

## Numerical Solution for a Non-Fickian Diffusion in a Periodic Potential

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**Abstract.** Numerical solutions of a non-Fickian diffusion equation belonging to a hyperbolic type are presented in one space dimension. The Brownian particle modelled by this diffusion equation is subjected to a symmetric periodic potential whose spatial shape can be varied by a single parameter. We consider a numerical method which consists of applying Laplace transform in time; we then obtain an elliptic diffusion equation which is discretized using a finite difference method. We analyze some aspects of the convergence of the method. Numerical results for particle density, flux and mean-square-displacement (covering both inertial and diffusive regimes) are presented.

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### 1 Introduction

In this paper we shall present numerical solutions of a non-Fickian diffusion equation in the presence of a symmetric periodic potential in one space dimension. Let us briefly recall that the familiar Fickian diffusion equation for a particle density  $n(\xi, \tau)$ , in the presence of a potential  $V(\xi)$  reads

$$\frac{\partial n}{\partial \tau}(\xi, \tau) = D \frac{\partial^2 n}{\partial \xi^2}(\xi, \tau) + \frac{1}{m\gamma} \frac{\partial}{\partial \xi} \left[ \frac{dV}{d\xi}(\xi) n(\xi, \tau) \right], \quad (1.1)$$

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where  $\xi$  is the space variable,  $\tau$  is time,  $\gamma$  is a friction parameter and  $D = k_B T / m\gamma$  is the diffusion coefficient,  $m$  being the mass of the Brownian particle whose overdamped (diffusive) dynamics is well described by (1.1);  $k_B$  is the Boltzmann's constant and  $T$  the temperature of the fluid.

The equation of our study is

$$\frac{1}{\gamma} \frac{\partial^2 n}{\partial \tau^2}(\xi, \tau) + \frac{\partial n}{\partial \tau}(\xi, \tau) = D \frac{\partial^2 n}{\partial \xi^2}(\xi, \tau) + \frac{1}{m\gamma} \frac{\partial}{\partial \xi} \left[ \frac{dV}{d\xi}(\xi) n(\xi, \tau) \right]. \quad (1.2)$$

Both equations, (1.1) and (1.2) can be derived from an underlying kinetic equation, e.g. the phase-space Kramers equation [9]

$$\frac{\partial f}{\partial \tau} + \frac{p}{m} \frac{\partial f}{\partial \xi} - \frac{dV}{d\xi} \frac{\partial f}{\partial p} = \gamma \frac{\partial}{\partial p} (pf) + mk_B T \gamma \frac{\partial^2 f}{\partial p^2}, \quad (1.3)$$

where  $f(\xi, p, \tau)$  is the probability density function for the position component  $\xi$  and momentum component  $p$  of the Brownian particle.

Eq. (1.2) in the absence of a potential field is sometimes referred to as the telegrapher equation although we shall call it a non-Fickian diffusion equation. We refer to [9] for a derivation of (1.2) from (1.3). It may be noted that for times larger than  $1/\gamma$ , the first term on the left hand side of (1.2) can be neglected and the Fickian regime is regained. Eq. (1.1) in the absence of a potential field leads to the well known result for the mean square displacement [11]

$$\langle \xi^2(\tau) \rangle = 2D\tau. \quad (1.4)$$

In the presence of a flexible symmetric potential, it was shown in [9] that  $\langle \xi^2(\tau) \rangle$  does not necessarily behave linearly with time. Eq. (1.2) retains some short time inertial behaviour of a Brownian particle and at long time results in a diffusive behaviour. The velocity  $v = d\xi/d\tau$  of a Brownian particle is not well defined in the diffusive regime for which (1.1) is applicable. Since (1.2) is applicable in an inertial regime, the velocity can be calculated with (1.2). Quite recently the instantaneous velocity of a Brownian particle has been experimentally investigated [12, 13, 18]. This provides an additional motivation for studying (1.2). There is also a recent paper [5] which models transport of ions in insulating media through a non-Fickian diffusion equation of the type discussed in our work. In [5] the non-Fickian diffusion equation is referred to as a hyperbolic diffusion equation.

To solve our problem we consider a numerical method based on a finite difference discretization and time Laplace transform. The latter is suitable for long times and also for solutions that are not necessarily smooth in time. It may be noted that iterative methods in time, including implicit methods such as the Crank-Nicolson [8], which allow a choice of large time steps, usually take too long to compute the solution.

The paper is organized as follows. In Section 2 we present the model problem in dimensionless variables. In Section 3 we describe a numerical method based on the time Laplace transform which is suitable for long time integration and also for solutions which