Applied Mathematical Sciences, Vol. 8, 2014, no. 155, 7727 - 7748
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/ams.2014.49723

Diffusion Through a Half Space: Equivalence Between Different Formulations of the Unique Solution

Michele Mantegna and Luigi Pietro Maria Colombo

Politecnico di Milano, Department of Energy
Via Lambruschini, 4 – 20156 Milano (Italy)

Abstract

Diffusion through a half space involves a classical parabolic partial differential equation that is encountered in many fields of physics and has significant engineering applications, concerning particularly heat and mass transfer. However, in the specialized literature, the solution is usually achieved restricting the problem to particular cases and attaining apparently different formulations, thus a comprehensive overview is hindered. In this paper, the solution of the diffusion equation in a half space with a boundary condition of the first kind is worked out by means of the Fourier's Transform, the Green's function and the similarity variable, with a proof of equivalence – not found elsewhere – of these different approaches. The keystone of the proof rests on the square completion method applied to Gaussian-like integrals, widely used in Quantum Field Theory.

Keywords: Parabolic PDE, Dirichelet problem, Mass diffusion, Heat Conduction, Square Completion Method

1 Introduction

One of the most important mathematical methods of Quantum Field Theory is square completion to compute Gaussian integrals that arise from the Path Integral

Approach pioneered by Feynman [1 - 2]. As Zee [3] says, "Believe it or not, a significant fraction of the theoretical physics literature consists of performing variations and elaborations of this basic Gaussian integral". Although all books at the advanced undergraduate and most books at the graduate level use the method of canonical quantization (which avoids Gaussian integrals) or defer path integrals to the last chapters, the book by Zee introduces path integrals from the beginning.

The purpose of this paper is to show how the square completion method to compute Gaussian-like integrals allows understanding the equivalence of apparently very different formulations of the solution of the standard parabolic PDE encountered in heat conduction and other diffusion problems that play an important role in many Engineering applications. A paper by Slutsky [4] applied the full-blown machinery of path integrals to diffusion in the context of polymer physics. A similar though shorter treatment of linear polymer molecules as random walks is found in earlier works such as the books by Schulman [5] and Carrà [6]. On the other hand, Hall [7] very recently discussed the connection between random walks and path integrals. Our purpose is somewhat more limited and, at the same time, more accessible to a broader audience. We want to show that an important integral, which lies at the core of the path integral approach to Quantum Field Theory, emerges naturally from the juxtaposition of classical methods to solve the diffusion PDE and highlights the hidden connections among them.

2 Problem Statement

We consider an important class of partial differential equations in the general form

$$\frac{\partial u}{\partial t} = D \cdot \nabla^2 u \tag{1}$$

belonging to the category of parabolic equations. They are used to represent in different contexts a kind of transport referred to as diffusion [8]. For instance, setting

- $u = T$, temperature [K] and $D = \alpha$, thermal diffusivity [m^2 s^{-1}], Eq. (1) describes heat conduction in a homogeneous isotropic continuum with constant properties and without heat sources. This equation was first derived by Fourier [9].
- $u = c_A$, molar concentration of the chemical species A [mol m^{-3}] and $D = D_{AB}$, binary diffusivity [m^2 s^{-1}], Eq. (1) describes ordinary diffusion of the chemical species A in a binary mixture A+B with constant total concentration $c = c_A + c_B$. This equation was first derived by Fick. A more general form would involve the chemical potential of the species [10] but this approximation still describes a wide field of applications. For example, a

classical problem in Metallurgy is the estimate of the decarburization depth in steel [11]. A variant of the diffusion PDE is also used in Nuclear Reactor Physics to model neutron density in the one-speed approximation [12].

- $u = \psi$, probability density function of the velocity of a particle and D, diffusion coefficient. This is known as the Fokker-Planck equation with zero drift coefficient [13]. It is interesting to note that this equation has been recently applied beyond Physics to study the volatility in financial markets [14].

A classical problem is the determination of $u = u(x,t)$ in a half space $(x > 0)$, initially at a uniform value u_0 with the interface subjected to a first kind boundary condition for $t > 0$ (Dirichelet's problem). The differential problem is stated as

$$\frac{\partial u}{\partial t} = D \cdot \frac{\partial^2 u}{\partial x^2} \qquad \{x > 0\} \times \{t > t_0\} \tag{2a}$$

$$u = u_0 \qquad \{x > 0\} \times \{t = t_0\} \tag{2b}$$

$$u = u_i(t) \qquad \{x = 0\} \times \{t > t_0\} \tag{2c}$$

$$u \to u_0 \qquad \{x \to +\infty\} \times \{t > t_0\} \tag{2d}$$

It is convenient to set $u_0 = 0$ (note that if u is a solution, $u + u_0$ is a solution as well) and $t_0 = 0$ conventionally.

