\lambda \xi^\lambda f_\lambda(\eta). \tag{A10}$$

We must have $\lambda \geq 0$ and $f_\lambda(\eta) = O(|\eta|^\lambda)$ as $\eta \to \pm\infty$, in order that $\Phi(y, v)$ shall remain bounded. The matching condition (A8) shows that the range of λ must include the values $0, 2, 3, \ldots$. From (A9) and (A10)

$$L_\lambda\{f_\lambda\} \equiv f''_\lambda - \tfrac{1}{3}\eta^2 f'_\lambda + \tfrac{1}{3}\lambda\eta f_\lambda = \eta f'_{\lambda-2} + p f_{\lambda-2} + 2\sum_m \alpha_m f'_{\lambda-3m-1}. \tag{A11}$$

Consider first the complementary functions $\phi_\lambda(\eta)$, given by

$$L_\lambda\{\phi_\lambda\} = 0. \tag{A12}$$

The general solution of this equation, namely

$$\phi_\lambda(\eta) = A\,{}_1F_1(-\tfrac{1}{3}\lambda; \tfrac{2}{3}; \tfrac{1}{9}\eta^3) + B\eta\,{}_1F_1(\tfrac{1}{3}(1-\lambda); \tfrac{4}{3}; \tfrac{1}{9}\eta^3) \tag{A13}$$

is exponentially large as $\eta \to +\infty$ and therefore inadmissible unless A and B are related so that $\phi_\lambda = O(\eta^\lambda)$. We therefore define

$$A = 3^{2\lambda/3}\frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{1}{3}(1-\lambda))} \qquad B = 3^{2(\lambda-1)/3}\frac{\Gamma(-\frac{1}{3})}{\Gamma(-\frac{1}{3}\lambda)} \tag{A14}$$

so that

$$\phi_\lambda(\eta) \sim \eta^\lambda\,{}_2F_0(-\tfrac{1}{3}\lambda, \tfrac{1}{3}(1-\lambda); (-9/\eta^3)) \qquad \text{as } \eta \to +\infty. \tag{A15}$$

We also have

$$\begin{aligned}\phi_\lambda(\eta) &= \exp(\tfrac{1}{9}\eta^3)[A\,{}_1F_1(\tfrac{1}{3}(\lambda+2); \tfrac{2}{3}; -\tfrac{1}{9}\eta^3) + B\eta\,{}_1F_1(\tfrac{1}{3}\lambda+1; \tfrac{4}{3}; -\tfrac{1}{9}\eta^3)]\\ &\sim 2\sin(\tfrac{1}{6}\pi(1-2\lambda))(-\eta)^\lambda\,{}_2F_0(-\tfrac{1}{3}\lambda, \tfrac{1}{3}(1-\lambda); (-9/\eta^3)) \qquad \text{as } \eta \to -\infty.\end{aligned} \tag{A16}$$

If $\lambda = 3m + \frac{1}{2}$, where m is an integer, this asymptotic form vanishes identically. The relevant values of m are $0, 1, 2, \ldots$, and then

$$\phi_{3m+1/2} = (-1)^m 3^{4m+2}(\tfrac{1}{6})_{m+1}(\tfrac{5}{6})_m \exp(\tfrac{1}{9}\eta^3)\phi_{-3m-5/2}(-\eta) \tag{A17}$$

so that the function is exponentially small as $\eta \to -\infty$. These values of λ are therefore eigenvalues, such that the corresponding eigensolutions $\xi^{3m+1/2}\phi_{3m+1/2}(\eta)$ make no contribution to the outer expansion in $v < 0$. From (A12) and (A15) we can establish the recurrence relation

$$\phi_{\lambda+3}(\eta) = (\eta^3 - 3\lambda - 6)\phi_\lambda(\eta) - 3\eta\phi'_\lambda(\eta). \tag{A18}$$

When $m = 0, 1, 2, \ldots$, the functions $\phi_{3m}(\eta)$ and $\phi_{3m+1}(\eta)$ are polynomials in η and the asymptotic expansions (A15) and (A16) terminate and are exact. The functions $\phi_{3m+2}(\eta)$ can be derived by means of (A18) from

$$\phi_{-1}(\eta) = \begin{cases} \frac{1}{3}(\eta/\pi)^{1/2} \exp(\frac{1}{18}\eta^3) K_{1/6}(\frac{1}{18}\eta^3) & (\eta > 0) \\ \frac{1}{3}(-\pi\eta)^{1/2} \exp(\frac{1}{18}\eta^3)[I_{-1/6}(-\frac{1}{18}\eta^3) + I_{1/6}(-\frac{1}{18}\eta^3)] & (\eta < 0) \end{cases} \tag{A19}$$

and the eigenfunctions $\phi_{3m+1/2}(\eta)$ from

$$\phi_{1/2}(\eta) = \pi^{1/2} \exp(\tfrac{1}{18}\eta^3)\left[12^{-1/6}\eta \operatorname{Ai}\left(\frac{\eta^2}{12^{2/3}}\right) - 12^{1/6} \operatorname{Ai}'\left(\frac{\eta^2}{12^{2/3}}\right)\right]. \tag{A20}$$

