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Brownian Motion Near an Absorbing Sphere

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The spherically symmetric solution of the Fokker–Planck equation with absorbing boundary is given in terms of a solution of an equivalent integral equation whose explicit form is found.

KEY WORDS: Brownian motion; Fokker–Planck equation; absorbing sphere.

1. INTRODUCTION

In this paper we shall consider the problem of determining the distribution function for a Brownian particle in the presence of an absorbing sphere. The problem was first raised some time ago by Wang and Uhlenbeck,[1] but until now only the one-dimensional case has been solved.[2,3] The three-dimensional problem, as a long-standing and well-defined one in statistical mechanics, has its own interest, but there is also a practical interest through its relationship with the theory of reaction rates.[4,5]

The main object of study is the spherically symmetric distribution function that satisfies the equation

$$Lf(\mathbf{r}, \mathbf{v}) \equiv (\mathbf{v} \cdot \nabla_{\mathbf{r}}) f(\mathbf{r}, \mathbf{v}) - \nabla_{\mathbf{v}}(\mathbf{v} \cdot f(\mathbf{r}, \mathbf{v})) - \Delta_v f(\mathbf{r}, \mathbf{v}) = 0 \qquad (1.1)$$

$$\mathbf{r} \in \mathbb{R}^3 \backslash S, \qquad \mathbf{v} \in \mathbb{R}^3$$

and the boundary conditions (BC)

$$f(a, v, \mu) = 0 \qquad \text{for} \quad \mu > 0, v = |\mathbf{v}| \in \mathbb{R}_+ \qquad (1.2a)$$

$$f(\mathbf{r}, \mathbf{v}) \equiv f(r, v, \mu) \xrightarrow[r \to \infty]{} g(r, v, \mu) \qquad \text{in an } L_2\text{-sense} \qquad (1.2b)$$

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Here $r = |\mathbf{r}|$, $S = \{\mathbf{r} \,|\, \mathbf{r}^2 \leqslant a^2\}$ is the sphere of radius a, $\mu = \cos \Omega$, Ω being the angle between the vectors $\mathbf{r}$ and $\mathbf{v}$, and $g(r, v, \mu)$ is a diffusion solution of Eq. (1.1). A diffusion solution is a solution of the form $P_1(r) f_1(v) + P_2(r) f_2(v)$, where P_1 and P_2 are polynomials in the variable r.

Because of the spherical symmetry the distribution function $f(\mathbf{r}, \mathbf{v}) = f(r, v, \mu)$ depends only on three variables r, v, μ. Until now no explicit analytic solution of the above problem has been found. However, many different numerical approaches have been used for solving the problem.[6-11] In all of them a problem arises: the BC (1.2a) cannot be correctly satisfied.

The aim of this paper is to transform the boundary value problem (1.1)–(1.2) into an integral equation of Fredholm type. The method makes explicit use of the fundamental solution of Eq. (1.1). We want to point out here that most of our results are at a purely formal level.

We want to point out also that our method is rather general and can be applied to boundary value problems of the form

$$Lf = \sum_{i,j=1}^{n} a_{ij}(x, y) \frac{\partial^2 f}{\partial y_i \, \partial y_j}(x, y) + \sum_{i=1}^{n} a_i(x, y) \frac{\partial f}{\partial y_i}(x, y)$$
$$+ a(x, y) f(x, y) + \sum_{i=1}^{m} b_i(x, y) \frac{\partial f}{\partial x_i}(x, y) = 0$$

+ appropriate boundary conditions.

Here $x = (x_1, ..., x_m)$, $y = (y_1, ..., y_n)$, $m \leqslant n$, and the matrix (a_{ij}) is supposed to be strictly positive. These conditions are the necessary conditions for the existence of the fundamental solution. See refs. 12 and 13.

In order to solve the problem (1.1)–(1.2a) it is necessary to solve first another problem, namely that with the following boundary conditions (BC):

$$f(a, v, \mu) = \varphi(v, \mu), \qquad \mu \in (0, 1), \quad v \in \mathbb{R}_+ \tag{1.2c}$$

Afterward by an elementary trick we obtain also the solution of the boundary value problem (1.1)–(1.2a).

The paper is organized as follows. In Section 2 we find the fundamental solution of Eq. (1.1) and in Section 3 we use it to transform the problem (1.1)–(1.2) into an integral equation. Section 4 presents our conclusions.