3 General Solution by Means of Fourier Analysis

The problem is approached by the Fourier analysis [15]. At first, we consider the Fourier transform of Eq. (2c) with respect to time

$$U(x = 0, \omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u(x = 0, t) \exp(-i\omega t) dt \tag{3}$$

where ω is the angular frequency [rad s^{-1}]. On the other hand, $u(x = 0, t)$ is recovered by the antitransform

$$u(x = 0, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} U(x = 0, \omega) \exp(i\omega t) d\omega \tag{4}$$

Notice that Eqs. (3) and (4) have the same coefficient $(2\pi)^{-1/2}$. However, different choices are possible. The reader is referred to Appendix A for a brief discussion on this subject.

The variable separation method is applied to Eq. (2a) looking for particular solutions in the form

$$u(x,t) = X(x)\exp(i\omega t) \tag{5}$$

as suggested by the integrand in Eq. (4).

Replacing in Eq. (2a) and dividing both members by $\exp(i\omega t)$, an ordinary differential equation is obtained:

$$\frac{d^2X}{dx^2} - \frac{i\omega}{D}X = 0 \tag{6}$$

The characteristic equation associated to Eq. (6) is

$$\beta^2 - \frac{i\omega}{D} = 0 \tag{7}$$

giving

$$\beta = \pm\sqrt{\frac{i\omega}{D}} \tag{8}$$

which is often called wavenumber [16] [rad m^{-1}].

Hence, the general solution of Eq. (6) turns out to be

$$X(x) = C^+(\omega)\exp\left(\sqrt{\frac{i\omega}{D}}x\right) + C^-(\omega)\exp\left(-\sqrt{\frac{i\omega}{D}}x\right) \tag{9}$$

Replacing in Eq. (5)

$$u(x,t;\omega) = C^+(\omega)\exp\left(i\omega t + \sqrt{\frac{i\omega}{D}}x\right) + C^-(\omega)\exp\left(i\omega t - \sqrt{\frac{i\omega}{D}}x\right) \tag{10}$$

which is often called a thermal wave even though the second-order derivative with respect to time, characteristic of the wave equation, does not appear in Eq. (1). A thorough discussion about the concept of wave and thermal waves is given by Salazar [17].

The boundary conditions Eqs. (2c) and (2d) are applied to calculate the coefficients $C^+(\omega)$ and $C^-(\omega)$.

From Eq. (2c)

$$u(x=0,t;\omega) = \left[C^+(\omega) + C^-(\omega)\right]\exp(i\omega t) = U(\omega, x=0)\exp(i\omega t) \tag{11}$$

then

$$C^+(\omega) + C^-(\omega) = U(x=0,\omega) \tag{12}$$

From Eq. (2d)

$$\lim_{x\to+\infty} u(x,t;\omega) = 0 \tag{13}$$

Eq. (13) is applied under the assumption that D is real and positive. This requirement is actually a consequence of the second principle of thermodynamics. On the other hand, if D were imaginary Eq. (1) would turn into the well-known Schrödinger equation which does not describe diffusive transport, hence is not treated here.

If $\omega > 0$, recalling that

$$\sqrt{\frac{i\omega}{D}} = (1+i)\sqrt{\frac{\omega}{2D}} \tag{14}$$

Eq. (10) becomes

$$\begin{aligned} u(x,t;\omega) = {} & C^{+}(\omega)\exp\left[i\left(\omega t + \sqrt{\frac{\omega}{2D}}x\right)\right]\exp\left(\sqrt{\frac{\omega}{2D}}x\right) \\ & + C^{-}(\omega)\exp\left[i\left(\omega t - \sqrt{\frac{\omega}{2D}}x\right)\right]\exp\left(-\sqrt{\frac{\omega}{2D}}x\right) \end{aligned} \tag{15}$$

Passing to the limit, Eq. (13), as u must be finite $C^{+}(\omega) = 0$ is obtained. Hence

$$u(x,t;\omega > 0) = U(x = 0, \omega > 0)\exp\left[i\omega t - (1+i)\sqrt{\frac{\omega}{2D}}x\right] \tag{16}$$

Repeating the same procedure for $\omega < 0$

$$u(x,t;\omega < 0) = U(x = 0, \omega < 0)\exp\left[-i|\omega|t - (1-i)\sqrt{\frac{|\omega|}{2D}}x\right] \tag{17}$$

If $\omega = 0$, Eq. (15) reduces to a constant that can be neglected as Eq. (2a) only contains derivatives of *u*.

