A drop of ink falls from my pen. . . it comes to earth, I know not when

1985 J. Phys. A: Math. Gen. 18 3531

(http://iopscience.iop.org/0305-4470/18/18/016)

J. Phys. A: Math. Gen. 18 (1985) 3531-3559. Printed in Great Britain

A drop of ink falls from my pen ... It comes to earth, I know not when

T W Marshall and E J Watson

Department of Mathematics, Manchester University, Manchester M13 9PL, UK

Received 5 December 1984, in final form 8 May 1985

Abstract. We obtain, for a Brownian particle in a uniform force field, the mean and asymptotic first-passage times as functions of the particle's initial position and velocity, with the recurrence times given as a special case. We discuss the region of phase space for which the diffusion model of Brownian motion provides an adequate approximation, and conclude that there is no possibility of obtaining the recurrence times within that model.

We find that the nature of the boundary-value problem is profoundly altered when the motion is treated as a process in phase rather than configuration space, because the time-development operator is then parabolic rather than elliptic. We argue that such a change in the treatment of Brownian motion places it within the sphere of transport theory rather than diffusion theory, and that, consequently, results such as ours have relevance to the study of phenomena such as radiative transfer and neutron transport.

1. Historical introduction

The mathematical theory of Brownian motion was established, by Einstein and Smoluchowski independently, in 1905 and 1906, though some important results had already been obtained more than a decade previously by Rayleigh. However, as emphasised by Nelson [1] the theory remained essentially descriptive, or kinematic, until 1930, when Uhlenbeck and Ornstein [2]†, starting with a dynamical equation of motion, that is, one involving the second time derivative of the particle's position, obtained the master equation for the distribution of the particle in phase space. Their result was generalised to Brownian motion in a force field by Kramers [3]. Solution of this master, or Fokker-Planck, equation gives the probability of transition from an initial point in phase space to any region of the space after a time t. As indicated by Rice [4], it also gives a formal expression for the first-passage-time distribution. However, Rice's expression is a series of increasingly complicated multiple integrals, and, mercifully, nobody has attempted to use it quantitatively. Since 1945, when Wang and Uhlenbeck [5] published their review article, little progress was made on the solution of the Kramers equation. Interest has recently revived, and some approximate solutions for the time-independent problem have been given by Titulaer and co-workers [6-8]. However, no progress has been made beyond Rice's expression, in inverting the transition probabilities to obtain first-passage times.

For this reason alone, our calculation of mean first-passage times for the Uhlenbeck-Ornstein process in a uniform field should be of interest, but we believe our results have a greater significance than this.

† References [2, 4, 5, 9] are reprinted in [2a].

0305-4470/85/183531+29$02.25

The stochastic differential equation for the process is

$$m\ddot{x} = g(x) - \beta\dot{x} + F(t), \tag{1.1}$$

where $F(t)$ is a stochastic force with mean value zero and autocorrelation

$$\langle F(t)F(t+\tau)\rangle = K(\tau). \tag{1.2}$$

The brackets denote ensemble averaging or, if the process is ergodic, time averaging. If we approximate this stochastic force by a white noise, so that

$$K(\tau) = 2\beta kT\delta(\tau), \tag{1.3}$$

then the Fokker–Planck equation for the phase-space distribution $W(x, u; t)(u = \dot{x})$ is

$$\frac{\partial W}{\partial t} = \frac{\beta kT}{m^2}\frac{\partial^2 W}{\partial u^2} + \frac{\beta}{m}\frac{\partial}{\partial u}(uW) - \frac{g(x)}{m}\frac{\partial W}{\partial u} - u\frac{\partial W}{\partial x}. \tag{1.4}$$

We express t in units of $\beta^{-1}m$ and x in units of $\beta^{-1}(mkT)^{1/2}$, so that this equation takes the non-dimensional form

$$\frac{\partial W}{\partial t} = \frac{\partial^2 W}{\partial u^2} + \frac{\partial}{\partial u}(uW) + 2\alpha(x)\frac{\partial W}{\partial u} - u\frac{\partial W}{\partial x}, \tag{1.5}$$

where

$$\alpha(x) = -\tfrac{1}{2}\beta^{-1}(m/kT)^{1/2}g(x). \tag{1.6}$$

Most discussions of Brownian motion have been based on the diffusion approximation, in which the inertia term in (1.1) is neglected

$$\dot{x} = \beta^{-1}g(x) + \beta^{-1}F(t). \tag{1.7}$$

In this case the non-dimensionalised Fokker–Planck equation is

$$\frac{\partial W}{\partial t} = \frac{\partial^2 W}{\partial x^2} + \frac{\partial}{\partial x}[2\alpha(x)W]. \tag{1.8}$$

The distribution of first-passage times may then, following Smoluchowski [9], be obtained by introducing an 'absorbing barrier' at $x = 0$, with the boundary condition

$$W(0+, t) = 0. \tag{1.9}$$

This approximation has been very fruitful. The number of independent variables has been reduced from three to two, and after Laplace transforming with respect to t, these reduce to the single variable x. The resulting ordinary differential equation may be solved for a large family of force fields [10]. Furthermore, for multidimensional processes the time-development operator† is always elliptic, which enables us to recast many problems about the first-passage times as classical Dirichlet-type boundary-value problems [11].

We believe, however, that probability theorists have concentrated their efforts too exclusively on this approximation. Within it one can obtain results only for those features of the motion which are (approximately) independent of the particle's initial velocity. Now, as Kramers [3] proved, at least informally, for large β the particle's memory of its initial velocity is a good deal shorter than its memory of its initial

† In an equation of the form $\mathrm{d}W/\mathrm{d}t = LW$, L will be referred to as 'the time-development operator'. It will be termed 'parabolic' or 'elliptic' depending on whether the equation $LW = 0$ is parabolic or elliptic.

position. It is therefore reasonable to expect that the first-passage times will be correctly given by the diffusion model, provided the initial position lies outside a certain region close to the absorbing barrier, and provided the initial velocity is not too large. Our more exact theory will indicate the orders of magnitude of such boundary regions.

When we come to the recurrence time, however, the diffusion model predicts incorrectly that, with probability one, it takes the value zero. Since Smoluchowski's original article [9] there has been almost no discussion of the recurrence time, except for Chandrasekhar's review article [12], and it is now known [13] that both of these are based on incorrect arguments. Ours is, therefore, the first reliable value for the mean recurrence time.

The boundary condition for an absorbing barrier in the Kramers equation (1.5) was given by Wang and Uhlenbeck [5] as

$$W(0+, u; t) = 0 \qquad u > 0. \tag{1.10}$$

They proposed this rather hesitantly ('We feel sure that this means the condition ...'), presumably because it seems to apply to only half of the boundary in phase space. Can one be sure that this condition, together with conditions of finiteness on the infinitely distant boundaries, will guarantee a unique solution in the half-space $x > 0$? In the following sections we shall see that this question can now be answered affirmatively.

Without going into details at this stage, we note that the reason why (1.10) is adequate to guarantee such a unique solution is that the time-development operator, because it contains no x derivatives beyond the first, is parabolic. This is also the feature which is responsible for the different memory time scales of x and u. Broadly speaking such behaviour is also characteristic of the linear transport processes [14] studied in connection with radiative transfer and neutron transport. Although in these processes the second derivative with respect to u is replaced by an integral operator, this parabolic nature of the time-development operator is again of crucial importance, and poses certain questions about half-range completeness of a family of eigenfunctions [15]. For the time-independent force-free case of equation (1.5), the half-range completeness of the eigenfunctions was proved by Beals and Protopopescu [16], and it seems very likely that their method can be applied to our problem.

2. The first-passage-time density

We consider the case of a uniform force field, for which the Fokker-Planck equation is

$$\frac{\partial W}{\partial t} = \frac{\partial^2 W}{\partial u^2} + \frac{\partial}{\partial u}[(u+2\alpha)W] - u\frac{\partial W}{\partial x} \qquad x > 0,\ t > 0. \tag{2.1}$$

In this article we shall consider in particular the case where the field attracts the particle towards the absorbing barrier, so that α is a positive constant. The transition probability for a particle initially at (y, v) satisfies (2.1) with the boundary conditions

$$W(x, u; 0) = \delta(x-y)\delta(u-v), \tag{2.2}$$

$$W(0+, u; t) = 0 \qquad u > 0, \tag{2.3}$$

$$W \to 0 \qquad \text{as } u \to \pm\infty \qquad \text{and as } x \to +\infty. \tag{2.4}$$

We denote this Green function by $W(x, u; y, v; t)$. Then the first-passage-time density is

$$\Phi(y, v; t) = -\int_{-\infty}^{0} uW(0+, u; y, v; t)\,\mathrm{d}u. \tag{2.5}$$

It is possible to find W by using the methods we shall describe in the next section, but it is somewhat easier to find Φ directly. This is because W satisfies the backward Fokker–Planck, or Kolmogorov [11] equation, and hence so does Φ, that is to say

$$\frac{\partial\Phi}{\partial t} = \frac{\partial^2\Phi}{\partial v^2} - (v+2\alpha)\frac{\partial\Phi}{\partial v} + v\frac{\partial\Phi}{\partial y} \qquad y>0,\ t>0. \tag{2.6}$$

Φ also satisfies the boundary and finiteness conditions

$$\Phi(y, v; 0+) = 0, \tag{2.7}$$

$$\int_0^t \Phi(y, v; t')\,\mathrm{d}t' \to 1 \qquad \text{as } y\to 0 \qquad v<0,\ t>0, \tag{2.8}$$

$$0 \leqslant \int_0^t \Phi(y, v; t')\,\mathrm{d}t' \leqslant 1, \tag{2.9}$$

$$\Phi \to 0 \qquad \text{as } y \to +\infty. \tag{2.10}$$

((2.8) says that a particle, released near to the absorbing barrier, is certain to be absorbed immediately.)

The Laplace transform $\bar\Phi(y, v; p)$ satisfies

$$\bar\Phi_{vv} - (v+2\alpha)\bar\Phi_v + v\bar\Phi_y - p\bar\Phi = 0, \tag{2.11}$$

$$\bar\Phi(0+, v; p) = 1 \qquad v<0, \tag{2.12}$$

$$0 \leqslant |\bar\Phi| \leqslant 1 \qquad \text{for } Rp \geqslant 0, \tag{2.13}$$

$$\bar\Phi - 0 \qquad \text{as } y \to +\infty. \tag{2.14}$$

Condition (2.13) originates in the probabilistic constraints

$$\Phi(y, v; t) \leqslant 0, \qquad \int_0^\infty \Phi(y, v; t)\,\mathrm{d}t \leqslant 1 \qquad \text{all } y, v.$$

In deriving the analytic solution in § 3 a very much weaker condition was imposed on $\bar\Phi$, as $|v|\to\infty$, in order to ensure a unique solution. Checks have, however, been made on the numerical solution in § 4 to establish that it does, in fact, satisfy (2.13). A separation of the variables gives a set of functions satisfying (2.11) and (2.14), namely

$$\Phi_n(y, v; p) = \exp[(\alpha - q_n)y + \alpha v + v^2/4]D_n(2q_n + v), \tag{2.15}$$

where D_n is a parabolic cylinder function (see appendix 1), and

$$q_n = (n + \alpha^2 + p)^{1/2}. \tag{2.16}$$

It is, therefore, natural to seek a solution for $\bar\Phi$ as a linear combination of Φ_n satisfying the remaining condition (2.12). We shall use the notation

$$f_n^-(v) = (n!)^{-1/2}\exp(-\alpha v)\Phi_n(0, v; p) = (n!)^{-1/2}\exp(v^2/4)D_n(2q_n + v). \tag{2.17}$$

The separation of variables in (2.15) is analogous to that of Burschka and Titulaer [6] for the time-independent case of equation (2.1). Their result generalised that of Pagani [17], who obtained the corresponding formula for the case $\alpha = 0$, in which there is no force field. It was proved by Beals and Protopopescu [16] that Pagani's functions form a complete set over the half-range $u > 0$. It seems very likely that their method will show that the set of functions $f_n^-(v)$ spans the space of functions $f(v)$, defined in $v < 0$, in which the inner product is given by

$$(f, g) = \int_{-\infty}^{0} f(v)g(v)(-v)\exp(-\tfrac{1}{2}v^2)\,\mathrm{d}v. \tag{2.18}$$

The proof of Beals and Protopopescu is one of pure existence, using functional analysis, and does not lead to a determination of the coefficients g_n in the expansion of an arbitrary function $g(v)$ as the series

$$g(v) = \sum_{n=0}^{\infty} g_n f_n^-(v) \qquad v < 0. \tag{2.19}$$

Our method gives explicitly a set of functions $F_n^-(v)$ such that

$$(F_m^-, f_n^-) = 0 \qquad \text{for } m \neq n, \tag{2.20}$$

and determines the coefficients g_n in (2.19).