From (A11) and (A8), the leading term of the inner expansion is

$$f_0(\eta) = \phi_0(\eta) = 1. \tag{A21}$$

Since $f_0'(\eta) = 0$ and $\phi_1(\eta)$ is not an eigenfunction, we must have

$$f_1(\eta) = 0. \tag{A22}$$

Hence

$$L_2\{f_2\} = p$$

of which the required solution is

$$f_2(\eta) = \tfrac{1}{2}p[\eta^2 + \tfrac{1}{2}\phi_2(\eta)]. \tag{A23}$$

We then have

$$L_3\{f_3\} = 2\alpha_0 f_2' = \alpha_0 p(2\eta + \tfrac{1}{2}\phi_2')$$

from which

$$f_3(\eta) = \tfrac{1}{2}\alpha_0 p\{\eta^3 - 2 + \tfrac{1}{2}\eta\phi_2(\eta)\}. \tag{A24}$$

These results satisfy the matching condition (A8) and there is no difficulty, in principle, about calculating higher terms.

The first eigenfunction to occur in the expansion (A10) is

$$f_{1/2}(\eta) = C_0\phi_{1/2}(\eta) \tag{A25}$$

where C_0 is not determined by the matching condition. This generates the further terms

$$f_{3/2}(\eta) = C_0\alpha_0\eta\phi_{1/2}(\eta) \tag{A26}$$

and

$$f_{5/2}(\eta) = C_0[\tfrac{1}{20}(18\alpha_0^2 + 1 + 8p)\eta^2\phi_{1/2}(\eta) + \tfrac{3}{5}(1 - 2\alpha_0^2 - 2p)\phi_{1/2}'(\eta)]. \tag{A27}$$

We then find that

$$f_{7/2}(\eta) = C_0\alpha_0[(\tfrac{1}{4} + \tfrac{1}{6}\alpha_0^2)\eta^3 - \tfrac{1}{2} + 3\alpha_0^2 + 3p]\phi_{1/2}(\eta) + C_1\phi_{7/2}(\eta) \tag{A28}$$

where C_1 is indeterminate and the second eigenfunction is given by

$$\phi_{7/2}(\eta) = (\eta^3 - \tfrac{15}{2})\phi_{1/2}(\eta) - 3\eta\phi_{1/2}'(\eta). \tag{A29}$$

The coefficients $C_0, C_1, \ldots,$ of the eigenfunctions in (A10) depend on the global behaviour of the solution and are determined by the boundary conditions on Φ as $v \to \pm\infty$ and $y \to +\infty$.

As $\eta \to +\infty$ we recover the outer expansion (A4) with

$$F_0(v) = 1 + C_0 v^{1/2} + C_0\alpha_0 v^{3/2} + \tfrac{3}{4}pv^2 + \tfrac{1}{20}C_0(18\alpha_0^2 + 1 + 8p)v^{5/2} + \tfrac{3}{4}\alpha_0 pv^3 + \mathrm{O}(v^{7/2}) \qquad \text{for } v > 0. \tag{A30}$$

At $\eta = 0$ we have

$$\Phi(y, 0) = 1 + 3^{1/3}\frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{1}{6})}C_0 y^{1/6} + \frac{3^{4/3}\Gamma(\frac{1}{3})}{4\Gamma(-\frac{1}{3})}py^{2/3} + \frac{3^{2/3}\Gamma(-\frac{1}{3})}{5\Gamma(-\frac{1}{6})}C_0(1 - 2\alpha_0^2 - 2p)y^{5/6} - \alpha_0 py + \mathrm{O}(y^{7/6}). \tag{A31}$$

The terms $\mathrm{O}(v^{7/2})$ and $\mathrm{O}(y^{7/6})$ in (A30) and (A31) involve C_1, the second indeterminate coefficient. Similarly

$$\Phi_v(y, 0) = 3^{-1/3}\frac{\Gamma(-\frac{1}{3})}{\Gamma(-\frac{1}{6})}C_0 y^{-1/6} + 3^{1/3}\frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{1}{6})}C_0\alpha_0 y^{1/6} + \frac{3^{1/3}\Gamma(-\frac{1}{3})}{4\Gamma(-\frac{2}{3})}py^{1/3} + \frac{3^{4/3}\Gamma(\frac{1}{3})}{4\Gamma(-\frac{1}{3})}\alpha_0 py^{2/3} + \mathrm{O}(y^{5/6}). \tag{A32}$$