A unique representation is obtained introducing the sign function, strictly related to the Heaviside step function as it will be shown in Section 5:

$$u(x,t;\omega) = U(x = 0, \omega)\exp\left\{i\omega t - [1 + i\cdot\operatorname{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\} \tag{18}$$

By integration over the angular frequency it is obtained

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} U(x = 0, \omega)\exp\left\{i\omega t - [1 + i\cdot\operatorname{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}d\omega \tag{19}$$

which, for $x = 0$, reduces to Eq. (4).

Finally, to eliminate the transformed function U it is convenient to express the boundary condition Eq. (2c) from Eq. (3) as follows

$$u(x,t)=\frac{1}{2\pi}\int_{\omega=-\infty}^{+\infty}\int_{t'=-\infty}^{+\infty}u(x=0,t')\exp\left\{i\omega(t-t')-[1+i\cdot\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}dt'd\omega \tag{20}$$

Handbooks usually report particular cases of Eq. (20). The reader should address in particular the book of Prestini [18] where the presented approach is developed in a less general way but with very interesting practical applications. Restricting the attention to the heat conduction problem, many authors deal with the cases of constant and periodic heating [19 - 26] though the general problem is not discussed in detail.

4 The Similarity Solution

Most of the cited bibliography directly refer to the similarity solution of (2a). Actually, dimensional analysis shows that the dependence on x and t is condensed in the combinations

$$B=\frac{x^2}{Dt}\quad\text{or}\quad\eta=\frac{x}{\sqrt{Dt}}=\sqrt{B} \tag{21}$$

The former is sometimes called the Boltzmann number, whereas the latter is simply known as the similarity variable. The physical meaning of B is discussed in Appendix B.

Generally speaking, similarity solutions are only a subset of the existing solutions. In this case, however, it can be shown that all the solutions are self-similar.

Adopting the Boltzmann number, the following identities hold

$$\frac{\partial B}{\partial t}=-\frac{B}{t}\quad\text{and}\quad\frac{\partial B}{\partial x}=\frac{2B}{x} \tag{22}$$

$$\frac{\partial u}{\partial t}=-\frac{B}{t}\frac{du}{dB} \tag{23}$$

$$\frac{\partial u}{\partial x}=\frac{2B}{x}\frac{du}{dB} \tag{24}$$

$$\frac{\partial^2 u}{\partial x^2}=\frac{2B}{x^2}\frac{du}{dB}+\frac{4B^2}{x^2}\frac{d^2u}{dB^2} \tag{25}$$

Hence, replacing in Eq. (2a), an ordinary differential equation is obtained:

$$\frac{d^2u}{dB^2} + \frac{2+B}{4B}\frac{du}{dB} = 0 \tag{26}$$

which is written as a first order equation setting $\dot{u} = du/dB$

$$\frac{d\dot{u}}{dB} + \frac{2+B}{4B}\dot{u} = 0 \tag{27}$$

Integration yields

$$\dot{u} = \frac{C_1}{\sqrt{B}\exp\left(\frac{B}{4}\right)} \tag{28}$$

Restoring $\dot{u} = du/dB$ and performing a second integration taking into account Eq. (21)

$$u = 2C_1 \int \exp\left(-\frac{\eta^2}{4}\right) d\eta + C_2 \tag{29}$$

The integral in Eq. (29) cannot be evaluated as a combination of elementary functions. It is a transcendental function as it is shown by the Liouville's theory [27].

It is customary to define the error function

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp\left(-x^2\right) dx \tag{30}$$

such that

$$erf(0) = 0 \quad \text{and} \quad \lim_{z \to +\infty} erf(z) = 1 \tag{31}$$

It is then obtained from Eq. (29)

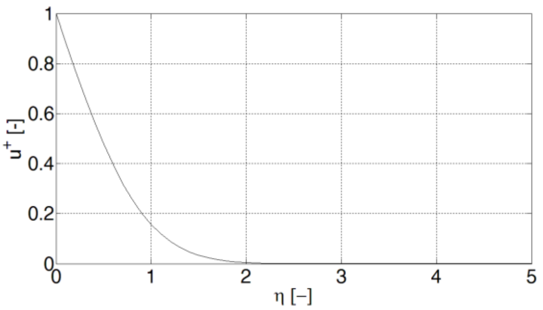
$$u = C_1' \operatorname{erf}\left(\frac{\eta}{2}\right) + C_2' \tag{32}$$

where multiplicative factors and additive constants have been lumped in C_1' and C_2' respectively.