3. Analytical solution

The substitution

$$\bar{\Phi}(y, v; p) = \exp[\alpha(v + y)]\phi(y, v; \tau), \tag{3.1}$$

where

$$\tau = p + \alpha^2, \tag{3.2}$$

converts equation (2.11) into

$$\phi_{vv} - v\phi_v + v\phi_y - \tau\phi = 0. \tag{3.3}$$

This is a parabolic equation with characteristics $y = \text{constant}$. The direction of evolution of the solution is that of increasing y when $v < 0$, but decreasing y when $v > 0$. Hence it is appropriate to look for a solution of (3.3) in $y > 0$, subject to the initial condition

$$\phi(0+, v; \tau) = g(v; \tau) \qquad \text{for } v < 0, \tag{3.4}$$

where $g(v; \tau)$ is a given function, together with the boundary conditions

$$\phi(y, v; \tau) = \mathrm{O}(\exp(A|v|)) \qquad \text{as } v \to \pm\infty \tag{3.5}$$

for some constant A. We also need a condition as $y \to \infty$ in $v > 0$, and so we further assume that

$$\phi(y, v; \tau) \to 0 \qquad \text{as } y \to \infty. \tag{3.6}$$

The boundary condition (2.12) corresponds to

$$g(v; \tau) = \exp(-\alpha v) \qquad \text{for } v < 0, \tag{3.7}$$

but it is useful to consider also the general case.

The method of solution is to split the region $y>0$ along the line $v=0$. Suppose that

$$\phi_v(y, 0; \tau) = \psi(y; \tau). \tag{3.8}$$

Then the solution of (3.3), (3.4) and (3.5) in $v \leqslant 0$ is of the form

$$\phi(y, v; \tau) = \int_0^\infty g(-w; \tau)\phi_1(y, v; \tau, w)\,\mathrm{d}w + \int_0^y \psi(z; \tau)\phi_2(y-z, v; \tau)\,\mathrm{d}z. \tag{3.9}$$

Here $\phi_1(y, v)$ and $\phi_2(y, v)$ are solutions of (3.3) and (3.5) in $v \leqslant 0$, such that

$$\phi_1(0+, v) = \delta(v+w) \qquad v<0, \qquad \phi_{1v}(y, 0) = 0, \tag{3.10}$$

and

$$\phi_2(0+, v) = 0 \qquad v<0, \qquad \phi_{2v}(y, 0) = \delta(y). \tag{3.11}$$

The solution of (3.3), (3.5) and (3.6) in $v \geqslant 0$ is then

$$\phi(y, v; \tau) = -\int_y^\infty \psi(z; \tau)\phi_2(z-y, -v; \tau)\,\mathrm{d}z. \tag{3.12}$$

The function $\psi(y; \tau)$ is determined by the condition that $\phi(y, v; \tau)$ must be continuous at $v=0$. Hence, from (3.9) and (3.12),

$$\int_0^\infty \phi_2(|y-z|, 0; \tau)\psi(z; \tau)\,\mathrm{d}z = \theta(y; \tau) \qquad \text{for } y>0, \tag{3.13}$$

where

$$\theta(y; \tau) = -\int_0^\infty g(-w)\phi_1(y, 0; \tau, w)\,\mathrm{d}w. \tag{3.14}$$

Equation (3.13) is an integral equation of the Wiener-Hopf type for $\psi(y; \tau)$. When $\psi(y; \tau)$ is known, the solution $\phi(y, v; \tau)$ is given by (3.9) and (3.12).

We define Laplace transforms with respect to y by

$$L\{u(y)\} = \tilde{u}(q) = \int_0^\infty u(y)\exp(-qy)\,\mathrm{d}y, \tag{3.15}$$

and Fourier transforms by

$$F\{u(y)\} = \int_{-\infty}^\infty u(y)\exp(-\mathrm{i}sy)\,\mathrm{d}y = \tilde{u}(\mathrm{i}s) + \tilde{u}_1(-\mathrm{i}s), \tag{3.16}$$

where

$$u_1(y) = u(-y). \tag{3.17}$$

The transforms $\tilde{\phi}_1(q, v)$ and $\tilde{\phi}_2(q, v)$ are easily obtained by transforming equation (3.3) and using the boundary conditions. In particular, we find that

$$\tilde{\phi}_1(q, 0) = -w\exp(-\tfrac{1}{4}w^2)D_\nu(2q+w)/D'_\nu(2q), \tag{3.18}$$

and

$$\tilde{\phi}_2(q, v) = -\exp(\tfrac{1}{4}v^2) D_\nu(2q - v)/D'_\nu(2q), \tag{3.19}$$

where

$$\nu = q^2 - \tau.$$

The solution of the integral equation (3.13) is found by the standard method as follows. Let

$$\chi(-y) = \int_0^\infty \phi_2(|y - z|, 0)\psi(z)\, dz \qquad \text{for } y < 0. \tag{3.20}$$

Then the Fourier transform of equations (3.13) and (3.20) combined is

$$K(s)\tilde{\psi}(is) = \tilde{\theta}(is) + \tilde{\chi}(-is), \tag{3.21}$$

where

$$K(s) = \tilde{\phi}_2(is, 0) + \tilde{\phi}_2(-is, 0) = \frac{(2\pi)^{1/2}}{\Gamma(s^2 + \tau) D'_\nu(2is) D'_\nu(-2is)}, \tag{3.22}$$

and now

$$\nu = -s^2 - \tau. \tag{3.23}$$

The result (3.22) is obtained from (3.19) with the use of the Wronskian relation (A1.4) for the parabolic cylinder functions.

Suppose that

$$K(s) = K_+(s) K_-(s), \tag{3.24}$$

where $K_+(s)$ and $K_-(s)$ are functions that are regular and non-zero in upper and lower half-planes respectively, and that

$$\tilde{\theta}(is)/K_+(s) = L(s) = L_+(s) + L_-(s), \tag{3.25}$$

where $L_+(s)$ and $L_-(s)$ are regular in upper and lower half-planes respectively. Then from (3.21) we obtain

$$K_-(s)\tilde{\psi}(is) - L_-(s) = L_+(s) + \tilde{\chi}(-is)/K_+(s), \tag{3.26}$$

where each side is regular in its appropriate half plane. If we can choose the decompositions (3.24) and (3.25) in such a way that the half planes overlap, and that each side tends to 0 as $s \to \infty$ in the appropriate half plane, then each side must vanish identically by Liouville's theorem, so that

$$\tilde{\psi}(is) = L_-(s)/K_-(s). \tag{3.27}$$

From the inverse Fourier transform

$$\psi(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\psi}(is) \exp(isz)\, ds \qquad z > 0,$$

we have in $v > 0$

$$\phi(y, v) = -\int_y^\infty \frac{\phi_2(z - y, -v)}{2\pi} \int_{-\infty}^{\infty} \tilde{\psi}(is) \exp(isz)\, ds\, dz.$$

If we can interchange the order of integration, we shall get

$$\phi(y, v) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{\psi}(\mathrm{i}s)\tilde{\phi}_2(-\mathrm{i}s, -v)\exp(\mathrm{i}sy)\,\mathrm{d}s$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{\psi}(\mathrm{i}s)\frac{D_\nu(v-2\mathrm{i}s)}{D'_\nu(-2\mathrm{i}s)}\exp(\mathrm{i}sy+\tfrac{1}{4}v^2)\,\mathrm{d}s, \tag{3.28}$$

where ν is given by (3.23).

The function $D'_{q^2-\tau}(-2q)$ is regular for all values of q, and (as shown in appendix 1) its zeros $q = d_n(\tau)$ $(n = 0, 1, 2, \ldots)$ all lie in $Rq > 0$, provided that $R\tau > 0$. The problem of factorising $K(s)$ therefore reduces to that of constructing the factorisation

$$\Gamma(s^2+\tau) = \gamma_+(s;\tau)\gamma_-(s;\tau). \tag{3.29}$$

The details of this factorisation are given in appendix 2; we note here that we can take

$$\gamma_-(s;\tau) = \gamma_+(-s;\tau). \tag{3.30}$$

Hence we put

$$K_+(s) = -\frac{(2\pi)^{1/4}}{\gamma_+(s;\tau)D'_\nu(-2\mathrm{i}s)}, \tag{3.31}$$

and

$$K_-(s) = K_+(-s). \tag{3.32}$$

From appendix 2 we have

$$K_+(s) \sim \frac{3^{1/3}\Gamma(\frac{1}{3})}{(2\pi)^{1/2}}(-\mathrm{i}s)^{-1/6} \tag{3.33}$$

as $|s| \to \infty$ with $|\arg(-\mathrm{i}s)| < \pi - \delta$.

If $g(v;\tau) = O(\mathrm{e}^{A|v|})$ as $v \to -\infty$, the integral

$$\tilde{\theta}(q;\tau) = -\int_0^{\infty} g(-w;\tau)\tilde{\phi}_1(q, 0; \tau, w)\,\mathrm{d}w$$

converges uniformly except near the poles $q = -d_n(\tau)$ of $\tilde{\phi}_1(q, 0)$, so that the singularities of $L(s)$ are poles at $s = \mathrm{i}d_n(\tau)$ and $s = -\mathrm{i}q_n(\tau)$ for $n = 0, 1, 2, \ldots$, where

$$q_n(\tau) = (n+\tau)^{1/2} \tag{3.34}$$

and the τ plane is cut along the negative real axis. The decomposition of $L(s)$ is also treated in appendix 2. From (3.27) it follows that $\tilde{\psi}(\mathrm{i}s)$ is regular except for poles at $s = \mathrm{i}q_n(\tau)$. The integrand of (3.28) has poles at $s = \mathrm{i}q_n(\tau)$ and $s = -\mathrm{i}d_n(\tau)$. If we can evaluate $\phi(y, v; \tau)$ from (3.28) in terms of the residues of the integrand in the upper half plane, we obtain after some reduction

$$\phi(y, v; \tau) = \sum_{n=0}^{\infty} \frac{L_-(\mathrm{i}q_n)D_n(v+2q_n)\exp(-q_ny+\frac{1}{4}v^2)}{2(2\pi)^{1/4}n!\,q_n\gamma_+(\mathrm{i}q_n;\tau)}. \tag{3.35}$$

For the case (3.7), we have when $\tau = \alpha^2$ (corresponding to $p = 0$)

$$\tilde{\theta}(\mathrm{i}s;\alpha^2) = -\frac{D'_\nu(2\mathrm{i}s) - \alpha D_\nu(2\mathrm{i}s)}{(\mathrm{i}s+\alpha)D'_\nu(2\mathrm{i}s)}, \tag{3.36}$$

where now

$$\nu = -s^2 - \alpha^2. \tag{3.37}$$

Hence

$$L(s) \equiv L(s;\alpha) = \frac{\{D'_\nu(2\mathrm{i}s) - \alpha D_\nu(2\mathrm{i}s)\}D'_\nu(-2\mathrm{i}s)\gamma_+(s;\alpha^2)}{(2\pi)^{1/4}(\mathrm{i}s+\alpha)D'_\nu(2\mathrm{i}s)}. \tag{3.38}$$

The Wronskian relation (A1.4) enables us to put

$$L(s;\alpha) = L_1(s;\alpha) + L_2(s;\alpha), \tag{3.39}$$

where

$$L_1(s;\alpha) = \frac{\{D'_\nu(-2\mathrm{i}s) + \alpha D_\nu(-2\mathrm{i}s)\}\gamma_+(s;\alpha^2)}{(2\pi)^{1/4}(\mathrm{i}s+\alpha)}, \tag{3.40}$$

and

$$L_2(s;\alpha) = \frac{(2\pi)^{1/4}\alpha}{(\mathrm{i}s+\alpha)D'_\nu(2\mathrm{i}s)\gamma_+(-s;\alpha^2)}. \tag{3.41}$$

The function $L_1(s;\alpha)$ is regular except at the poles $s = -\mathrm{i}q_n(\alpha^2)$ of $\gamma_+(s;\alpha^2)$, since $\{D'_\nu(-2\mathrm{i}s) + \alpha D_\nu(-2\mathrm{i}s)\} = 0$ when $s = \mathrm{i}\alpha$, and $L_1(s;\alpha) = \mathrm{O}(|s|^{-5/6})$ as $|s| \to \infty$ with $|\arg(-\mathrm{i}s)| < \pi - \delta$. $L_2(s;\alpha)$ is regular except at the zeros $s = \mathrm{i}d_n(\alpha^2)$ of $D'_\nu(2\mathrm{i}s)$, and possibly at $s = \mathrm{i}\alpha$; as $|s| \to \infty$ with $|\arg(\mathrm{i}s)| < \pi - \delta$, $L_2(s;\alpha) = \mathrm{O}(|s|^{-7/4})$.