2. FUNDAMENTAL SOLUTION

The fundamental solution of our problem satisfies the equation

$$L^* G = (-\mathbf{v} \cdot \nabla_{\mathbf{r}} + \mathbf{v} \cdot \nabla_{\mathbf{v}} - \Delta_{\mathbf{v}})\, G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) = \delta(\mathbf{r} - \boldsymbol{\rho})\, \delta(\mathbf{v} - \boldsymbol{\omega}) \tag{2.1}$$

Looking at (2.1), it seems very difficult to solve such an equation. Instead of (2.1) we shall consider the time-dependent equation

$$\frac{\partial \phi}{\partial t} + L^{*}\phi = \delta(t)\,\delta(\mathbf{r}-\boldsymbol{\rho})\,\delta(\mathbf{v}-\boldsymbol{\omega}) \tag{2.1a}$$

whose solution can be obtained easily. By making the change of variables

$$\mathbf{u} = \mathbf{v}e^{-t}, \qquad \mathbf{p} = \mathbf{r} + \mathbf{v}$$

we get for the left hand side of (2.1a)

$$\frac{\partial f}{\partial t} + L^{*}f = \frac{\partial f}{\partial t} - e^{-2t}\Delta_{\mathbf{u}} f - 2e^{-t}\nabla_{\mathbf{u}}\nabla_{\mathbf{p}} f - \Delta_{\mathbf{p}} f = 0$$

The fundamental solution of the last equation is known[1,14] and as a consequence the solution of Eq. (2.1a) is given by

$$\begin{aligned}\phi(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) &= (8\pi^3\Delta^{3/2})^{-1}\exp[-E(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})] &\quad \text{for} \quad t \geqslant 0\\ &= 0 &\quad \text{for} \quad t < 0\end{aligned}$$

where

$$\begin{aligned}E(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) = \frac{1}{2\Delta}\,&[(2t(\mathbf{v}e^{-t} - \boldsymbol{\omega})^2 - 4(1-e^{-t})(\mathbf{v}e^{-t} - \boldsymbol{\omega})(\mathbf{r}+\mathbf{v}-\boldsymbol{\rho}-\boldsymbol{\omega}))\\ &+ (1-e^{2t})(\mathbf{r}+\mathbf{v}-\boldsymbol{\rho}-\boldsymbol{\omega})^2]\end{aligned}$$

and

$$\Delta = 2t(1-e^{2t}) - 4(1-e^{-t})^2$$

It is easily seen that

$$\begin{aligned}\Delta &= 2t + O(1) &\quad \text{as} \quad t \to \infty\\ \Delta &= \frac{t^4}{3} + O(t^5) &\quad \text{as} \quad t \to 0\end{aligned}$$

and

$$\begin{aligned}E(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) &= \frac{\boldsymbol{\omega}^2}{2} + \frac{(\mathbf{r}+\mathbf{v}+\boldsymbol{\omega}-\boldsymbol{\rho})^2}{4t} + O(t^{-2}) &\quad \text{as} \quad t \to \infty\\ E(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) &= 3\,\frac{(\boldsymbol{\rho}-\mathbf{r})^2}{t^3} + O(t^{-2}) &\quad \text{as} \quad t \to 0\end{aligned} \tag{2.2}$$

These properties show that the time dependence of the function ϕ is such that the integral

$$G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\int_0^{\infty} \phi(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\, dt \tag{2.3}$$

does exist, and since we know that ϕ satisfies Eq. (2.1a) it follows that (2.3) gives the fundamental solution of the time-independent Eq. (2.1). Because we are interested in the spherically symmetric case, we shall write

$$G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) \equiv G(r, v, \rho, \omega, \alpha, \varphi, \beta, \theta, \Omega, \gamma)$$

where (v, α, φ) denote the spherical coordinates of $\mathbf{v}$, (ρ, β, θ) those of $\boldsymbol{\rho}$, $\boldsymbol{\omega}$ is pointing out in the positive direction of the z axis of the rectangular system, and (r, Ω, γ) are the spherical coordinates of $\mathbf{r}$, where now the z axis is taken along the direction of $\mathbf{v}$. This means that the scalar products entering (2.3) have the following form:

$$\mathbf{r} \cdot \mathbf{v} = rv \cos \Omega$$

$$\begin{aligned} \boldsymbol{\rho} \cdot \mathbf{r} = \rho r[&\sin \alpha \sin \beta \cos \Omega \cos(\theta - \varphi) + \sin \beta \sin \Omega \cos \gamma \sin(\theta - \varphi) \\ &- \sin \beta \sin \Omega \sin \gamma \cos \alpha \cos(\theta - \varphi) + \cos \alpha \cos \beta \cos \Omega \\ &+ \sin \alpha \sin \gamma \sin \Omega \cos \beta] \end{aligned}$$

etc.

