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The Fokker–Planck equation with absorbing boundary

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Abstract. An analytic solution of the stationary one-dimensional Fokker–Planck equation with absorbing boundary is explicitly constructed.

1. Introduction

The purpose of this paper is to solve the stationary one-dimensional Fokker–Planck equation

$$v\frac{\partial f(x, v)}{\partial x}=\zeta\frac{\partial}{\partial v}\left(v+\alpha\frac{\partial}{\partial v}\right)f(x, v) \tag{1.1}$$

subject to the boundary condition

$$f(0, v)=0, \qquad v\in[0, \infty). \tag{1.2a}$$

In (1.1), $f(x, v)$ is the distribution function of a Brownian particle of mass m, ζ is the friction coefficient, $\alpha = kT/m$ is supposed to be constant, x and v are the position and velocity coordinates. The case studied here is that of a motion in a half-space $x \geqslant 0$ bounded by a plane wall at $x = 0$.

In this form the problem was raised by Wang and Uhlenbeck (1945), but until now only approximate numerical solutions have been published (Harris 1981, Burschka and Titulaer 1981).

The boundary condition (1.2a) is not sufficient for obtaining an unique solution as it will become clear from what follows, and it must be supplemented by a condition at $x=\infty$, which we take as

$$f(x, v)\to h(x, v) \qquad \text{as } x\to\infty \tag{1.2b}$$

where $h(x, v)=(x-v\zeta^{-1})\exp(-v^2/2\alpha)$ is the diffusion solution found by Pagani (1970).

Exactly solvable problems in which a kinetic boundary layer occurs are extremely rare and then the solving proceeds in two steps. One constructs first a set of stationary solutions which are complete on a half-range interval and secondly one combines them in order to fulfil the boundary conditions.

The paper is organised as follows. The construction of a complete system of functions on the half-range interval $[0, \infty)$ is given in § 2. This system is used in § 3 for obtaining the analytical solution of the problem (1.1)-(1.2). The paper ends with some conclusions.

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2. Construction of a complete set of functions on the half-range interval

It is useful to make the following transformation

$$f(x, v)=\exp(-t^2/2)g(x, t)$$

where $t=(2\alpha)^{-1/2}v$.

Equation (1.1) takes the form

$$\frac{(2\alpha)^{1/2}}{\zeta}\frac{\partial g(x, t)}{\partial x}=\frac{1}{2t}\left(\frac{\partial^2 g(x, t)}{\partial t^2}+(1-t^2)g(x, t)\right). \tag{2.1}$$

Solutions of (2.1) can be obtained if we make the ansatz

$$g(x, t)=\exp(-\lambda_1 x)h(t).$$

We get for $h(t)$ the differential equation

$$\frac{1}{2t}\left(-\frac{\mathrm{d}^2 h}{\mathrm{d}t^2}+(t^2-1)h\right)=\lambda h \tag{2.2}$$

where $\lambda=(2\alpha)^{1/2}\zeta^{-1}\lambda_1$.

Two independent solutions of (2.2) are $D_{\lambda^2/2}(\sqrt{2}(t-\lambda))$ and $D_{-\lambda^2/2-1}(\mathrm{i}\sqrt{2}(t-\lambda))$, where $D_\nu(z)$ denotes the parabolic cylinder function.

In order to have a functional calculus, i.e. spectral decompositions, expansion theorems and so on, we have to supplement (2.2) with suitable boundary conditions. The relations (1.2) do not impose a definite boundary condition upon $h(t)$. However they suggest looking at the differential operator (2.2) on the half-range interval $(0, \infty)$. Consequently we make the change of variable

$$t=\sqrt{s} \tag{2.3}$$

and (2.2) takes the form

$$\begin{aligned} &-(\mathrm{d}/\mathrm{d}s)(2\sqrt{s}\,\mathrm{d}y/\mathrm{d}s)+\tfrac{1}{2}(\sqrt{s}-1/\sqrt{s})y=\lambda y \\ &y(s)=h(t(s)), \qquad s\in[0, \infty). \end{aligned} \tag{2.4}$$

We remark that the transformation (2.3) has changed the differential equation (2.2) into a standard formally self-adjoint Sturm-Liouville problem. Thus, with suitable boundary conditions, the differential operator

$$L_s=-(\mathrm{d}/\mathrm{d}s)(2\sqrt{s}\,\mathrm{d}/\mathrm{d}s)+\tfrac{1}{2}(\sqrt{s}-1/\sqrt{s}) \tag{2.5}$$

will provide us with a complete system of orthonormal functions, which will be a necessary ingredient in solving the problem (1.1)-(1.2).