If $R\alpha > 0$ the first pole of $\gamma_+(-s;\alpha^2)$ is at $s = \mathrm{i}\alpha$, and therefore cancels the zero of $(\mathrm{i}s+\alpha)$ in $L_2(s;\alpha)$. Hence, provided that $R\alpha^2 > 0$ also, we can take

$$L_+(s;\alpha) = L_1(s;\alpha), \qquad L_-(s;\alpha) = L_2(s;\alpha). \tag{3.42}$$

In particular, $L_-(\mathrm{i}q_n(\alpha^2);\alpha) = 0$ when $n = 1, 2, 3, \ldots$ and

$$L_-(\mathrm{i}\alpha;\alpha) = 2(2\pi)^{1/4}\alpha\exp(\alpha^2)\gamma_+(\mathrm{i}\alpha;\alpha^2). \tag{3.43}$$

The series (3.35) therefore reduces to the single term $n = 0$, giving

$$\phi(y, v;\alpha^2) = \exp(\alpha^2)D_0(v+2\alpha)\exp(-\alpha y + \tfrac{1}{4}v^2) = \exp[-\alpha(v+y)], \tag{3.44}$$

which corresponds to

$$\bar{\Phi}(y, v; 0) = 1. \tag{3.45}$$

If we change α into $-\alpha$ (keeping $R\alpha > 0$), we see that $L_2(s;-\alpha)$ has a pole $s = -\mathrm{i}\alpha$ in the lower half plane. Consequently we must now take

$$\begin{aligned} L_+(s;-\alpha) &= L_1(s;-\alpha) + \frac{(2\pi)^{1/4}\exp(\alpha^2)}{(\mathrm{i}s-\alpha)\gamma_+(\mathrm{i}\alpha;\alpha^2)}, \\ L_-(s;-\alpha) &= L_2(s;-\alpha) - \frac{(2\pi)^{1/4}\exp(\alpha^2)}{(\mathrm{i}s-\alpha)\gamma_+(\mathrm{i}\alpha;\alpha^2)}, \end{aligned} \tag{3.46}$$

again assuming that $R\alpha^2 > 0$, so that

$$L_-(\mathrm{i}q_n(\alpha^2);-\alpha) = \frac{(2\pi)^{1/4}\exp(\alpha^2)}{(q_n+\alpha)\gamma_+(\mathrm{i}\alpha;\alpha^2)}. \tag{3.47}$$

The series (3.35) now takes the form

$$\phi(y, v; \alpha^2) = \sum_{n=0}^{\infty} \frac{D_n(v+2q_n)\exp(\alpha^2 - q_n y + \frac{1}{4}v^2)}{2q_n(q_n+\alpha)n!\gamma_+(\mathrm{i}\alpha; \alpha^2)\gamma_+(\mathrm{i}q_n; \alpha^2)}$$

$$= \frac{\alpha\exp(\alpha^2+\frac{1}{4}v^2)}{\gamma_+(\mathrm{i}\alpha; \alpha^2+1)} \sum_{n=0}^{\infty} \frac{D_n(v+2q_n)\,\mathrm{e}^{-q_n y}}{n!q_n\gamma_+(\mathrm{i}q_n; \alpha^2+1)}. \tag{3.48}$$

from (A2.25), where $q_n = (n+\alpha^2)^{1/2}$.

The solutions (3.44) and (3.48) for $g(v) = \mathrm{e}^{\mp\alpha v}$ were derived on the assumptions that $v>0$ and $R\alpha^2>0$. Clearly (3.44) is valid also for $v\leqslant 0$ provided only that $R\alpha>0$. In (3.48) the nth term of the series

$$\sim \frac{\mathrm{Ai}(n^{1/6}v)\,\mathrm{e}^{-n^{1/2}y}}{(2\pi)^{1/4}n^{13/12}} \qquad \text{as } n\to\infty, \tag{3.49}$$

(from (A1.30) and (A2.20)) so that the series converges uniformly in v and y when $y\geqslant 0$ and $R\alpha>0$, and satisfies equation (3.3) with $\tau=\alpha^2$ for all v with $y>0$. Hence (3.48) is valid for all v when $y\geqslant 0$ and $R\alpha>0$. From the construction of the series we infer that

$$\mathrm{e}^{\alpha v} = \frac{\alpha\,\mathrm{e}^{\alpha^2+v^2/4}}{\gamma_+(\mathrm{i}\alpha; \alpha^2+1)} \sum_{n=0}^{\infty} \frac{D_n(v+2q_n)}{n!q_n\gamma_+(\mathrm{i}q_n; \alpha^2+1)} \qquad \text{for } v<0 \tag{3.50}$$

provided that $R\alpha>0$. The temporary restriction to $R\alpha^2>0$ was an artificial consequence of the device of splitting the region $y>0$ along the line $v=0$, and the necessity of this restriction disappeared with the factors $D'_n(\pm 2q_n)$.

The solutions for $g(v) = \exp(\mp\alpha v)$, with $\tau=\alpha^2$, can be generalised. We define, for $n = 0, 1, 2, \ldots$

$$f_n^{\pm}(v; \tau) = (n!)^{-1/2}\exp(\tfrac{1}{4}v^2)D_n(2q_n(\tau)\mp v). \tag{3.51}$$

Thus if $R\alpha>0$

$$\exp(\mp\alpha v) = \exp(\alpha^2)f_0^{\mp}(v; \alpha^2).$$

If we take $\tau=\alpha^2$ and

$$g(v) = f_m^{\mp}(v; \alpha^2) \tag{3.52}$$

we obtain, in place of (3.40) and (3.41),

$$L_1(s) = \frac{\{D_m(2q_m)D'_\nu(-2\mathrm{i}s) \mp D'_m(2q_m)D_\nu(-2\mathrm{i}s)\}\gamma_+(s; \alpha^2)}{(2\pi)^{1/4}(m!)^{1/2}(\mathrm{i}s\pm q_m)}, \tag{3.53}$$

$$L_2(s) = \frac{\mp(2\pi)^{1/4}D'_m(2q_m)}{(m!)^{1/2}(\mathrm{i}s\pm q_m)D'_\nu(2\mathrm{i}s)\gamma_+(-s; \alpha^2)}. \tag{3.54}$$

When we take the upper signs in (3.52)-(3.54), assuming temporarily that $R\alpha^2>0$, we have $L_+(s) = L_1(s)$, $L_-(s) = L_2(s)$, and hence

$$\phi(y, v; \alpha^2) = f_m^-(v; \alpha^2)\exp(-q_m y). \tag{3.55}$$

With the lower signs we must take

$$L_-(s) = L_2(s) - \frac{(2\pi)^{1/4}}{(m!)^{1/2}(\mathrm{i}s-q_m)\gamma_+(\mathrm{i}q_m; \alpha^2)}, \tag{3.56}$$

from which we obtain

$$\phi(y, v; \alpha^2) = \sum_{n=0}^{\infty} \frac{f_n^-(v; \alpha^2) \exp(-q_n y)}{2q_n(q_n + q_m) Q_m(\alpha^2) Q_n(\alpha^2)}, \tag{3.57}$$

where we define, for each $n = 0, 1, 2, \ldots$ and τ in the cut plane,

$$Q_n(\tau) = (n!)^{1/2} \gamma_+(\mathrm{i}q_n(\tau); \tau). \tag{3.58}$$

As in the cases $g(v) = \exp(\mp \alpha v)$, the solutions (3.55) and (3.57) are valid for all v with $y \geqslant 0$, provided only that $R\alpha > 0$. In particular, we can replace α^2 by τ to obtain the expansion

$$f_m^+(v; \tau) = \sum_{n=0}^{\infty} \frac{f_n^-(v; \tau)}{2q_n(q_n + q_m) Q_m(\tau) Q_n(\tau)} \qquad \text{for } v < 0. \tag{3.59}$$

For the general case, with an arbitrary function $g(v; \tau)$ defined in $v < 0$, we have

$$L(s; \tau) = -\int_0^{\infty} g(-w; \tau) w \exp(-\tfrac{1}{4}w^2) D_\nu(2\mathrm{i}s + w)\, \mathrm{d}w \frac{D'_\nu(-2\mathrm{i}s)\gamma_+(s; \tau)}{(2\pi)^{1/4} D'_\nu(2\mathrm{i}s)}. \tag{3.60}$$

Because we are assuming that $g(v; \tau) = O(\exp(A|v|))$, the integral in (3.60) is a regular function of s. As shown in appendix 2, we can evaluate $L_+(s; \tau)$ in terms of the residues of $L(s; \tau)$ at the poles $s = -\mathrm{i}q_n(\tau)$. This gives

$$L_+(s; \tau) = \sum_{m=0}^{\infty} \frac{(g, f_m^+)}{2(2\pi)^{1/4} q_m Q_m (q_m - \mathrm{i}s)}, \tag{3.61}$$

where q_m, Q_m have argument τ, and the inner product is defined by

$$(F, G) = \int_{-\infty}^{0} F(v) G(v)(-v) \exp(-\tfrac{1}{2}v^2)\, \mathrm{d}v. \tag{3.62}$$

Then $L_-(s; \tau) = L(s; \tau) - L_+(s; \tau)$, and the series (3.35) gives

$$\phi(y, v; \tau) = \sum_{n=0}^{\infty} \left((g, f_n^-) - \sum_{m=0}^{\infty} \frac{(g, f_m^+)}{2q_m(q_m + q_n) Q_m Q_n} \right) \frac{f_n^-(v) \exp(-q_n y)}{(8\pi)^{1/2} q_n}. \tag{3.63}$$

As with (3.48) and (3.57), this result, although derived initially for $v > 0$ and $R\tau > 0$, extends to all values of v and all τ in the cut plane. Corresponding to (3.50) we have the general expansion

$$g(v; \tau) = \sum_{n=0}^{\infty} \frac{(g, F_n^-)}{(8\pi)^{1/2} q_n} f_n^-(v) \qquad \text{for } v < 0, \tag{3.64}$$

where

$$F_n^-(v) = f_n^-(v) - \sum_{m=0}^{\infty} \frac{f_m^+(v)}{2q_m(q_m + q_n) Q_m Q_n}. \tag{3.65}$$