3. INTEGRAL EQUATION

We shall denote by D the domain

$$D = \{\mathbf{r}, \mathbf{v} \mid \mathbf{r} \in \mathbb{R}^3 \backslash S, \mathbf{v} \in \mathbb{R}^3\}$$

where $S = \{\mathbf{r} \mid \mathbf{r}^2 \leqslant a^2\}$ is the sphere of radius a centered at the origin of the system of coordinates.

Let $f(r, v, \mu)$ denote the spherically symmetric solution of Eq. (1.1) with the boundary conditions (BC). Now we integrate the equation

$$G(r, v, \rho, \omega. \alpha, \varphi, \beta, \theta, \Omega, \gamma)\, Lf(r, v, \mu) = 0$$

over the domain D, and we get

$$f(\rho, \omega, v) + \int_0^{\infty} v^3\, dv \int_{-1}^{1} \mu\, d\mu\, f(a, v, \mu)\, K(a, \rho, v, \omega, \mu, v) = 0 \tag{3.1}$$

where $\mu = \cos \Omega$, $v = \cos \beta$, and

$$K(a, v\,\rho, \omega, v) = \frac{a^2}{2\pi} \int_0^{\pi} d\alpha \int_0^{2\pi} d\varphi \int_0^{2\pi} d\gamma \int_0^{2\pi} d\theta \sin \alpha\, G(a, v, \rho, \omega, \alpha, \varphi, \beta, \theta, \Omega, \gamma)$$

The factor $1/2\pi$ in front of the last integral arises from an integration over the azimuthal angle θ, $f(\rho, \omega, v)$ being independent of it. Equation (3.1) shows that $f(\rho, \omega, v)$ is completely determined by the function $f(a, \omega, v)$, $v \in (-1, 1)$, $\omega \in \mathbb{R}_+$. For this last function we obtain an integral equation. Indeed, by making $\rho \to a+$ and by using the relation (1.2c) in Eq. (3.1), we find

$$\begin{aligned} f(a, \omega, v) &+ \int_0^{\infty} u^3\, du \int_{-1}^{0} \mu f(a, u, v)\, K(a, u, a, \omega, \mu, v)\, d\mu \\ &= -\int_0^{\infty} u^3\, du \int_0^1 \mu \cdot \phi(u, \mu) \cdot K(a, u, a, \omega, \mu, v)\, d\mu \\ &\equiv \psi(\omega, v) \end{aligned} \tag{3.2}$$

which is satisfied by the distribution function $f(\rho, \omega, v)$ on the surface of the sphere S. The right-hand side of Eq. (3.2) is a known function depending on the boundary value $\varphi(u, \mu)$, for $\mu > 0$. After we know the solution of Eq. (3.2), the distribution function $f(\rho, \omega, v)$ that solves the boundary value problem (1.1)–(1.1c) is given by the integral transform (3.1). Unfortunately, there is no hope to solve explicitly Eq. (3.2), its kernel being a very complicated function.

We want to point out here that this is the first time that an integral equation for the distribution function of the steady-state spherically symmetric Fokker–Planck equation has been obtained. All the previous approaches for solving the problem (1.1)–(1.2) were based on the moments problems, and various schemes of truncated expansions have been attempted. See ref. 10 and the references therein for a discussion of the shortcomings of these expansions.

In most applications[1–11] the interesting physical problem is the boundary value problem (1.1)–(1.2a), i.e., the solution of Eq. (1.1) that satisfies at

$$r = a, \qquad f(a, v, \mu) = 0, \qquad \mu \in (0, 1), \quad v \in \mathbb{R}_+$$

This means that all particles falling upon sphere are absorbed by it.

In order to obtain a unique solution we have to impose also the condition (1.2b), namely

$$f(r, v, \mu) \to g(r, v, \mu) \qquad \text{as} \quad r \to \infty, \quad \text{in an } L_2\text{-sense}$$

where $g(r, v, \mu)$ is a diffusion solution.