Two independent solutions of (2.4) for $\lambda=\mathrm{i}$ are $y_1=D_{-1/2}(\sqrt{2s}-\mathrm{i}\sqrt{2})$ and $y_2=D_{-1/2}(\mathrm{i}\sqrt{2s}+\sqrt{2})$. From the asymptotic behaviour of $D_\nu(z)$ we conclude that $y_1\in L_2(0, \infty)$ and $y_2\notin L_2(0, \infty)$, so that L_s has deficiency indices (1, 1). Thus L_s will become self-adjoint if we impose one boundary condition at the non-singular end $s=0$. The general form of this boundary condition is

$$y(0)\cos\alpha-2\sqrt{s}\,\mathrm{d}y/\mathrm{d}s|_{s=0}\sin\alpha=0, \qquad \alpha\in[0, 2\pi). \tag{2.6}$$

By imposing (2.6) we get for each α a self-adjoint extension, each extension providing us with a complete set of functions. Since for solving the problem (1.1)-(1.2) it is sufficient to know one complete system, we have freedom in choosing the parameter α. The operator L_s subject to the boundary conditions (2.6) having a discrete spectrum, our choice is $\alpha = 0$, which gives the simplest eigenvalue equation.

In the following we will find the spectrum and the eigenfunctions of the differential operator L_s subject to the boundary condition

$$y(0) = 0. \tag{2.7}$$

The spectrum of the operator (2.5)-(2.7) is determined by the Weyl's m function (Titchmarsh 1962). In order to find it we construct two solutions of (2.3), $u(s, \lambda)$ and $v(s, \lambda)$, which satisfy the boundary conditions

$$u(0, \lambda) = 1, \qquad 2\sqrt{s}\, u'(s, \lambda)|_{s=0} = -1$$

and

$$v(0, \lambda) = 1, \qquad 2\sqrt{s}\, v'(s, \lambda)|_{s=0} = \tfrac{1}{2}.$$

They are

$$\begin{aligned} u(s, \lambda) = {} & \mathrm{i}2^{-1/2} \exp(\pi\lambda^2\mathrm{i}/4)[D_{-\lambda^2/2-1}(-\mathrm{i}\lambda\sqrt{2}) D_{\lambda^2/2}(\sqrt{2s} - \lambda\sqrt{2}) \\ & - D_{\lambda^2/2}(-\lambda\sqrt{2}) D_{-\lambda^2/2-1}(\mathrm{i}\sqrt{2s} - \mathrm{i}\lambda\sqrt{2})] \\ v(s, \lambda) = {} & \mathrm{i} \exp(\pi\lambda^2\mathrm{i}/4)\{[\mathrm{i}D'_{-\lambda^2/2-1}(-\mathrm{i}\lambda\sqrt{2}) - 2^{-3/2} D_{-\lambda^2/2-1}(-\mathrm{i}\lambda\sqrt{2})] D_{\lambda^2/2}(\sqrt{2s} - \lambda\sqrt{2}) \\ & + [2^{-3/2} D_{\lambda^2/2}(-\lambda\sqrt{2}) - D'_{\lambda^2/2}(-\lambda\sqrt{2})] D_{-\lambda^2/2-1}(\mathrm{i}\sqrt{2s} - \mathrm{i}\lambda\sqrt{2})\} \end{aligned}$$

$(D'_\nu(z) = (\mathrm{d}/\mathrm{d}z) D_\nu(z))$.

The m function is determined by the condition $v(s, \lambda) + m(\lambda) u(s, \lambda) \in L_2(0, \infty)$. Taking into account the asymptotic behaviour of $D_\nu(z)$ we find

$$m(\lambda) = \tfrac{1}{2} - \sqrt{2}\, D'_{\lambda^2/2}(-\lambda\sqrt{2}) / D_{\lambda^2/2}(-\lambda\sqrt{2}). \tag{2.8}$$

The singularities of $m(\lambda)$ on the real line give the spectrum of the operator.