In the case $\alpha(y) = \alpha_0$, a constant, the coefficient C_0 can be determined from the analytical solution of [1] which gives

$$\Phi_v(y, 0) = \tfrac{1}{2}p \sum_{n=0}^{\infty} g_n \frac{\alpha_0 D_n(2q_n) + D_n'(2q_n)}{q_n(n!)^{1/2}} \exp[-(q_n - \alpha_0)y] \tag{A33}$$

where

$$g_n = a_n + \sum_{m=0}^{\infty} \frac{b_m}{2q_m(q_m + q_n)Q_m Q_n}$$

and

$$\begin{aligned} a_n &= (n!)^{-1/2}(q_n - \alpha_0)^{n-1}\exp(\alpha_0 q_n - \tfrac{1}{2}n - \tfrac{1}{2}p) \\ b_n &= (n!)^{-1/2}(q_n + \alpha_0)^{n-1}\exp(-\alpha_0 q_n - \tfrac{1}{2}n - \tfrac{1}{2}p) \\ q_n &= (n + p + \alpha_0^2)^{1/2} \qquad Q_n = (n!)^{1/2}\gamma_+(\mathrm{i}q_n; p + \alpha_0^2). \end{aligned} \tag{A34}$$

The sum of any finite number of terms of the series (A33) remains bounded as $y \to 0+$, so that we need the asymptotic form of the nth term as $n \to \infty$. As in [1], appendix 3,

$$g_n \sim \sum_{r=0}^{\infty} G_r q_n^{-r/2-1} \qquad \text{as } n \to \infty \tag{A35}$$

where

$$G_0 = (8\pi)^{-1/2}S_0 = (8\pi)^{-1/2}\sum_{m=0}^{\infty}\frac{b_m}{q_m Q_m}. \tag{A36}$$

We also have from [1], (A1.32) and (A1.33),

$$\frac{\alpha_0 D_n(2q_n) + D_n'(2q_n)}{q_n(n!)^{1/2}} = \left(\frac{2\pi}{n!}\right)^{1/2} q_n^{n+1/3}\exp(-\tfrac{1}{2}q_n^2)[\mathrm{Ai}'(0) + \mathrm{O}(q_n^{-1/3})] = (2\pi)^{1/4}n^{-5/12}\left(-\frac{3^{-1/3}}{\Gamma(\frac{1}{3})} + \mathrm{O}(n^{-1/6})\right). \tag{A37}$$

It follows that

$$g_n \frac{\alpha_0 D_n(2q_n)+D'_n(2q_n)}{q_n(n!)^{1/2}} = -\frac{S_0 n^{-11/12}}{2(2\pi)^{1/4}3^{1/3}\Gamma(\frac{1}{3})} + O(n^{-13/12}) \tag{A38}$$

so that as $y \to 0+$

$$\Phi_v(y,0) = -\frac{S_0 p}{4(2\pi)^{1/4}3^{1/3}\Gamma(\frac{1}{3})} Z(\tfrac{11}{12}, y) + O(1) \tag{A39}$$

where

$$Z(\nu, y) = \sum_{m=1}^{\infty} m^{-\nu} e^{-y\sqrt{m}} \tag{A40}$$

is the function defined by Titulaer [10]. Since

$$Z(\nu, y) = 2\Gamma(2-2\nu)y^{2\nu-2} + \sum_{m=0}^{\infty} \zeta(\nu - \tfrac{1}{2}m)(-y)^m/m! \tag{A41}$$

we have

$$\Phi_v(y,0) = -\frac{S_0\Gamma(\frac{1}{6})p}{2(2\pi)^{1/4}3^{1/3}\Gamma(\frac{1}{3})} y^{-1/6} + O(1). \tag{A42}$$

Comparison with (A32) therefore gives

$$C_0 = -3^{1/2}(2\pi)^{-1/4}S_0 p. \tag{A43}$$

The constant S_0 depends on p and α_0. We are particularly interested in the case when p is small, so that C_0 is proportional to p. With $p=0$, from [1], (A3.14),

$$d_m = \frac{b_m}{q_m Q_m} \sim \sum_{r=0}^{\infty} D_r q_m^{-r-5/2} \qquad \text{as } m \to \infty. \tag{A44}$$

In the case $\alpha_0 = 1$, for which $q_m = (m+1)^{1/2}$, numerical values of d_0–d_{15}, and of D_0–D_4, were computed, and D_5 was estimated. These values give

$$S_0 = \sum_{m=0}^{\infty} d_m \simeq \sum_{m=0}^{14} d_m + \sum_{r=0}^{5} D_r \zeta(\tfrac{1}{2}r + \tfrac{5}{4}, 16)$$
$$\simeq 0.6831 \tag{A45}$$

so that

$$C_0 \simeq -0.7473p \tag{A46}$$

for $\alpha_0 = 1$ and p small.

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