A spherically symmetric diffusion solution of Eq. (1.1) is

$$g(r, v, \mu) = \left(r\mu \frac{v^2 + 1}{v^2} + \frac{3 - v^2}{v} \right) \exp\left(-\frac{v^2}{2} \right)$$

The function

$$h(r, v, \mu) = g(r, v, \mu) - f(r, v, \mu)$$

where $f(r, v, \mu)$ is a solution of the problem (1.1)–(1.2a), is a solution of Eq. (1.1) and satisfies the boundary conditions (BC)

$$h(a, v, \mu) = g(a, v, \mu) \equiv \left(a\mu \frac{v^2 + 1}{v^2} + \frac{3 - v^2}{v} \right) \exp\left(-\frac{v^2}{2} \right), \quad \mu \in (0, 1), \ v \in \mathbb{R}_+$$

and by construction $h(r, v, \mu) \to 0$ as $r \to \infty$.

We see that the function $h(r, v, \mu)$ satisfies the BC (1.2c) and consequently $h(a, v, \mu)$ can be obtained by solving the integral equation (3.2), where the function $\varphi(u, \mu)$ entering the right-hand side is given by the above explicit expression. The solution $h(r, v, \mu)$ and as a consequence $f(r, v, \mu)$, is obtained via the integral transform (3.1).

Finally we want to point out that the integral operator (3.2) can be studied in detail, although we shall not pursue this here. The key point is the asymptotic relation (2.2), which allows an estimate of the fundamental solution $G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})$ as follows.

Let A be a constant such that for $t > A$ we have

$$E(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) \geqslant \frac{\boldsymbol{\omega}^2}{2} + \frac{(\mathbf{r} + \mathbf{v} + \boldsymbol{\omega} - \boldsymbol{\rho})^2}{4t}$$

We shall write $G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})$ in the form

$$G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) = \int_0^A \phi(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\, dt + \int_A^\infty \phi(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\, dt$$

and note that the first integral on the right-hand side can be written as $A \cdot \phi(t_0, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\, dt$, where $0 < t_0 < A$.

As concerns the second integral we have

$$\begin{aligned} \int_A^\infty \phi(t, \mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega})\, dt &\leqslant \frac{1}{8\pi} \int_A^\infty \frac{\exp\{-\boldsymbol{\omega}^2/2 - (\mathbf{r} + \mathbf{v} + \boldsymbol{\omega} - \boldsymbol{\rho})^2/4t\}}{(2t - 4)^{3/2}}\, dt \\ &\leqslant \frac{A \exp(-\boldsymbol{\omega}^2/2)}{8\pi(A - 2)} \int_A^\infty \frac{\exp\{-(\mathbf{r} + \mathbf{v} + \boldsymbol{\omega} - \boldsymbol{\rho})^2/4t\}}{(2t)^{3/2}}\, dt \\ &= \frac{B \exp(-\boldsymbol{\omega}^2/2)}{|\mathbf{r} + \mathbf{v} + \boldsymbol{\omega} - \boldsymbol{\rho}|}, \qquad B^{-1} = (2\pi)^{1/2} \frac{A - 2}{A} \end{aligned}$$

Thus,

$$G(\mathbf{r}, \mathbf{v}, \boldsymbol{\rho}, \boldsymbol{\omega}) \cong \frac{B \exp(-\omega^2/2)}{|\mathbf{r} + \mathbf{v} + \boldsymbol{\omega} - \boldsymbol{\rho}|} + \text{smooth terms}$$

The behavior reflects itself into an explicit dependence of the kernel of the integral equation (3.2) and makes possible an almost complete analysis of the corresponding operator.

4. CONCLUSION

In this paper we have shown that the boundary value problems (1.1)–(1.2) are equivalent to an integral equation. In this way we have succeeded in taking exactly into account the boundary condition (1.2a), which caused much trouble when implementing it in numerical calculations. We hope to find an approximation scheme for solving the integral equation (3.2) and show that the approximation converges to the true solution.

Our work also sugests that this method can be extended to other interesting transport equations, the sole proviso being the knowledge of the fundamental solution of the corresponding partial differential equation. In this way this paper suggests a new route for solving such boundary value problems, since by transforming them into Fredholm integral equations, the existence and uniqueness theory is considerably simplified.

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