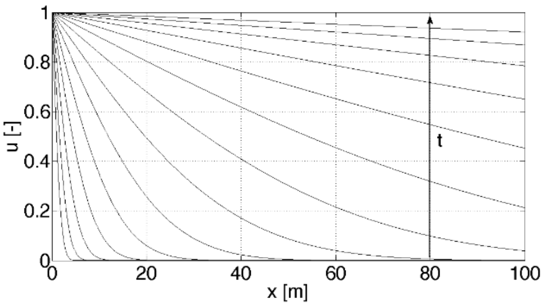
A particularly useful case study is obtained if Eq. (2c) is written as $t > 0, x = 0, u = 1$. This implies $C_2 = 1$ whereas the initial condition Eq. (2b) yields $C_1 = -1$ so that

$$u = 1 - \operatorname{erf}\left(\frac{\eta}{2}\right) \tag{33}$$

This is the response of the half-space to a step variation of u on its interface. Figures 1a and 1b report $u(\eta/2)$ and $u(x,t)$, respectively, to clarify the meaning of the term similarity. It is evident that each spatial distribution of u at a certain time instant is self-similar because, when reported in terms of the similarity variable η, all the distributions collapse into a unique curve.



(a)



(b)

Figure 1 – Response of the half-space to a step variation of u on its interface in terms of the similarity variable (a) and of the natural variables (b).

It is also evident that the diffusive transport described by (1) occurs instantaneously in contrast with the basic tenets of Special Relativity. Actually, since $u > 0 \ \forall(x,t)$, the propagation speed turns out to be infinite, meaning that the effect of a perturbation at the interface $x = 0$ is immediately felt at any distance from the interface. This is a theoretical problem arising from the constitutive equations relating the diffusive flux to the gradient of u, such as Fourier's law and Fick's first law. However, this effect is quite small in the most common situations and it is usually neglected [28].

To show that all the solutions of the problem defined by Eqs. (2a) to (2d) are self-similar, it is convenient to switch to a dimensionless formulation. Recalling the definition of the Boltzmann number, Eq. (21), characteristic time t_c and length L_c are chosen arbitrarily such that

$$\frac{L_c^2}{Dt_c} = 1 \tag{34}$$

As $t_c > 0$, $L_c = \sqrt{Dt_c}$ and, choosing u_c as a characteristic value of *u*, the following set of dimensionless quantities is identified

$$x^{+} = \frac{x}{L_c}, \quad t^{+} = \frac{t}{t_c}, \quad u^{+} = \frac{u}{u_c} \tag{35}$$

Replacing in Eqs. (2a) to (2d) the dimensionless problem results

$$\frac{\partial u^{+}}{\partial t^{+}} = \frac{\partial^2 u^{+}}{\partial x^{+2}} \quad \{x^{+} > 0\} \times \{t^{+} > 0\} \tag{36a}$$

$$u^{+} = 1 \quad \{x^{+} > 0\} \times \{t^{+} = 0\} \tag{36b}$$

$$u^{+} = u_i^{+}(t^{+}) \quad \{x^{+} = 0\} \times \{t^{+} > 0\} \tag{36c}$$

$$u^{+} \to 1 \quad \{x^{+} \to +\infty\} \times \{t^{+} > 0\} \tag{36d}$$

Hence, $u^{+} = u^{+}(x^{+}, t^{+}; u_i^{+})$ or $u = u_c \cdot u^{+}\left(x/\sqrt{Dt_c}, t/t_c; u_i/u_c\right)$, the latter showing that a double infinity of solutions is derived by choosing arbitrarily u_c and t_c, i.e. the set of all the solutions is split into two equivalence classes. As each class includes only self-similar solutions, all the possible solutions are self-similar.

At this point it is interesting to seek a general solution of problem defined by Eqs. (2a) to (2d) in the form of infinite series of particular solutions like Eq. (33) where self-similarity is evident rather than Eq. (20). In the following it is discussed the method for representing the new form of the solution and the equivalence with Eq. (20).