The expansion coefficients can also be expressed in terms of the pseudo product

$$[F, G] = \int_{-\infty}^{\infty} F(v) G(v) v \exp(-\tfrac{1}{2}v^2)\, \mathrm{d}v, \tag{3.66}$$

since the relation (3.59) shows that $F_n^-(v) = 0$ if $v > 0$. Thus

$$g(v; \tau) = \sum_{n=0}^{\infty} -\frac{[g, F_n^-]}{(8\pi)^{1/2} q_n} f_n^-(v) \qquad \text{for } v < 0, \tag{3.67}$$

independently of the form of $g(v;\tau)$ when $v>0$, and

$$\phi(y,v;\tau)=\sum_{n=0}^{\infty}-\frac{[g,F_n^-]}{(8\pi)^{1/2}q_n}f_n^-(v)\exp(-q_n y). \tag{3.68}$$

For the case

$$g(v;\tau)=\exp(-\alpha v) \qquad \alpha>0, \tag{3.69}$$

we have (see appendix 1)

$$[g,f_n^{\pm}]=\pm\left[\frac{2\pi}{n!}\right]^{1/2}(\tau-\alpha^2)(q_n\pm\alpha)^{n-1}\exp(\mp\alpha q_n-\tfrac{1}{2}q_n^2+\tfrac{1}{2}\alpha^2), \tag{3.70}$$

so that from (3.68) and (3.1)

$$\begin{aligned}\bar\Phi(y,v;p)=\tfrac{1}{2}p\sum_{n=0}^{\infty}&\left(a_n(p)+\sum_{m=0}^{\infty}\frac{b_m(p)}{2q_m(q_m+q_n)Q_mQ_n}\right)\\&\times\frac{\exp(\alpha v)f_n^-(v)\exp[-(q_n-\alpha)y]}{q_n},\end{aligned} \tag{3.71}$$

where

$$\left.\begin{aligned}a_n(p)&=(n!)^{-1/2}(q_n-\alpha)^{n-1}\exp[\alpha q_n-\tfrac{1}{2}(n+p)],\\ b_n(p)&=(n!)^{-1/2}(q_n+\alpha)^{n-1}\exp[-\alpha q_n-\tfrac{1}{2}(n+p)],\end{aligned}\right\} \tag{3.72}$$

$$q_n\equiv q_n(p+\alpha^2)=(n+p+\alpha^2)^{1/2}, \qquad Q_n\equiv Q_n(p+\alpha^2), \tag{3.73}$$

and the p plane is cut along the negative real axis from $-\infty$ to $-\alpha^2$.

4. Numerical solution

The Laplace inversion of (3.71) to give $\Phi(y,v;t)$ appears to be out of the question. We can, however, obtain valuable information about the first-passage times from the behaviour of (3.71) near $p=0$ and near $p=-\alpha^2$.

For example, from (3.72) we deduce that, as $p\to 0+$, the coefficients $a_n(p)$ and $b_n(p)$ all remain finite except that

$$a_0(p)=\frac{\exp(\alpha^2)}{p}\left\{2\alpha+\frac{p}{2\alpha}+O(p^2)\right\}. \tag{4.1}$$

It follows that

$$\int_0^{\infty}\Phi(y,v;t)\,dt=\bar\Phi(y,v;0+)=1, \tag{4.2}$$

which means that the total probability of absorption is 1, so the process is recurrent.

Similarly, the mean first-passage time is obtained from the first derivative of ϕ at $p=0$, that is

$$\bar t=\Psi(y,v)=-\bar\Phi_p(y,v;0+). \tag{4.3}$$

Using (4.1) again, we obtain

$$\Psi(y,v)=\frac{y+v}{2\alpha}+1+\frac{1}{4\alpha^2}-\frac{\exp(-\alpha^2)}{4\alpha Q_0}\sum_{m=0}^{\infty}\frac{b_m(0)}{q_m(q_m+\alpha)Q_m}$$
$$-\tfrac{1}{2}\sum_{n=1}^{\infty}\left(a_n(0)+\frac{1}{2Q_n}\sum_{m=0}^{\infty}\frac{b_m(0)}{q_m(q_m+q_n)Q_m}\right)$$
$$\times\frac{\exp(\alpha v)f_n^-(v)\exp[(\alpha-q_n)y]}{q_n}, \tag{4.4}$$

where q_m and Q_m now take their values at $p=0$, that is

$$q_m=(m+\alpha^2)^{1/2}, \qquad Q_m=(m!)^{1/2}\gamma_+(\mathrm{i}q_m;\,\alpha^2). \tag{4.5}$$

We may also obtain the leading term in the asymptotic expansion of $\Phi(y,v;t)$ as $t\to+\infty$, by examining the behaviour of $\bar{\Phi}(y,v;p)$ near its first branch-point at $p=-\alpha^2$. We find that

$$\bar{\Phi}(y,v;p)=\bar{\Phi}(y,v;-\alpha^2)-(p+\alpha^2)^{1/2}F(y,v;\alpha)+\mathrm{O}(p+\alpha^2) \tag{4.6}$$

so that, asymptotically

$$\Phi(y,v,t)\sim\frac{1}{2(\pi t^3)^{1/2}}F(y,v;\alpha)\exp(-\alpha^2 t). \tag{4.7}$$

The function $F(y,v)$ was obtained from the second term in the Taylor series of (3.71) expanded in powers of q_0. We find that

$$F(y,v;\alpha)=\exp[\alpha(y+v)]H(\alpha)G(y,v), \tag{4.8}$$

where

$$H(\alpha)=\exp(\alpha^2/2)\left\{1-\alpha\zeta(\tfrac{1}{2})+\alpha^2-\tfrac{1}{2}\alpha^2\sum_{m=1}^{\infty}\frac{(\sqrt{m}+\alpha)^{m-1}\exp(-\alpha\sqrt{m}-m/2)}{m!\sqrt{m}\gamma_+(\mathrm{i}\sqrt{m};1)}\right\}, \tag{4.9}$$

and

$$G(y,v)=y+v-\zeta(\tfrac{1}{2})-\frac{1}{2}\sum_{n=1}^{\infty}\frac{\exp(-y\sqrt{n}+v^2/4)D_n(2\sqrt{n}+v)}{n!\sqrt{n}\gamma_+(\mathrm{i}\sqrt{n};1)}. \tag{4.10}$$

The task of obtaining numerical values from (4.4) falls naturally into three parts: (a) the computation of the coefficients appearing in the sum; (b) the summations over m; (c) the summation over n. We describe these in turn. The computation of (4.8) is somewhat easier, owing to the factorisation, but broadly similar.

4.1. *The computation of the coefficients*

Since a_n and b_m are given explicitly by (3.72), the only problem is in the computation of Q_n. One of three different routines was used, depending on the value taken by q_n. For $q_n>3.2$, the asymptotic expansion (A2.31)

$$\log Q_n\sim\tfrac{1}{2}\log(2\pi)-\sum_{r=0}^{\infty}\frac{\zeta(-r-\tfrac{1}{2},\alpha^2)}{(2r+1)q_n^{2r+1}}, \tag{4.11}$$

was used. The other two routines both made repeated use of the relation (A2.25)

$$\gamma_+(\mathrm{i}q_n;\,q_{m+1}^2)=(q_n+q_m)\gamma_+(\mathrm{i}q_n;\,q_m^2). \tag{4.12}$$

Within the range $1.6 < q_n \leqslant 3.2$, the above relation was used to express Q_n in terms of $\gamma_+(\mathrm{i}q_n; q_n^2)$, which was computed with the aid of the asymptotic expansion (A2.39). Finally, for $q_n \leqslant 1.6$, Q_n was expressed in terms of $\gamma_+(\mathrm{i}q_n; q_{25+n}^2)$, which was computed from the Taylor expansion (A2.37) with N put equal to 25.

These routines, over the whole range of q_n, give values of Q_n correct to seven decimal places.

4.2. *The m-summations*

We define

$$g_n = a_n + \frac{1}{2Q_n} \sum_{m=0}^{\infty} \frac{b_m}{q_m(q_m+q_n)Q_m}. \tag{4.13}$$

For large m, Q_m is represented by the asymptotic expansion (4.11). The corresponding expansion for b_m is

$$\log b_m \sim -\tfrac{1}{4}\log(2\pi) - \tfrac{3}{2}\log q_m - \sum_{r=1}^{\infty} \frac{\alpha^{2r-1}}{(2r-1)q_m^{2r-1}}\left(1+\frac{2\alpha^2}{2r+1}\right)$$
$$+ \sum_{r=1}^{\infty} \frac{\alpha^{2r}}{2rq_m^{2r}}\left(1+\frac{\alpha^2}{r+1}+(-1)^{r-1}\zeta(-r;\alpha^2)\right). \tag{4.14}$$

It will be evident that the summand in (4.13) is asymptotically a multiple of $m^{-7/4}$, so that the sum converges rather slowly. Our summation routine summed the terms explicitly for $0 \leqslant m \leqslant 50$ and replaced the 'tail' of the series by an Euler-Maclaurin expansion, whose first term, the integral of the summand with respect to m, is

$$4(2\pi)^{-3/4}q_n^{-3/2}(\beta - \tan^{-1}\beta) \qquad \text{with} \qquad \beta = q_n^{1/2}(50+\alpha^2)^{-1/4}. \tag{4.15}$$

4.3. *The n-summation*

Here the nature of the convergence varies greatly with the values of y and v. For y well separated from zero, the series is rapidly convergent on account of the factor $\exp[(\alpha - q_n)y]$ in the summand. It therefore suffices to take a small number of terms, and the appropriate functions $f_n^-(v)$ are computed with the aid of the recurrence relations for the Hermite polynomials. For $y=0$, the series is very slowly convergent, as may be seen (see (A1.30)) from the fact that, for large n

$$f_n^-(v) \sim n^{-1/24}\,\mathrm{Ai}(n^{1/6}v). \tag{4.16}$$

Consequently another Euler-Maclaurin routine had to be devised for values of y close to zero with v negative, and for $y=0$ with v positive. For such a routine it was necessary to know the asymptotics, for large n, of the coefficients g_n. These were obtained (see appendix 3) as

$$g_n \sim \tfrac{1}{2}a_n + \frac{1}{2Q_n}\sum_{r=0}^{\infty}\frac{(-1)^r S_r}{q_n^{r+1}}, \tag{4.17}$$

where

$$S_r = \sum_{m=0}^{\infty}\left(d_m q_m^r - \sum_{s=1}^{r} D_{r-s} q_m^{s-5/2}\right) + \sum_{s=1}^{r} D_{r-s}\zeta(\tfrac{5}{4}-\tfrac{1}{2}s;\alpha^2) \tag{4.18}$$

$$d_m = \frac{b_m}{q_m Q_m} \sim \sum_{s=0}^{\infty} \frac{D_s}{q_m^{s+5/2}}. \qquad (4.19)$$

Thus the leading term in the summand behaves, for large n, like $n^{-25/24}\mathrm{Ai}(n^{1/6}v)$.

By increasing the number of terms taken in the various asymptotic and power series expansions, we may increase without limit the accuracy of $\Psi(y, v)$ and $F(y, v)$. We were able to submit our computing procedures to a particularly stringent test by computing the values of $\Psi(y, v)$ for negative v and small y. It is obvious from the form of (2.6)-(2.8) and also from elementary dynamics, that

$$\Psi(y, v) \sim -y/v, \qquad \text{as} \qquad y \to 0+ (v<0). \qquad (4.20)$$

This result is, however, not at all obvious from the form of (4.4), and indeed this is the region of phase space for which the n-summation has the slowest convergence. Nevertheless, for moderate values of v we were able to verify numerically that (4.20) is satisfied.