The function $D_\nu(z)$ is an entire function of both ν and z, so that $D_{\lambda^2/2}(-\lambda\sqrt{2})$ is an entire function of λ. Thus (2.8) can be written

$$m(\lambda) = \tfrac{1}{2} + \sqrt{2} \sum_n (\lambda_n - \lambda)^{-1}$$

where the summation is over all n for which λ_n is a root of the equation

$$D_{\lambda^2/2}(-\lambda\sqrt{2}) = 0. \tag{2.9}$$

The m function (2.8) being meromorphic, the spectrum is discrete and the eigenvalues λ_n are simple. The residue at the pole $\lambda = \lambda_n$ is $\sqrt{2}$ and consequently the orthonormal eigenfunctions are

$$\begin{aligned} u_n(s, \lambda_n) &= \mathrm{i}2^{-1/4} \exp(\pi\lambda_n^2\mathrm{i}/4) D_{\lambda_n^2/2-1}(-\mathrm{i}\lambda_n\sqrt{2}) D_{\lambda_n^2/2}(\sqrt{2s} - \lambda_n\sqrt{2}) \\ &= 2^{-1/4} D_{\lambda_n^2/2}(\sqrt{2s} - \lambda_n\sqrt{2}) [D'_{\lambda_n^2/2}(-\lambda_n\sqrt{2})]^{-1}. \end{aligned} \tag{2.10}$$

The spectrum of the operator (2.5)-(2.7) is positive although this is not evident from the eigenvalue equation (2.9).

We do not produce a direct argument showing that (2.9) has no roots for $\lambda < 0$, but use an indirect method.

First we remark that $\lambda = 0$ is not an eigenvalue. By the transformation

$$y(s) = u^{-1/6} v(u)$$

where $u=s^{3/4}$, (2.4) can be written in the form

$$d^2v/du^2+[\tfrac{8}{9}\lambda-q(u)]v=0 \qquad (2.11)$$

where $q(u)=\frac{4}{9}(u^{2/3}-u^{-2/3})-\frac{5}{36}u^{-2}$.

Now we can use the results of chapter 5 from Titchmarsh's book (1962). By the above transformation the end $u=0$ is becoming singular, but since $q(u)>-\frac{1}{4}u^{-2}+A$, for u sufficiently close to zero, the results are the same as if there were no singularities at $u=0$. When $q(u)\to\infty$ as $u\to\infty$, which is precisely our case, there are discrete eigenvalues and the eigenfunction associated with λ_n has n zeros.

Up to constant factors the eigenfunctions of (2.11) are the functions (2.10) multiplied by $u^{1/6}$

$$v_n(u,\lambda_n)=u^{1/6}D_{\lambda_n^2/2}(\sqrt{2}(u^{2/3}-\lambda_n)).$$

We introduce the notation $g(\lambda)=D_{\lambda^2/2}(-\lambda\sqrt{2})$ and notice that $g(0)>0$ and $g(\sqrt{2})<0$. Thus we have at least one eigenvalue in $(0,\sqrt{2})$ which we let be λ_0. On the other hand $D_\nu(z)$ has $[\nu+1]$ zeros on $(-\infty,\infty)$, where $[x]$ denotes the integral part of x (Erdélyi 1953). Since $0<\lambda_0<\sqrt{2}$, $[1+\lambda_0^2/2]=1$ and we conclude that $v_0(u,\lambda_0)$ has only one zero on the real line. However we know that this zero is at $u=0$ since $D_{\lambda_0^2/2}(-\lambda_0\sqrt{2})=0$.

Thus we have found that $v_0(u,\lambda_0)$ has no nodes on the interval $(0,\infty)$, i.e. λ_0 is the eigenvalue which corresponds to the fundamental state.

Since $\lambda_0>0$ the operator (2.5)-(2.7) is positive.