5 Integral Representations of the Dirac's δ Function and Heaviside's Step Applied to the Diffusion Problem

The Dirac's delta function is defined as [29]

$$\begin{aligned} &\delta(x) = 0, \quad x \in R \\ &\delta(0) = +\infty \\ &\int_{-\infty}^{+\infty} \delta(x)\,dx = 1 \end{aligned} \tag{37}$$

Accordingly, an important property is that any function $f(y)$ can be represented as

$$f(y) = \int_{-\infty}^{+\infty} f(x)\,\delta(y - x)\,dx \tag{38}$$

There are different representations [30] of such a function that today mathematicians prefer to call more properly a distribution. A useful one for the purpose of this paper is found in Mandl [31]

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(ixy) dy \tag{39}$$

The following developments justify this choice. Actually, if Eq. (3) is replaced in Eq. (4), it yields

$$u(x,t) = \frac{1}{2\pi} \int_{\omega=-\infty}^{+\infty} \int_{t'=-\infty}^{+\infty} u(x,t') \exp[i\omega(t-t')] dt' d\omega \tag{40}$$

On the other hand, according to Eq. (38)

$$u(x,t) = \int_{t'=-\infty}^{+\infty} u(x,t') \delta(t'-t) dt' \tag{41}$$

Comparing Eq. (40) and Eq. (41) it is seen that

$$\delta(t'-t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp[i\omega(t-t')] d\omega \tag{42}$$

which is equivalent to Eq. (39).

The Heaviside's step function is defined as [3]

$$H(t<0)=0, \quad H(t=0)=1/2, \quad H(t>0)=1 \tag{43}$$

The relation between H and the sign function used in Eq. (20) is formally expressed as

$$\operatorname{sgn}(t) = 2H(t) - 1 \tag{44}$$

The application of the step function usually requires, as seen for the Dirac's delta, suitable representations. For the purpose of this paper, it is convenient to use the following [32]:

$$H(t) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\exp(itz)}{z} dz \tag{45}$$

Considering Eq. (39) it can be shown that

$$\frac{dH(t)}{dt} = \delta(t) \tag{46}$$

which is more easily understood if H is thought as the limit of a ramp that rises from 0 to 1 about $t = 0$.

This relation is useful to transform Eq. (38) in another useful representation of any continuous function. Integrating by parts

$$\begin{aligned} f(t) &= \int_{-\infty}^{+\infty} f(t')\delta(t-t')dt' = -\int_{-\infty}^{+\infty} f(t')\frac{dH(t-t')}{d(t-t')}dt' = \\ &= -\left[f(t')H(t-t')\right]_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} H(t-t')\frac{df}{dt'}dt' = \\ &= f(-\infty) + \int_{-\infty}^{+\infty} H(t-t')\frac{df}{dt'}dt' \end{aligned} \tag{47}$$

The geometrical meaning of Eq. (47) is a representation of $f(t)$ as the superposition of elementary steps of height df (Duhamel's formula) [20].

Equation (47) is then applied to the solution of problem defined by Eqs. (2a) to (2d) as follows:

$$u(x=0,t) = u(0,-\infty) + \int_{-\infty}^{+\infty} H(t-t')\frac{\partial u(0,t')}{\partial t'}dt' \tag{48}$$

where $u(0,-\infty)=0$ since no perturbation is applied at the interface before the initial time. In any case, the value of $u(0,-\infty)$ would be only an additive constant. The same holds for $u(0,+\infty)$ since any physical perturbation has finite duration. The solution is then built as a continuous linear combination of the particular solution, Eq. (33), corresponding to the response of the half space to a constant perturbation at the interface, that is

$$u(x,t) = \int_{-\infty}^{+\infty} H(t-t')\frac{\partial u(0,t')}{\partial t'}\left\{1 - erf\left[\frac{x}{2\sqrt{D(t-t')}}\right]\right\}dt' \tag{49}$$

It is worthwhile noting that the argument of the error function is prevented from assuming imaginary values when $t<t'$ because, in this case, $H(t-t')=0$.

Equation (49) clearly shows that the diffusion process obeys to the principle of delayed causality. Actually, a generic boundary condition at the interface is decomposed as the superposition of elementary steps, the response to which is delayed by the time interval $t-t'$. Some attempts to modify the Fourier's law in order to prevent an infinite speed of propagation of the perturbations, as observed in the previous section, happened to violate the delayed causality principle [33].

6 Solution by Means of the Green's Function

The solution of Eq. (2a) in the same form as Eq. (20) is also obtained by means of the Green's function [34]. Since the derivation is less straightforward than making use of the Fourier's transform, only an outline will be given in the following. For this purpose, it is convenient to consider the inhomogeneous diffusion equation:

$$\frac{\partial u}{\partial t} - D \cdot \frac{\partial^2 u}{\partial x^2} = S(x,t) \tag{50}$$

where $S(t,x)$ physically represents a source term.