In figures 1 and 2 we have plotted the mean first-passage and recurrence times $\Psi(y, 0)$ and $\Psi(0, v)$. We have found it convenient to change the independent variables to $y/2\alpha$ and $v/2\alpha$, because this enables us to display (as a bold curve) the deterministic limit, for which

$$t_D = y/2\alpha + (1 + v/2a)[1 - \exp(-t_D)] \qquad \alpha \to +\infty. \qquad (4.21)$$

It is also convenient to plot, as dependent variable, the function $\Psi(y, v) - \Psi_{\mathrm{diff}}(y, v)$ where $\Psi_{\mathrm{diff}}(y, v)$ is obtained by solving the equation for $\bar{\Phi}$ in the diffusion limit, that is

$$\mathrm{d}^2\bar{\Phi}/\mathrm{d}y^2 - 2\alpha\, \mathrm{d}\bar{\Phi}/\mathrm{d}y - p\bar{\Phi} = 0, \qquad \bar{\Phi}(0+; p) = 1, \qquad (4.22)$$

giving

$$\bar{\Phi}(y; p) = \exp[(\alpha^2 + p)y], \qquad (4.23)$$

and hence

$$\bar{\Psi}_{\mathrm{diff}}(y, v) = y/2\alpha. \qquad (4.24)$$

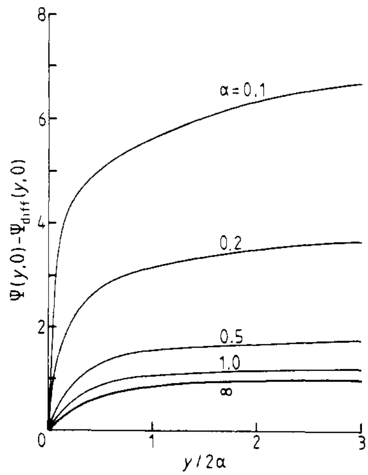

Figure 1. Mean first-passage time for a particle, released with zero velocity at distance y from an absorbing barrier in a uniform force field α, given as a divergence from the prediction $\Psi_{\mathrm{diff}}(y, 0) = y/2\alpha$ of the diffusion model.

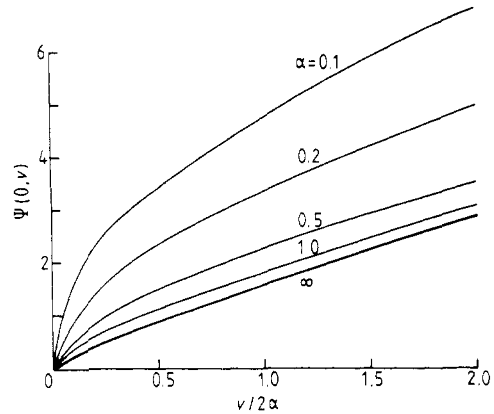

Figure 2. Mean recurrence time for a particle, released with velocity v in a uniform force field α.

It will be noted from figures 1 and 2 that, as $\alpha \to \infty$, the recurrence and first-passage times both approach their deterministic limiting values. It may seem rather surprising, however, that this limit is approached from above rather than from below, since intuitively, the diffusion limit and the deterministic limit represent two extreme cases. Such an intuition proves unreliable here. This is because the case $\alpha \to 0$ does not correspond very well to the diffusion limit. Indeed, as $\alpha \to 0$, one obtains the limiting behaviour

$$\Psi(y, v) = G(y, v)/2\alpha + \mathrm{O}(1),$$

where $G(y, v)$ is as defined in (4.10) above.

Because of the factorisation of (4.8), the asymptotic first-passage and recurrence times may be represented in tabular form. In table 1 we give the functions $G(y, 0)$ and $G(0, v)$, while in table 2 we give the function $H(\alpha)$.

We observe that, from (4.10), the asymptotic form of $G(y, v)$, for large positive y or v, is

$$G(y, v) \sim y + v + 1.4603\ldots \qquad (y, v \to +\infty). \tag{4.25}$$

We may compare the result for $G(y, 0)$ with the diffusion limit by looking at the right-hand side of (4.23) in the neighbourhood of $p = -\alpha^2$, obtaining

$$\Phi_{\text{diff}}(y, v; t) \sim \frac{1}{2(\pi t^3)^{1/2}} y \exp(\alpha y - \alpha^2 t), \tag{4.26}$$

which is equivalent to

$$F_{\text{diff}}(y, v; \alpha) = y \exp(\alpha y). \tag{4.27}$$

It will be seen that our exact result bears little resemblance to this:

$$F(y, 0; \alpha) = H(\alpha) \exp(\alpha y) G(y, 0), \tag{4.28}$$

and in particular, for large y (4.27) and (4.28) differ by a factor of $H(\alpha)$. It would therefore seem that the greatest divergence between the diffusion model and our more exact model is in their predicted values of asymptotic first-passage times.

Table 1. The function $G(y, v)$ for $v=0$ and $y=0$.

y, v	$G(y, 0)$	$G(0, v)$
0.1	1.1341	0.6948
0.2	1.3485	0.9803
0.3	1.5152	1.2031
0.4	1.6609	1.3931
0.5	1.7947	1.5627
0.6	1.9208	1.7184
0.7	2.0416	1.8639
0.8	2.1585	2.0018
0.9	2.2724	2.1337
1.0	2.3840	2.2609
1.1	2.4938	2.3841
1.2	2.6022	2.5042
1.3	2.7093	2.6216
1.4	2.8154	2.7368
1.5	2.9208	2.8501
1.6	3.0254	2.9618
1.7	3.1294	3.0721
1.8	3.2329	3.1812
1.9	3.3360	3.2893
2.0	3.4387	3.3964

Table 2. The function $H(\alpha)$.

α	$H(\alpha)$
0	1.0000
0.1	1.1601
0.2	1.3524
0.3	1.5845
0.4	1.8658
0.5	2.2085
0.6	2.6282
0.7	3.1448
0.8	3.7843
0.9	4.5804
1.0	5.5774

We make two final remarks which establish points of contact between our work and investigations of the stationary problem.

Firstly the exact solution of the 'Milne problem' of Selinger and Titulaer (7) is related to our function $G(y, v)$. The Milne problem is to find the stationary solution of (2.1) for the case $\alpha=0$ such that

$$W(x, u) \sim (2\pi)^{-1/2}(x-u+x_{\mathrm{M}}) \exp(-\tfrac{1}{2}u^2) \qquad \text{as } x \to +\infty, \tag{4.29}$$

$$W(x, u) \to 0 \qquad \text{for } u \to \pm\infty \tag{4.30}$$

$$W(0+, u) = 0 \qquad \text{for } u > 0. \tag{4.31}$$

The solution is

$$W(x, u) = (2\pi)^{-1/2} \exp(-\tfrac{1}{2}u^2) G(x, -u), \tag{4.32}$$

as can be shown with the aid of the expansion (4.4) and the explicit formula (4.10). It follows that the 'Milne length' $x_M = -\zeta(\frac{1}{2}) \simeq 1.460\,35$, in good agreement with the estimates of Selinger and Titulaer [7] and Titulaer [8].

Secondly we stress that there is no real difference in difficulty between solving (2.1) and (2.6). We have chosen to present here the solution for Φ rather than W because of the greater simplicity of notation gained by integrating over u. It should be noted that the albedo problem, as defined by Selinger and Titulaer, is solved by integrating W with respect to t. More precisely, the probability that a particle, released from $x = 0$ with velocity v, will be absorbed at $x = 0$ with velocity between u and $u + du$ is

$$w(u; v)\, du = -u \int_0^\infty W(0+, u; 0, v; t)\, dt\, du = -u\bar{W}(0+, u; 0, v; 0)\, du \tag{4.33}$$

Further details on both of these matters will be given in a later paper.

Acknowledgment

We acknowledge with pleasure the assistance of Professor U M Titulaer, who showed us how our results are related to other recent studies of the Kramers equation.

Appendix 1. Parabolic cylinder functions

The function $D_\nu(z)$ is the solution of Weber's equation

$$d^2w/dz^2 + (\nu + \tfrac{1}{2} - \tfrac{1}{4}z^2)w = 0 \tag{A1.1}$$

such that

$$D_\nu(z) \sim \exp(-\tfrac{1}{4}z^2) z^\nu \left(1 - \frac{\nu(\nu-1)}{2z^2} + \frac{\nu(\nu-1)(\nu-2)(\nu-3)}{2.4z^4} - \dots\right) \tag{A1.2}$$

as $z \to +\infty$. $D_\nu(z)$ is a regular function of both z and ν for all finite values of the variables. It can be expressed in terms of the confluent hypergeometric function as

$$D_\nu(z) = 2^{\nu/2} \exp(-\tfrac{1}{4}z^2) \left(\frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2} - \frac{1}{2}\nu)}\, {}_1F_1(-\tfrac{1}{2}\nu; \tfrac{1}{2}; \tfrac{1}{2}z^2) + \frac{\Gamma(-\frac{1}{2})z}{\Gamma(-\frac{1}{2}\nu)\sqrt{2}}\, {}_1F_1(\tfrac{1}{2} - \tfrac{1}{2}\nu; \tfrac{3}{2}; \tfrac{1}{2}z^2) \right), \tag{A1.3}$$

and the asymptotic expansion (A1.2) is valid as $|z| \to \infty$ in $|\arg z| < \frac{3}{4}\pi - \delta$.

Weber's equation is also satisfied by the functions $D_\nu(-z)$ and $D_{-\nu-1}(\pm iz)$. The Wronskian relation

$$D_\nu(z) D'_\nu(-z) + D'_\nu(z) D_\nu(-z) = -(2\pi)^{1/2}/\Gamma(-\nu) \tag{A1.4}$$

shows that $D_\nu(\pm z)$ are independent solutions of (A1.1) unless $\nu = 0, 1, 2, \dots$. Any three solutions of (A1.1) are connected by a linear relation, and

$$D_\nu(z) = \exp(\nu\pi i) D_\nu(-z) + \frac{(2\pi)^{1/2}}{\Gamma(-\nu)} \exp[(\nu+1)\pi i/2] D_{-\nu-1}(-iz), \tag{A1.5}$$

so that if $n = 0, 1, 2, \ldots$

$$D_n(-z) = (-1)^n D_n(z). \tag{A1.6}$$

In the case $\nu = n = 0, 1, 2, \ldots$ the expansion (A1.2) terminates and is identical with (A1.3). Using Kummer's first theorem we can express (A1.3) in this case as

$$D_n(z) = (-1)^n \exp(\tfrac{1}{4}z^2)(\mathrm{d}^n/\mathrm{d}z^n)\exp(-\tfrac{1}{2}z^2), \tag{A1.7}$$

from which we can establish the orthogonality relation

$$\int_{-\infty}^{\infty} D_m(z) D_n(z)\, \mathrm{d}z = (2\pi)^{1/2} n!\, \delta_{mn}, \tag{A1.8}$$

where m and n take the values $0, 1, 2, \ldots$.

We can also use (A1.7) to prove the result (3.70). With $q = q_n(\tau)$, we have

$$\begin{aligned}(n!)^{1/2}[\exp(-\alpha v), f_n^-] &= \int_{-\infty}^{\infty} v \exp(-\alpha v - \tfrac{1}{4}v^2) D_n(2q + v)\, \mathrm{d}v \\ &= \int_{-\infty}^{\infty} v \exp[-\alpha v - \tfrac{1}{4}v^2 + \tfrac{1}{4}(2q+v)^2](-\mathrm{d}/\mathrm{d}v)^n \exp[-\tfrac{1}{2}(2q+v)^2]\, \mathrm{d}v.\end{aligned}$$

Integration by parts n times now gives

$$\begin{aligned}&\int_{-\infty}^{\infty} \exp[-\tfrac{1}{2}(2q+v)^2](\mathrm{d}/\mathrm{d}v)^n\{v \exp[(q-\alpha)v + q^2]\}\, \mathrm{d}v \\ &\quad = \int_{-\infty}^{\infty} [(q-\alpha)^n v + n(q-\alpha)^{n-1}] \exp[-\tfrac{1}{2}v^2 - (q+\alpha)v - q^2]\, \mathrm{d}v \\ &\quad = (q-\alpha)^{n-1} \int_{-\infty}^{\infty} [(q-\alpha)(v+q+\alpha) - q^2 + \alpha^2 + n] \\ &\qquad \times \exp[-\tfrac{1}{2}(v+q+\alpha)^2 + \tfrac{1}{2}(q+\alpha)^2 - q^2]\, \mathrm{d}v \\ &\quad = (2\pi)^{1/2}(q-\alpha)^{n-1}(n - q^2 + \alpha^2)\exp(-\tfrac{1}{2}q^2 + \alpha q + \tfrac{1}{2}\alpha^2).\end{aligned} \tag{A1.9}$$

This is equivalent to the result stated in (3.70). The case $[\mathrm{e}^{-\alpha v}, f_n^+]$ is evaluated by the substitution $v = -u$ and a change of sign of α.