The above arguments can be extended to show that

$$(2n)^{1/2}<\lambda_n<(2n+2)^{1/2} \qquad n=1,2,\ldots.$$

A more precise estimate for λ_n can be obtained only for large n. From the asymptotic behaviour of $D_\nu(z)$ when both ν and z are large (Abramovitz and Stegun 1964) we get

$$\lambda_n=(2n+3/4)^{1/2}(1+O(1/n)), \qquad n\to\infty.$$

3. Solution of the Fokker–Planck equation

In the preceding section we have constructed a complete system on the half-range interval $[0,\infty)$ of orthonormal eigenfunctions $u_n(s,\lambda_n)$. Consequently the functions

$$g_n(x,s)=\exp(-s/2-\zeta(2\alpha)^{-1/2}\lambda_n x)u_n(s,\lambda_n) \qquad n=0,1,\ldots \qquad (3.1)$$

are elementary solutions of the Fokker–Planck equation (1.1). Recalling that $v=(2\alpha s)^{1/2}$ the elementary solutions (3.1) can be written as

$$\begin{aligned}g_n(x,s)&=f_n(x,v)\\ &=2^{-1/4}\exp(-v^2/4\alpha-\zeta(2\alpha)^{-1/2}\lambda_n x)\\ &\quad\times D_{\lambda_n^2/2}(\alpha^{-1/2}v-\lambda_n\sqrt{2})/D'_{\lambda_n^2/2}(-\lambda_n\sqrt{2}), \qquad n=0,1,\ldots.\end{aligned} \qquad (3.1a)$$

Since $D_\nu(z)$ is an entire function of both ν and z, $f_n(x,v)$ are well defined in all the complex plane and $(3.1a)$ makes sense for $v<0$.

Since $f_n(x,v)$ is a complete system, an arbitrary solution $F(x,v)$ of (1.1) can be written

$$F(x,v)=\sum c_n f_n(x,v). \qquad (3.2a)$$

If we try to satisfy the boundary condition (1.2a)

$$F(0, v) = \sum_n c_n f_n(0, v) = 0,$$

we find that $c_n = 0$, i.e. the null solution. We remark that with the solution (3.2a) we cannot satisfy the boundary condition (1.2b). We can bypass this difficulty by adding to the independent set of functions $\{f_n(x, v)\}_{n=0}^{\infty}$, one or more functions which are solutions of (1.1). In this way we obtain a linearly dependent system of functions and we can write an expansion like (3.2a) in which not all the coefficients are identically zero. If we add more functions we have to give supplementary boundary conditions in order to find a unique solution. The solution we propose here is, in some sense, minimal. We add only such a function to $\{f_n(x, v)\}$, and this function is the diffusion solution $h(x, v)$.

Thus $F(x, v)$ can be written as

$$F(x, v) = a\left(h(x, v) + \sum_{n=0}^{\infty} c_n f_n(x, v)\right). \tag{3.2b}$$

This function must satisfy the boundary conditions (1.2a)-(1.2b). From (1.2b) we get $a = 1$, and from (1.2a)

$$F(0, v) = -v\zeta^{-1} \exp(-v^2/2\alpha) + \sum_{n=0}^{\infty} c_n f_n(0, v) = 0.$$

For $v \geqslant 0$ the above relation can be written

$$\sum_{n=0}^{\infty} c_n u_n(s, \lambda_n) = \zeta^{-1}(2\alpha s)^{1/2} \, \mathrm{e}^{-s/2}$$

whence we obtain

$$c_n = \zeta^{-1}(2\alpha)^{1/2} \int_0^{\infty} s^{1/2} \, \mathrm{e}^{-s/2} u_n(s, \lambda_n) \, \mathrm{d}s \qquad n = 0, 1, \ldots.$$

Instead of using the boundary condition (1.2b), we may use, alternatively, the asymptotic behaviour of the particle density, or the particle flux as $x \to \infty$.

The formula (3.2b) with $a = 1$ and c_n given by (3.3) is our solution of the Fokker-Planck equation with absorbing boundary. A numerical computation of the solution will be given elsewhere.

4. Conclusion

In this paper we have found a method for obtaining an analytic solution to a boundary value problem that, until now, has resisted all attempts to solve it.

It is easily seen that our method can be applied to a large class of kinetic equations, that by separation of variables lead to a Sturm-Liouville operator like (2.2). In most cases, although the problems are indefinite, the boundary conditions allow them to be treated as definite ones. This is precisely our case here, where the operator (2.2) is not definite on the whole interval ($-\infty < v < \infty$), but on the half-range interval $[0, \infty)$, suggested by the boundary conditions (1.2), it becomes definite, and we could apply the standard methods for solving the problem.

The method can be used to solve kinetic equations with a boundary condition like $f(0, v) = \varphi(v)$ for $v > 0$. Work in this direction is in progress.

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