The Green's function $G(t,x)$ is the solution of Eq. (50) if

$$S(x,t) = \delta(x)\delta(t) = \delta^2(x,t) \tag{51}$$

under appropriate initial and boundary conditions, that is

$$\frac{\partial G}{\partial t} - D \cdot \frac{\partial^2 G}{\partial x^2} = \delta^2(x,t) \tag{52}$$

The relation between u and G is found as

$$u(x,t) = \int_{t'=-\infty}^{+\infty} \int_{x'=-\infty}^{+\infty} S(x',t')G(x-x',t-t')dx'dt' \tag{53}$$

The Green's function is determined as follows.
At first, $G(x,t)$ is written as Fourier's back-transform of $g(\beta,\omega)$:

$$G(x,t) = \frac{1}{(2\pi)^2} \int_{\omega=-\infty}^{+\infty} \int_{\beta=-\infty}^{+\infty} g(\beta,\omega)\exp[i(\omega t + \beta x)]d\beta d\omega \tag{54}$$

Then the partial derivatives that appear in Eq. (52) result respectively

$$\frac{\partial G}{\partial t} = \frac{1}{(2\pi)^2} \int_{\omega=-\infty}^{+\infty} \int_{\beta=-\infty}^{+\infty} i\omega g(\beta,\omega)\exp[i(\omega t + \beta x)]d\beta d\omega \tag{55}$$

$$\frac{\partial^2 G}{\partial x^2} = \frac{1}{(2\pi)^2} \int_{\omega=-\infty}^{+\infty} \int_{\beta=-\infty}^{+\infty} -\beta^2 g(\beta,\omega)\exp[i(\omega t + \beta x)]d\beta d\omega \tag{56}$$

Furthermore, from Eq. (39) it is found

$$\delta^2(x,t) = \frac{1}{(2\pi)^2} \int_{\omega=-\infty}^{+\infty} \int_{\beta=-\infty}^{+\infty} \exp[i(\omega t + \beta x)]d\beta d\omega \tag{57}$$

Replacing Eqs. (55), (56) and (57) in Eq. (52) the Fourier's back-transform of the Green's function results

$$g(\beta,\omega) = \frac{1}{i\omega - D\beta^2} \tag{58}$$

Hence, from Eq. (54)

$$G(x,t)=\frac{1}{(2\pi)^2}\int_{\omega=-\infty}^{+\infty}\int_{\beta=-\infty}^{+\infty}\frac{\exp[i(\omega t+\beta x)]}{i\omega-D\beta^2}d\beta d\omega \tag{59}$$

which is more conveniently rewritten as

$$G(x,t)=\frac{1}{(2\pi)^2}\int_{\omega=-\infty}^{+\infty}\exp(i\omega t)I(x,\omega)d\omega \tag{60}$$

with

$$I(x,\omega)=\int_{\beta=-\infty}^{+\infty}\frac{\exp(i\beta x)}{i\omega-D\beta^2}d\beta \tag{61}$$

Integration is performed by means of the residuals theorem and the Jordan's lemma in the complex plane along the loop depicted in Figure 2. The integration loop is suitably selected so that, when $R_l \to +\infty$, only the contribution along the diameter (which extends to the whole real axis) is different from zero, as a consequence of the Jordan's lemma.

The integrand poles are:

$$\begin{cases} P(\omega>0)=(\pm 1\pm i)\sqrt{\dfrac{|\omega|}{2D}} \\ P(\omega<0)=(\pm 1\mp i)\sqrt{\dfrac{|\omega|}{2D}} \end{cases} \tag{62}$$