The function

$$\phi(x; q, \tau) = D_{q^2-\tau}(x - 2q) \tag{A1.10}$$

satisfies the equation

$$\phi''(x) + (\tfrac{1}{2} - \tau - \tfrac{1}{4}x^2 + qx)\phi(x) = 0, \tag{A1.11}$$

with the condition $\phi(x) \to 0$ as $x \to +\infty$. The further condition $\phi'(0) = 0$ determines an infinite set of eigenvalues

$$q = d_n(\tau) \tag{A1.12}$$

which are the zeros of the function $D'_{q^2-\tau}(-2q)$. The eigenfunction that corresponds to (A1.12) is

$$\phi_n(x; \tau) = \phi(x; d_n(\tau), \tau). \tag{A1.13}$$

These eigenfunctions satisfy the orthogonality relation

$$\int_0^\infty x\phi_m(x)\phi_n(x)\,\mathrm{d}x = 0 \qquad \text{if } d_m \neq d_n, \tag{A1.14}$$

and it follows that if τ is real, so also are the eigenvalues $d_n(\tau)$.

If q is any function of τ, it follows from (A1.11) that

$$\int_0^\infty \left(1 - \frac{\mathrm{d}q}{\mathrm{d}\tau}x\right)\phi^2(x)\,\mathrm{d}x = -\phi(0)\frac{\mathrm{d}\phi'(0)}{\mathrm{d}\tau}, \tag{A1.15}$$

so that, taking $q = d_n(\tau)$, we see that

$$(\mathrm{d}/\mathrm{d}\tau)\{d_n(\tau)\} > 0 \tag{A1.16}$$

if τ is real. The eigenvalues must be distinct if τ is real, and they can be labelled by the condition $d_n(-2n) = 0$. Since the functions $d_n(\tau)$ are analytic, this labelling can be extended to complex τ; singularities can occur only where eigenvalues coalesce.

If q_a and q_b are any two eigenvalues belonging respectively to τ_a and τ_b, and $\phi_i(x) = \phi(x; q_i, \tau_i)$ for $i = a$ and $i = b$, then

$$\int_0^\infty \{2(\phi_a' + \tfrac{1}{2}x\phi_a)(\phi_b' + \tfrac{1}{2}x\phi_b) + [\tau_a + \tau_b - (q_a + q_b)x]\phi_a\phi_b\}\,\mathrm{d}x = 0. \tag{A1.17}$$

If τ_a and τ_b are complex conjugates, then we can suppose that so are q_a and q_b. In this case (A1.17) shows that

$$\int_0^\infty [|\phi_a' + \tfrac{1}{2}x\phi_a|^2 + (R\tau_a - Rq_a x)|\phi_a|^2]\,\mathrm{d}x = 0, \tag{A1.18}$$

so that if $R\tau_a \geqslant 0$ we must have $Rq_a \geqslant 0$, and further $Rq_a > 0$ unless $\phi_a \propto \exp(-\frac{1}{4}x^2)$, which is possible only when $\tau_a = q_a = 0$.

Equation (A1.1) has turning points at $z = \pm(4\nu + 2)^{1/2}$, and when q is large the corresponding values of x in (A1.11) are near 0 and $4q$. Thus the behaviour of $\phi(x; q, \tau)$ for moderate values of x and τ, but large $|q|$ depends on that of $D_\nu(z)$ near a turning point for large $|\nu|$. Approximations to the solutions of a differential equation in a region containing a turning point can be obtained by the method described by Olver [18].

We put

$$N = 2\nu + 1, \qquad z = (2N)^{1/2}t, \tag{A1.19}$$

and define

$$\eta = \left(\frac{3}{2}\int_1^t (s^2 - 1)^{1/2}\,\mathrm{d}s\right)^{2/3}. \tag{A1.20}$$

Then

$$D_\nu(z) = \left(\frac{\eta}{t^2 - 1}\right)^{1/4} U(\eta), \tag{A1.21}$$

where

$$U''(\eta) - N^2\eta U(\eta) = F(\eta)U(\eta), \tag{A1.22}$$

and

$$F(\eta)=\tfrac{5}{16}\,\eta^{-2}-\frac{3t^2+2}{4(t^2-1)^3}\,\eta. \tag{A1.23}$$

We look for an asymptotic solution of (A1.22) for large N in terms of the Airy functions in the form

$$U(\eta)=L(N)\left(\mathrm{Ai}(\zeta)\sum_{n=0}^{\infty}\alpha_n(\eta)N^{-2n}+\mathrm{Ai}'(\zeta)\sum_{n=0}^{\infty}\beta_n(\eta)N^{-2n-4/3}\right), \tag{A1.24}$$

$$U'(\eta)=L(N)\left(\mathrm{Ai}(\zeta)\sum_{n=0}^{\infty}\gamma_n(\eta)N^{-2n}+\mathrm{Ai}'(\zeta)\sum_{n=0}^{\infty}\delta_n(\eta)N^{-2n+2/3}\right), \tag{A1.25}$$

where

$$\zeta=N^{2/3}\eta \tag{A1.26}$$

and

$$\alpha_0(\eta)=\delta_0(\eta)=1. \tag{A1.27}$$

Then we find that

$$\beta_0(\eta)=-\tfrac{5}{48}\,\eta^{-2}-\frac{t^3-6t}{24(t^2-1)^{3/2}\eta^{1/2}},\qquad \gamma_0(\eta)=\eta\beta_0(\eta), \tag{A1.28}$$

and that this solution matches the asymptotic expansion (A1.2) provided that

$$L(N)=(2\pi)^{1/2}N^{1/6}(\tfrac{1}{2}N)^{(N-1)/4}\exp(-\tfrac{1}{4}N)\{1-\tfrac{1}{24}N^{-1}+\mathrm{O}(N^{-2})\}. \tag{A1.29}$$

From these results we find that, as $|q|\to\infty$ with $|\arg q|<\frac{1}{2}\pi-\delta$,

$$D_{q^2-\tau}(2q+w)=(2\pi)^{1/2}q^{q^2-\tau+1/3}\exp(-\tfrac{1}{2}q^2)[\mathrm{Ai}(q^{1/3}w)+\mathrm{O}(q^{-2/3})], \tag{A1.30}$$

$$D'_{q^2-\tau}(2q)=(2\pi)^{1/2}q^{q_2-\tau+2/3}\exp(-\tfrac{1}{2}q^2)[\mathrm{Ai}'(0)+\mathrm{O}(q^{-4/3})]. \tag{A1.31}$$

It can be shown by use of (A1.5) that (A1.30) and (A1.31) are valid throughout $|\arg q|<\pi-\delta$. Another application of (A1.5) leads to

$$\begin{aligned} D_{q^2-\tau}(-2q+w)\sim(2\pi)^{1/2}q^{q^2-\tau+1/3}\exp(-\tfrac{1}{2}q^2)\{&\exp[(q^2-\tau+\tfrac{1}{3})\pi\mathrm{i}]\mathrm{Ai}[\exp(\tfrac{1}{3}\pi\mathrm{i})q^{1/3}w]\\ &+\exp[-(q^2-\tau+\tfrac{1}{3})\pi\mathrm{i}]\mathrm{Ai}[\exp(-\tfrac{1}{3}\pi\mathrm{i})q^{1/3}w]\} \end{aligned} \tag{A1.32}$$

$$D'_{q^2-\tau}(-2q)\sim(8\pi)^{1/2}\,\mathrm{Ai}'(0)q^{q^2-\tau+2/3}\exp(-\tfrac{1}{2}q^2)\cos(q^2-\tau+\tfrac{2}{3})\pi, \tag{A1.33}$$

as $|q|\to\infty$ with $|\arg q|<\frac{1}{2}\pi-\delta$. Equation (A1.33) shows that the large zeros of $D'_{q^2-\tau}(-2q)$ are approximately of the form $q=(n+\tau-\frac{1}{6})^{1/2}$, where n is an integer.

It is possible to obtain further coefficients $\alpha_n(\eta)$ to $\delta_n(\eta)$ in (A1.24) and (A1.25), and hence to extend the asymptotic formulae (A1.30) to (A1.33), but the calculations are tedious and the results are complicated.

Appendix 2. The Wiener–Hopf decompositions

Given a function $F(s)$, regular in a strip $-a\leqslant Is\leqslant a$ and vanishing as $Rs\to\pm\infty$, we can express it in the form

$$F(s)=F_+(s)+F_-(s), \tag{A2.1}$$

where $F_+(s)$ is regular in $Is \geqslant -b$ and $F_-(s)$ is regular in $Is \leqslant b$, for any b with $0<b<a$. This can be done by defining

$$F_\pm(s) = \frac{1}{2\pi\mathrm{i}} \int_{C_\pm} \frac{F(z)}{z-s}\,\mathrm{d}z, \tag{A2.2}$$

where the paths of integration $C_\pm$ are the lines $Is = \mp c$, $b<c<a$, and Rz increases along C_+ from $-\infty$ to $+\infty$, but decreases along C_- from $+\infty$ to $-\infty$.

This method cannot be applied directly to the function $\log\Gamma(s^2+\tau)$, because it is large when $Rs \to \pm\infty$. However, we can take

$$F(s) = \frac{\mathrm{d}^3}{\mathrm{d}s^3} \log\Gamma(s^2+\tau) = 8s^3\psi''(s^2+\tau) + 12s\psi'(s^2+\tau), \tag{A2.3}$$

where

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} = -\gamma + \sum_{n=0}^{\infty}\left(\frac{1}{n+1} - \frac{1}{n+z}\right) \tag{A2.4}$$

and γ is Euler's constant. From the decomposition of $F(s)$ we can then derive a decomposition of $\log\Gamma(s^2+\tau)$ by integration. From (A2.3) and (A2.4) we have

$$F(s) = \sum_{n=0}^{\infty} \frac{-4s^3 + 12(n+\tau)s}{(n+s^2+\tau)^3}, \tag{A2.5}$$

which we can express in partial fractions to give (A2.1) with

$$F_\pm(s) = -2\sum_{n=0}^{\infty} (s \pm \mathrm{i}q_n(\tau))^{-3}, \tag{A2.6}$$

where

$$q_n(\tau) = (n+\tau)^{1/2} \tag{A2.7}$$

and the τ plane is cut along the negative real axis. The results (A2.6) can also be established from (A2.2) by completing the contours $C_\pm$ in the appropriate half planes.

When we integrate (A2.6) three times, with appropriate conditions at $s=0$, we obtain after exponentiation

$$\Gamma(s^2+\tau) = \Gamma_+(s;\tau)\Gamma_-(s;\tau), \tag{A2.8}$$

where

$$\Gamma_+(s;\tau) = [\Gamma(\tau)]^{1/2} \exp[\tfrac{1}{2}\psi(\tau)s^2] \prod_{n=0}^{\infty} \left(\frac{\exp(s/\mathrm{i}q_n + s^2/2q_n^2)}{1+s/\mathrm{i}q_n}\right) \tag{A2.9}$$

and

$$\Gamma_-(s;\tau) = \Gamma_+(-s;\tau). \tag{A2.10}$$

The functions $\Gamma_\pm(s;\tau)$ are regular and non-zero in their respective half planes, but they are not the only such functions to satisfy (A2.8). We shall need to modify them by defining

$$\gamma_\pm(s;\tau) = \Gamma_\pm(s;\tau)\{f(s;\tau)\}^{\pm 1}, \tag{A2.11}$$

where $f(s;\tau)$ is a suitable function that is regular and non-zero for all s. The choice of $f(s;\tau)$ must be made so that the subsequent decomposition (3.25) of $L(s)$ is possible and leads to functions $L_\pm(s)$ that tend to 0 in their respective half planes as $|s|\to\infty$. For this reason we must determine the asymptotic behaviour of $\Gamma_+(s;\tau)$ as $|s|\to\infty$.

