Physica A 444 (2016) 530–537

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

General method to solve the heat equation

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HIGHLIGHTS

- We present a unified method to obtain various solutions of the heat equation.
- Separable and nonseparable solutions are treated on an equal footing.
- A new nonseparable solution is derived for the first time.
- A physical phenomenon described by the new solution is demonstrated by simulations.
- It is confirmed that there is no more solution in the exponential form.

ARTICLE INFO

Article history:
Received 22 July 2015
Received in revised form 9 September 2015
Available online 23 October 2015

Keywords:
Heat equation
Diffusion equation
Random walk
Koopman–Darmois exponential function

ABSTRACT

General solutions of the heat equation are presented in terms of the Koopman–Darmois family of exponential functions, which include both the separable solution and the fundamental solution. In particular, we derive a new closed-form solution, which may not be obtained via the separation of variables or via an integral transform. It is demonstrated that the new solution describes the time evolution of the distribution of random walkers under an absorbing boundary.

1. Introduction

Diffusion is one of the fundamental mechanism for transport of materials in nature and has key importance not only in physical and biological sciences but also in financial mathematics. Diffusive motion of particles is described widely by a partial differential equation, called the diffusion equation or the heat equation, which corresponds to the continuity equation combined with Fick's law [1]. A simple solution of the heat equation is in general written as an expansion of basis functions, which is obtained via the separation of variables. On the other hand, another solution, which is the nonseparable fundamental solution, may usually be found through the integral transform of the partial differential equation.

In this study, we present a unified method, employing the Koopman–Darmois family of exponential functions [2,3], to obtain various solutions of the heat equation. The obtained solutions turn out to include both the (separable) Fourier series solution and the fundamental solution. In addition, the unified method also discloses a new nonseparable solution in a closed form. To our knowledge, this is the first time to derive the new solution as well as the conventional separable and fundamental solutions within a unified framework.

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http://dx.doi.org/10.1016/j.physa.2015.10.044

The heat equation in one dimension reads

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}, \tag{1}$$

where D is a positive constant called diffusivity. (The generalization to higher dimensions will be considered in Section 5.) We consider the solution in the form of an exponential function

$$f(x,t) = \exp[a(t)b(x) + c(t) + d(x)], \tag{2}$$

which may be derived via the maximum entropy principle [4,5] and is used to represent a family of probability density functions [6,7]. Inserting Eq. (2) into Eq. (1), we obtain

$$b(x)a'(t) + c'(t) = Db'(x)^2 a(t)^2 + D[2b'(x)d'(x) + b''(x)]a(t) + D[d'(x)^2 + d''(x)], \tag{3}$$

where $a'(t) \equiv \mathrm{d}a(t)/\mathrm{d}t$, $b'(x) \equiv \mathrm{d}b(x)/\mathrm{d}x$, and so on. Eq. (2) with $a(t)$, $b(x)$, $c(t)$, and $d(x)$ satisfying Eq. (3) constitutes a basis function of the solution space of the heat equation.

This paper is organized as follows: we first describe derivation of separable and nonseparable solutions in Sections 2 and 3, respectively. Then a numerical example of random walk is presented in Section 4, which demonstrates that the new solution gives a convenient description of the system with an absorbing boundary condition. Finally, Section 5 discusses a general form of the basis function and extension to higher dimensions, and gives a summary.

2. Separable solutions

In this section, we seek for the solution $f(x,t)$ in Eq. (2) with $a(t)b(x) \equiv 0$, which corresponds to the separable solution. Without the terms of $a(t)$ or $b(x)$, Eq. (3) reduces to

$$c'(t) = D\left[d'(x)^2 + d''(x)\right]. \tag{4}$$

It is obvious that for Eq. (4) to bear solutions, both left- and right-hand sides should be a constant, namely,

$$c'(t) = \zeta_0 = D[d'(x)^2 + d''(x)] \tag{5}$$

with ζ_0 being a constant.

We first consider the case that $\zeta_0 = 0$. Eq. (5) then yields

$$\begin{aligned} c(t) &= \alpha_1 \\ d(x) &= \ln|x-\alpha_2| + \alpha_3, \end{aligned} \tag{6}$$

where α_1, α_2, and α_3 are all constants. (Throughout this paper, Greek letters with integer subscripts, e.g., ζ_0, α_1, and β_2, represent constants.) Inserting Eq. (6) into Eq. (2), we obtain the first basis function of the heat equation

$$f(x,t) = \alpha_4|x-\alpha_2|, \tag{7}$$

which is trivial.

We next suppose that $\zeta_0 \neq 0$ in Eq. (5), which leads to

$$\begin{aligned} c(t) &= \zeta_0 t + \beta_1 \\ d(x) &= \ln\left[\exp\left(\sqrt{\frac{\zeta_0}{D}}x\right) - \exp\left(\beta_2 - \sqrt{\frac{\zeta_0}{D}}x\right)\right] + \beta_3. \end{aligned} \tag{8}$$

Then, from Eq. (2) with Eq. (8), we obtain the second basis function of the heat equation

$$f(x,t) = \beta_4 \exp(\zeta_0 t)\left[\exp\left(\sqrt{\frac{\zeta_0}{D}}x\right) - \exp\left(\beta_2 - \sqrt{\frac{\zeta_0}{D}}x\right)\right]. \tag{9}$$

Depending on the constants ζ_0 and β_2, this basis function assumes simple forms: In case that $\zeta_0 < 0$, taking $\beta_2 = -\infty$ reduces Eq. (9) to

$$f(x,t) = \beta_4 e^{\zeta_0 t}\exp\left(\mathrm{i}\sqrt{-\frac{\zeta_0}{D}}x\right) \tag{10}$$

with $\mathrm{i} \equiv \sqrt{-1}$, which is just the basis function for the Fourier series solution. When $\zeta_0 > 0$, on the other hand, Eq. (9) takes the form

$$f(x,t) = \beta_5 e^{\zeta_0 t}\sinh\left(\sqrt{\frac{\zeta_0}{D}}x - \frac{\beta_2}{2}\right), \tag{11}$$