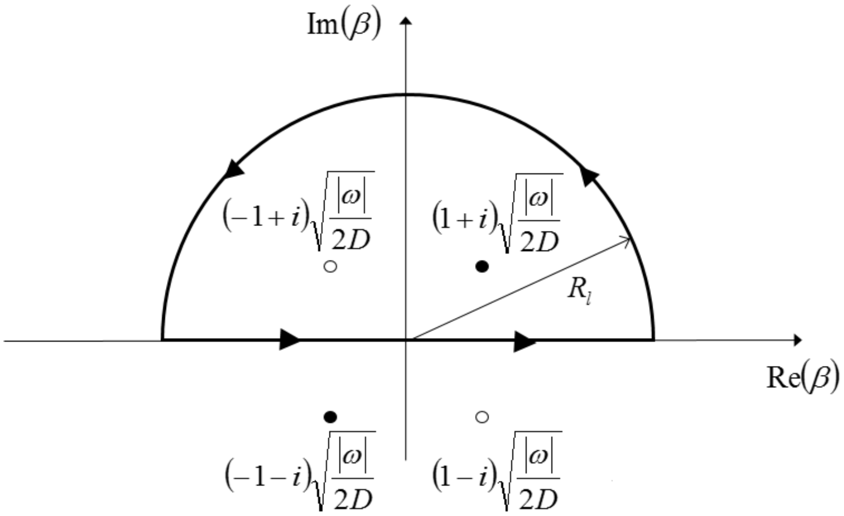


Figure 2 – Integration loop and poles of the integrand for Eq. (61). Black dots represent the poles for $\omega>0$, the white ones for $\omega<0$.

As $R_l \to +\infty$ the integration loop only includes two poles, one for $\omega > 0$ and the other for $\omega < 0$, which are unified by the sign function:

$$P = \mathrm{sgn}(\omega)[1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}} \tag{63}$$

The residual is then

$$R = \lim_{\beta \to P}(\beta - P)\frac{\exp(i\beta x)}{i\omega - D\beta^2} = -\frac{\exp\left\{[-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}}{[\mathrm{sgn}(\omega) + i]\sqrt{\frac{2|\omega|}{D}}} \tag{64}$$

Hence, the residuals theorem allows writing

$$I(x,\omega) = \frac{2\pi \exp\left\{[-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}}{[-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{2|\omega|}{D}}} \tag{65}$$

Finally, replacing Eq. (65) in Eq. (60)

$$G(x,t) = \frac{1}{2\pi}\int_{\omega=-\infty}^{+\infty} \frac{\exp\left\{i\omega t + [-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}}{[-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{2|\omega|}{D}}} d\omega \tag{66}$$

The partial derivative of Eq. (66) with respect to x

$$\frac{\partial G}{\partial x} = \frac{1}{4\pi}\int_{\omega=-\infty}^{+\infty} \exp\left\{i\omega t + [-1 + i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\} d\omega \tag{67}$$

coincides with Eq. (20) if the boundary condition is set as

$$u(x = 0, t) = \frac{\delta(t)}{2} \tag{68}$$

Actually, replacing Eq. (68) in Eq. (20) it follows

$$u(x > 0, t) = \frac{1}{4\pi}\int_{\omega=-\infty}^{+\infty} \exp\left\{i\omega t + [-1 - i\,\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\} d\omega \tag{69}$$

Despite the different sing in the square brackets, Eqs. (67) and (69) describe the same scalar field: it is sufficient to replace simultaneously ω with $-\omega$ and t with $-t$.

In summary, it has been shown that the solution of Eq. (2a) with the boundary condition Eq. (68) is equivalent to the solution of Eq. (52). In other words, through the Green's function the solution of the homogeneous diffusion equation is derived from the inhomogeneous one endowed with a suitable source term.

7 Equivalence of the General Solutions by Means of the Square Completion Method

Apparently, the two general solutions developed in Sections 3 and 5, respectively, are quite different. In particular, Eq. (20) involves two improper integrals whereas only one appears in Eq. (49); Eq. (20) involves complex functions, whereas Eq. (49) is restricted to the real field; Eq. (20) involves the boundary condition $u(0,t')$, whereas its derivative with respect to time appears in Eq. (49). Nevertheless, the boundary value problems involving Eq. (1) do have a unique solution [19] so that Eq. (20) and Eq. (49) must be equivalent. The proof of equivalence is given in the following.

Equation (20) is written as

$$u(x,t)=\frac{1}{2\pi}\int_{\omega=-\infty}^{+\infty}\left\{\int_{t'=-\infty}^{+\infty}u(x=0,t')\exp[i\omega(t-t')]dt'\right\}\exp\left\{-[1+i\cdot\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}d\omega \tag{70}$$

The inner integral is solved by parts considering that $u(x=0,t'\to-\infty)=u(x=0,t'\to+\infty)=0$

$$\int_{t'=-\infty}^{+\infty}u(x=0,t')\exp[i\omega(t-t')]dt'=\frac{1}{i\omega}\int_{-\infty}^{+\infty}\frac{\partial u(x=0,t')}{\partial t'}\exp[i\omega(t-t')]dt' \tag{71}$$