The Mellin transform

$$\hat{F}_+(Z;\tau)=\int_0^\infty s^{Z-1}F_+(s;\tau)\,\mathrm{d}s \tag{A2.12}$$

can be evaluated, from either the integral (A2.2) or the series (A2.6), as

$$\hat{F}_+(Z;\tau)=-\frac{\pi\mathrm{i}}{\sin\pi Z}(Z-1)(Z-2)\exp(\tfrac{1}{2}\pi\mathrm{i}Z)\,\zeta\left(\frac{3-Z}{2},\tau\right) \tag{A2.13}$$

for $0<RZ<1$, where

$$\zeta(z,a)=\sum_{n=0}^{\infty}(n+a)^{-z} \tag{A2.14}$$

is the generalised zeta function. The inversion theorem for Mellin transforms now gives

$$F_+(s;\tau)=-\frac{1}{2}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{(Z-1)(Z-2)}{\sin\pi Z}\exp(\tfrac{1}{2}\pi\mathrm{i}Z)\zeta\left(\frac{3-Z}{2},\tau\right)s^{-Z}\,\mathrm{d}Z, \tag{A2.15}$$

where $0<c<1$ and $s>0$. Since

$$|\zeta(x+\mathrm{i}y,\tau)|\leqslant[1+\exp(y\arg\tau)]\sum_{n=0}^{\infty}|n+\tau|^{-x}\qquad\text{for } x>1, \tag{A2.16}$$

the integral (A2.15) converges absolutely for all complex s such that both $|\arg(-\mathrm{i}s)|\leqslant\pi-\delta$ and $|\arg(-\mathrm{i}s\tau^{-1/2})|\leqslant\pi-\delta$, so that analytic continuation extends (A2.15) to all such s. Integration three times now gives

$$\log\Gamma_+(s;\tau)=\frac{1}{2\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\zeta(\frac{1}{2}(3-Z),\tau)(-\mathrm{i}s)^{3-Z}}{(Z-3)\sin\pi Z}\,\mathrm{d}Z+\tfrac{1}{2}\psi(\tau)s^2+\tfrac{1}{2}\log\Gamma(\tau). \tag{A2.17}$$

The power-series expansion for $\log\Gamma_+(s;\tau)$ can be obtained by evaluating the integral in (A2.17) by means of the residues at the poles of the integrand to the left of the path of integration. This can be justified by means of (A2.16), and gives

$$\log\Gamma_+(s;\tau)=\tfrac{1}{2}\log\Gamma(\tau)+\tfrac{1}{2}\psi(\tau)s^2+\sum_{n=0}^{\infty}\frac{\zeta(\frac{1}{2}(n+3),\tau)}{n+3}(\mathrm{i}s)^{n+3}, \tag{A2.18}$$

provided that $|s|^2<|n+\tau|$ for all $n=0,1,2,\ldots$. The function $\zeta(z,\tau)$ can be continued analytically to all z except for a simple pole at $z=1$, and it can be proved that

$$|\zeta(x+\mathrm{i}y,\tau)|<A(x,\tau,\delta)[1+\exp(y\arg\tau)]|y|^{1/2-x}\exp(\delta|y|) \tag{A2.19}$$

for any $\delta>0$ and sufficiently great $|y|$. Using this result, we can move the path of integration in (A2.17) to the right and show that as $|s|\to\infty$

$$\log\Gamma_+(s;\tau)\sim[\log(-\mathrm{i}s)-\tfrac{1}{2}]s^2-\mathrm{i}\zeta(\tfrac{1}{2},\tau)s+(\tau-\tfrac{1}{2})\log(-\mathrm{i}s)+\tfrac{1}{4}\log(2\pi)$$
$$+\sum_{n=0}^{\infty}\frac{\zeta(-\frac{1}{2}(n+1),\tau)}{n+1}(\mathrm{i}s)^{-n-1}. \tag{A2.20}$$

Although the argument requires both $|\arg(-\mathrm{i}s)|<\pi-\delta$ and $|\arg(-\mathrm{i}s\tau^{-1/2})|<\pi-\delta$, we can drop the second condition by using the relation $\Gamma_+(s;\tau)\Gamma_+(-s;\tau)=\Gamma(s^2+\tau)$. This relation, combined with $\Gamma(s^2+\tau)\Gamma(1-s^2-\tau)=\pi\operatorname{cosec}(s^2+\tau)\pi$, enables the behaviour of $\Gamma_+(s;\tau)$ to be determined near the negative imaginary axis and the poles $s=-\mathrm{i}q_n(\tau)$.

The function $f(s;\tau)$ in (A2.11) must be chosen so that

$$K_+(s) = -\frac{(2\pi)^{1/4}}{\Gamma_+(s;\tau)f(s;\tau)D'_{-s^2-\tau}(-2\mathrm{i}s)} \tag{A2.21}$$

shall behave asymptotically like a power of s. From (A1.31) and (A2.20)

$$\Gamma_+(s;\tau)D'_{-s^2-\tau}(-2\mathrm{i}s) \sim -\frac{(2\pi)^{3/4}}{3^{1/3}\Gamma(\frac{1}{3})}(-\mathrm{i}s)^{1/6}\exp[-\mathrm{i}\zeta(\tfrac{1}{2},\tau)s], \tag{A2.22}$$

so that we choose

$$\gamma_+(s;\tau) = \Gamma_+(s;\tau)\exp[\mathrm{i}\zeta(\tfrac{1}{2},\tau)s], \tag{A2.23}$$

and then

$$K_+(s) \sim \frac{3^{1/3}\Gamma(\frac{1}{3})}{(2\pi)^{1/2}}(-\mathrm{i}s)^{-1/6}, \tag{A2.24}$$

as $|s|\to\infty$ with $|\arg(-\mathrm{i}s)|<\pi-\delta$.

Using the product form for $\gamma_+(s;\tau)$, derived from (A2.9) and (A2.23), we can show that

$$\gamma_+(s;\tau+1) = (\tau^{1/2}-\mathrm{i}s)\gamma_+(s;\tau), \tag{A2.25}$$

$$(2s\,\partial/\partial\tau - \partial/\partial s)\log\gamma_+(s;\tau) = -\mathrm{i}\zeta(\tfrac{1}{2},\tau), \tag{A2.26}$$

$$2^{s^2+\tau-1/2}\gamma_+(s;\tau)\gamma_+(s;\tau+\tfrac{1}{2}) = \pi^{1/4}\gamma_+(2^{1/2}s;2\tau). \tag{A2.27}$$

In order to evaluate the series (3.71) we need to compute numerical values of

$$Q_n(\tau) = (n!)^{1/2}\gamma_+(\mathrm{i}q_n(\tau);\tau). \tag{A2.28}$$

When n is large, this can be done from the asymptotic expansion (A2.20), where the term $-\mathrm{i}\zeta(\frac{1}{2},\tau)s$ is omitted when Γ_+ is replaced by γ_+. If we write

$$q = q_n(\tau), \qquad n = q^2-\tau, \tag{A2.29}$$

we have

$$\log(n!) \sim [\log(q^2)-1]q^2 + (\tfrac{1}{2}-\tau)\log(q^2) + \tfrac{1}{2}\log(2\pi) - \sum_{m=0}^{\infty}\frac{\zeta(-m-1,\tau)}{(m+2)q^{2m+2}}, \tag{A2.30}$$

so that as $n\to\infty$

$$\log Q_n(\tau) \sim \tfrac{1}{2}\log(2\pi) - \sum_{k=0}^{\infty}\frac{\zeta(-k-\frac{1}{2},\tau)}{(2k+1)q^{2k+1}}. \tag{A2.31}$$

If n is not large, it is convenient to apply the formula (A2.25) repeatedly to give

$$\gamma_+(\mathrm{i}q;\tau) = \gamma_+(\mathrm{i}q;\tau+N)\left(\prod_{m=0}^{N-1}[q+(\tau+m)^{1/2}]\right)^{-1} \tag{A2.32}$$

for a suitably large value of N. We now define

$$P(q,a) = \log\gamma_+(\mathrm{i}q;q^2+a), \tag{A2.33}$$

so that from (A2.26)

$$\partial P(q, a)/\partial q = -\zeta(\tfrac{1}{2}, q^2 + a), \tag{A2.34}$$

and hence

$$\partial^2 P(q, a)/\partial q^2 = q\zeta(\tfrac{3}{2}, q^2 + a). \tag{A2.35}$$

Provided $a > 0$, and $|q|^2 < a$, we can express (A2.35) as

$$\begin{aligned}\frac{\partial^2 P}{\partial q^2} &= q \sum_{m=0}^{\infty} (m+a)^{-3/2} \sum_{k=0}^{\infty} \frac{(\frac{3}{2})_k}{k!}\left(-\frac{q^2}{m+a}\right)^k \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k(\frac{3}{2})_k}{k!} \zeta(k+\tfrac{3}{2}, a) q^{2k+1}.\end{aligned} \tag{A2.36}$$

It follows on integration that

$$P(q, a) = \tfrac{1}{2}\log\Gamma(a) - \sum_{m=0}^{\infty} \frac{(-1)^m(\frac{1}{2})_m \zeta(m+\frac{1}{2}, a)}{m!(2m+1)} q^{2m+1} \tag{A2.37}$$

for $|q|^2 < a$.

We can also obtain an asymptotic expansion for $P(q, a)$ as $q \to \infty$. The integral

$$I = \frac{1}{2\pi \mathrm{i}} \int_{C-\mathrm{i}\infty}^{C+\mathrm{i}\infty} \frac{\Gamma(-s)\Gamma(s+\frac{1}{2})\zeta(s+\frac{1}{2}, a) q^{2s+1}}{\Gamma(\frac{1}{2})(2s+1)} \mathrm{d}s \tag{A2.38}$$

converges absolutely for all $a > 0$, provided that $|\arg q| \leq \frac{1}{2}\pi - \delta$. The poles of the integrand belong to two classes, namely

$$(1) \quad s = m, \qquad (2) \quad s = -\tfrac{1}{2} - m,$$

where $m = 0, 1, 2, \ldots$. The pole at $s = -\frac{1}{2}$ is double, but the rest are simple. If the path of integration is chosen to separate the two classes of poles, we can evaluate I in terms of the residues at the poles of class (1), provided that $|q|^2 < a$. This gives

$$I = \sum_{m=0}^{\infty} \frac{(-1)^m(\frac{1}{2})_m \zeta(m+\frac{1}{2}, a) q^{2m+1}}{m!(2m+1)} = \tfrac{1}{2}\log\Gamma(a) - P(q, a).$$

We can also move the path of integration across the poles of class (2), and thus derive the asymptotic expansion of I as $|q| \to \infty$, namely

$$I \sim -q^2 + (\tfrac{1}{2} - a)\log(2q) + \tfrac{1}{2}\log\left(\frac{\Gamma(a)}{(2\pi)^{1/2}}\right) + \sum_{m=1}^{\infty} \frac{(-1)^{m-1}(\frac{1}{2})_m \zeta(-m, a)}{m!\,2mq^{2m}}.$$

Combining these results, we have

$$P(q, a) \sim q^2 + (a - \tfrac{1}{2})\log(2q) + \tfrac{1}{4}\log(2\pi) + \sum_{m=1}^{\infty} \frac{(-1)^{m-1}(\frac{1}{2})_m \phi_{m+1}(a)}{(m+1)!\,2mq^{2m}} \tag{A2.39}$$

as $|q| \to \infty$ with $|\arg q| \leq \frac{1}{2}\pi - \delta$. Here the Bernoulli polynomials $\phi_m(a)$ are defined by

$$\sum_{m=0}^{\infty} \phi_m(a) \frac{z^m}{m!} = \frac{z\exp(az)}{\mathrm{e}^z - 1}. \tag{A2.40}$$

In applying these results to (A2.28) with the aid of (A2.32) we have

$$a = \tau + N - q^2 = N - n. \tag{A2.41}$$

For (A2.37) a, and hence N, should be large, but in (A2.39) it is best to take $a \mp 1$, and hence $N = n+1$, since

$$P(q, 1) \sim q^2 + \tfrac{1}{4}\log(8\pi q^2) + \sum_{k=0}^{\infty} \frac{(-1)^k (\frac{1}{2})_{2k+1} B_{k+1}}{(2k+2)!(4k+2)q^{4k+2}}, \tag{A2.42}$$

where the Bernoulli numbers are given by

$$\frac{z}{1-\mathrm{e}^{-z}} = 1 + \tfrac{1}{2}z + \sum_{m=1}^{\infty} (-1)^{m-1} B_m \frac{z^{2m}}{(2m)!}. \tag{A2.43}$$

We consider the decomposition of the function $L(s; \tau)$ given by (3.60). We can use the formula (A2.2) in this case, since $L(s; \tau)$ vanishes as $|s| \to \infty$. This can be shown if we approximate to the integral in (3.60) by means of (A1.26). It follows that unless s is near the positive imaginary axis we have

$$L(s; \tau) \sim -(2\pi)^{1/2} \int_0^{\infty} g(-w; \tau) w \exp(-\tfrac{1}{4}w^2)\, \mathrm{Ai}((\mathrm{i}s)^{1/3} w))\, \mathrm{d}w\, \Lambda(s), \tag{A2.44}$$

where

$$\Lambda(s) = \begin{cases} \exp(-\frac{1}{4}\pi \mathrm{i}) s^{-1/6} & \text{if } |\arg s| \le \frac{1}{2}\pi - \delta, \\ \exp(\frac{1}{4}\pi \mathrm{i})(-s)^{-1/6} & \text{if } |\arg(-s)| \le \frac{1}{2}\pi - \delta, \\ \dfrac{\cos(s^2 + \tau - \frac{2}{3})\pi}{\sin(s^2+\tau)\pi} (\mathrm{i}s)^{-1/6} & \text{if } |\arg(\mathrm{i}s)| \le \frac{1}{2}\pi - \delta. \end{cases} \tag{A2.45}$$

The Airy function in (A2.44) is exponentially small as $|s| \to \infty$, since $|\arg(\mathrm{i}s)| \le \pi - \delta$, unless $w = 0$. Consequently the integral is given asymptotically by the behaviour of the integrand as $w \to 0$, as with Watson's lemma for Laplace transforms. (Compare Olver [18] p 337.) The integral therefore vanishes as $|s| \to \infty$, and if $g(-w; \tau)$ is analytic at $w = 0$, then $L(s, \tau) = \mathrm{O}(|s|^{-5/6})$.

Because $L(s; \tau)$ is small at infinity, we can evaluate $L_+(s; \tau)$ by deforming the contour C_+ of (A2.2) into a loop round the negative imaginary axis. By considering integrals across this loop along lines $s = -\mathrm{i}(N + \tau + \frac{1}{2} + \mathrm{i}y)^{1/2}$, where N is an integer, we can then show that

$$L_+(s; \tau) = -\sum_{m=0}^{\infty} \operatorname{Re} s\left(\frac{L(z; \tau)}{z - s}; z = -\mathrm{i}q_m(\tau)\right). \tag{A2.46}$$

It also follows from (A2.2) that since $L(s; \tau) = \mathrm{O}(|s|^{-\lambda})$ as $|s| \to \infty$ on C_+, for some λ with $0 < \lambda < 1$, then also $L_\pm(s; \tau) = \mathrm{O}(|s|^{-\lambda})$. We can now conclude that both sides of (3.26) vanish as $|s| \to \infty$. This is why we had to make $K_+(s)$ behave like a power of s at infinity, and define $\gamma_+(s; \tau)$ by (A2.23).

Appendix 3

We wish to find an asymptotic expansion, as $q \to +\infty$, for the function

$$g(q) = a(q) + \frac{1}{2Q(q)} \sum_{m=0}^{\infty} \frac{b(q_m)}{q_m Q(q_m)(q + q_m)}, \tag{A3.1}$$

where

$$q_m = (m+\alpha^2)^{1/2}, \tag{A3.2}$$

$$Q(q) = [(q^2-\alpha^2)!]^{1/2}\gamma_+(\mathrm{i}q;\alpha^2), \tag{A3.3}$$

$$a(q) = (q-\alpha)^{q^2-\alpha^2-1}\exp(\alpha q - \tfrac{1}{2}q^2 + \tfrac{1}{2}\alpha^2)[(q^2-\alpha^2)!]^{-1/2}, \tag{A3.4}$$

$$b(q) = (q+\alpha)^{q^2-\alpha^2-1}\exp(-\alpha q - \tfrac{1}{2}q^2 + \tfrac{1}{2}\alpha^2)[(q^2-\alpha^2)!]^{-1/2}. \tag{A3.5}$$

The asymptotic expansions, as $q \to +\infty$, of these latter functions are

$$Q(q) \sim (2\pi)^{1/2}\exp\left(-\sum_{r=0}^{\infty}\frac{\zeta(-r-\frac{1}{2};\alpha^2)}{(2r+1)q^{2r+1}}\right), \tag{A3.6}$$

$$a(q) \sim (2\pi)^{-1/4}q^{-3/2}\exp(\Sigma_1+\Sigma_2), \tag{A3.7}$$

$$b(q) \sim (2\pi)^{-1/4}q^{-3/2}\exp(-\Sigma_1+\Sigma_2), \tag{A3.8}$$

$$\Sigma_1 = \sum_{r=1}^{\infty}\frac{\alpha^{2r-1}}{(2r-1)q^{2r-1}}\left(1+\frac{2\alpha^2}{2r+1}\right), \tag{A3.9}$$

$$\Sigma_2 = \sum_{r=1}^{\infty}\frac{1}{2rq^{2r}}\left[\alpha^{2r}\left(1+\frac{\alpha^2}{r+1}\right)+\zeta(-r;\alpha^2)\right]. \tag{A3.10}$$

Define now

$$c(q) = a(q)Q(q)/q, \tag{A3.11}$$

$$d(q) = b(q)/qQ(q). \tag{A3.12}$$

Then from (A3.6)-(A3.8) we may obtain asymptotic expansions for these functions

$$c(q) \sim \sum_{r=0}^{\infty} C_r q^{-r-5/2}, \tag{A3.13}$$

$$d(q) \sim \sum_{r=0}^{\infty} D_r q^{-r-5/2}, \tag{A3.14}$$

and we note that

$$C_r = (-1)^r 2\pi D_r. \tag{A3.15}$$

Now the sum appearing in (A3.1) can be written

$$\begin{aligned}\Sigma\frac{d_m}{q+q_m} &= \frac{\Sigma\, d_m}{q} - \frac{\Sigma\,(d_m q_m - D_0 q_m^{-3/2})}{q^2} + \ldots + (-1)^r\frac{\Sigma\,(d_m q_m^r - \Sigma_{s=1}^r D_{r-s}q_m^{s-5/2})}{q^{r+1}} \\ &\quad - \left(\frac{D_0}{q}-\frac{D_1}{q^2}+\ldots-(-1)^r\frac{D_{r-1}}{q^r}\right)\Sigma\frac{q_m^{-3/2}}{q+q_m} + \mathrm{O}(q^{-r-3/2}).\end{aligned} \tag{A3.16}$$

Consider now the function

$$\sigma(q) = \sum_{m=0}^{\infty}\frac{q_m^{-3/2}}{q+q_m}. \tag{A3.17}$$

For $|q|<\alpha$ this function is regular, with the Taylor expansion

$$\sigma(q)=\sum_{s=0}^{\infty}\zeta[\tfrac{5}{4}+\tfrac{1}{2}s,\alpha^2](-q)^s, \tag{A3.18}$$

and it may be analytically continued to give a function which is regular in the right half of the q plane

$$\sigma(q)=-\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\pi\zeta[\frac{5}{4}+\frac{1}{2}s,\alpha^2]}{\sin\pi s}q^s\,\mathrm{d}s \qquad (-\tfrac{1}{2}<c<0). \tag{A3.19}$$

Then the asymptotic expansion of $\sigma(q)$, as $q\to+\infty$, is obtained as the sum of the residues of the integrand lying to the left of the contour, that is

$$\sigma(q)\sim 2\pi q^{-1/2}+\sum_{s=1}^{\infty}\frac{\zeta[\frac{5}{4}-\frac{1}{2}s,\alpha^2]}{(-q)^s}. \tag{A3.20}$$

Hence we have obtained

$$\begin{aligned}\sum\frac{d_m}{q+q_m}=&-2\pi(D_0q^{-3/2}-D_1q^{-5/2}+\ldots-(-1)^rD_{r-1}q^{-r-1/2})\\&+\frac{\Sigma\, d_m}{q}-\frac{\Sigma\,(d_mq_m-D_0q_m^{-3/2})+D_0\zeta[\frac{3}{4},\alpha^2]}{q^2}+\ldots\\&+(-1)^r\frac{\Sigma\,(d_mq_m^r-\Sigma_{s=1}^r D_{r-s}q_m^{s-5/2})+\Sigma_{s=1}^r D_{r-s}\zeta[\frac{5}{4}-\frac{1}{2}s;\alpha^2]}{q^{r+1}}\\&+\mathrm{O}(q^{-r-3/2}).\end{aligned} \tag{A3.21}$$

Using (A3.15), the first bracketed expression on the right-hand side of (A3.21) is recognised as the beginning of the asymptotic expansion for $qc(q)$. It therefore follows that

$$\frac{1}{2Q(q)}\sum\frac{d_m}{q+q_m}\sim-\frac{1}{2}a(q)+\frac{1}{2Q(q)}\sum_{r=0}^{\infty}\frac{(-1)^rS_r}{q^{r+1}}, \tag{A3.22}$$

where

$$S_r=\sum_{m=0}^{\infty}\left(d_mq_m^r-\sum_{s=1}^{r}D_{r-s}q_m^{s-5/2}\right)+\sum_{s=1}^{r}D_{r-s}\zeta[\tfrac{5}{4}-\tfrac{1}{2}s;\alpha^2]. \tag{A3.23}$$

References

[1] Nelson E 1967 *Dynamical theories of Brownian motion* (Princeton, NJ: Princeton University Press)
[2] Uhlenbeck G E and Ornstein L S 1930 *Phys. Rev.* **36** 823
[2a] Wax N (ed) 1954 *Selected papers in noise and stochastic processes* (New York: Dover)
[3] Kramers H A 1940 *Physica* **7** 284
[4] Rice S O 1945 *Bell Syst. Tech. J.* **25** 46 equation (3.4-11)
[5] Wang M C and Uhlenbeck G E 1945 *Rev. Mod. Phys.* **17** 323
[6] Burschka M A and Titulaer U M 1982 *Physica* **112A** 315
[7] Selinger J V and Titulaer U M 1984 *J. Stat. Phys.* **36** 293
[8] Titulaer U M 1984 *J. Stat. Phys.* **37** 589
[9] Smoluchowski M 1916 *Z. Phys.* **17** 557-71, 585-99
[10] Darling D A and Siegert A J F 1953 *Ann. Math. Stat.* **24** 624

[11] Gikhman I I and Skorokhod A V 1969 *Introduction to the theory of random processes* (Philadelphia: Saunders) Ch 8

[12] Chandrasekhar S 1943 *Rev. Mod. Phys.* **15** 1

[13] Bartlett M S 1950 *Nature* **165** 767

[14] Case K M and Zweifel P F 1967 *Linear transport theory* (Reading, Mass.: Addison-Wesley)

[15] Larsen E W and Mullikin T W 1981 *J. Math. Phys.* **22** 856

[16] Beals R and Protopopescu V 1983 *J. Stat. Phys.* **32** 565

[17] Pagani C D 1970 *Boll. Un. Math. Ital.* **3** 961

[18] Olver F W J 1974 *Asymptotics and Special Functions* (London: Academic)