Replacing in Eq. (70)

$$u(x,t)=\int_{t'=-\infty}^{+\infty}\frac{1}{2\pi i}\int_{\omega=-\infty}^{+\infty}\frac{\exp[i\omega(t-t')]}{\omega}\exp\left\{-[1+i\cdot\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}d\omega\frac{\partial u(x=0,t')}{\partial t'}dt' \tag{72}$$

Comparison between Eq. (49) and Eq. (72) shows that their equivalence would imply

$$\begin{aligned}&H(t-t')\left\{1-erf\left[\frac{x}{2\sqrt{D(t-t')}}\right]\right\}=\\&=\frac{1}{2\pi i}\int_{\omega=-\infty}^{+\infty}\frac{\exp[i\omega(t-t')]}{\omega}\exp\left\{-[1+i\cdot\mathrm{sgn}(\omega)]\sqrt{\frac{|\omega|}{2D}}x\right\}d\omega\end{aligned} \tag{73}$$

Denoting the left hand side as M_1 and the right hand side as M_2, both are rewritten eliminating $H(\cdot)$ and $\operatorname{sgn}(\cdot)$

$$M_1 = \frac{2}{\sqrt{\pi}} \int_{x/\left[2\sqrt{D(t-t')}\right]}^{+\infty} \exp\left(-\eta^2\right) d\eta \tag{74}$$

$$M_2 = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{1}{\omega} \exp\left\{ i\omega(t-t') - \sqrt{\frac{i\omega}{D}}x \right\} d\omega \tag{75}$$

It will be shown that

$$\frac{\partial M_1}{\partial x} = \frac{\partial M_2}{\partial x} \tag{76}$$

which implies $M_1 = M_2$ apart from an integration constant that is equal to zero according to the initial condition Eq. (2b).

From the Leibnitz formula

$$\frac{\partial M_1}{\partial x} = -\frac{1}{\sqrt{\pi D(t-t')}} \exp\left\{ -\frac{x^2}{4D(t-t')} \right\} \tag{77}$$

$$\frac{\partial M_2}{\partial x} = -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \sqrt{\frac{i}{\omega D}} \exp\left\{ i\omega(t-t') - \sqrt{\frac{i\omega}{D}}x \right\} d\omega \tag{78}$$

The latter expression is manipulated as first by applying to the argument of the exponential the square completion method [35], widely used in Quantum Field Theory to compute path integrals [5], [36].

$$i\omega(t-t') - \sqrt{\frac{i\omega}{D}}x = \left[\sqrt{i\omega(t-t')} - \frac{x}{2\sqrt{D(t-t')}} \right]^2 - \frac{x^2}{4D(t-t')} \tag{79}$$

Hence

$$\frac{\partial M_2}{\partial x} = -\frac{1}{2\pi i} \exp\left\{ -\frac{x^2}{4D(t-t')} \right\} \int_{-\infty}^{+\infty} \sqrt{\frac{i}{\omega D}} \exp\left\{ \left[\sqrt{i\omega(t-t')} - \frac{x}{2\sqrt{D(t-t')}} \right]^2 \right\} d\omega \tag{80}$$

The integral in Eq. (80) is solved by substitution setting

$$y = \sqrt{i\omega(t-t')} - \frac{x}{2\sqrt{D(t-t')}} \tag{81}$$

Hence

$$\int_{-\infty}^{+\infty} \sqrt{\frac{i}{\omega D}} \exp\left\{\left[\sqrt{i\omega(t-t')} - \frac{x}{2\sqrt{D(t-t')}}\right]^2\right\} d\omega = \frac{2}{\sqrt{D(t-t')}} \int_{-\infty}^{+\infty} \exp\left(y^2\right) dy \tag{82}$$

Further replacing $y^2 = -\frac{z^2}{2}$ implying $dy = -\frac{\sqrt{2}}{2i} dz$

$$\int_{-\infty}^{+\infty} \exp\left(y^2\right) dy = -\frac{\sqrt{2}}{2i} \int_{-\infty}^{+\infty} \exp\left(-\frac{z^2}{2}\right) dz \tag{83}$$

It is known [36] that

$$\int_{-\infty}^{+\infty} \exp\left(-\frac{z^2}{2}\right) dz = \sqrt{2\pi} \tag{84}$$

Incidentally, it is worthwhile mentioning that the first mathematician who studied the so-called Gaussian integrals was not Gauss but De Moivre in 1733 [37].

Replacing Eqs. (62) to (64) in Eq. (80) yields, finally

$$\frac{\partial M_2}{\partial x} = -\frac{1}{\sqrt{\pi D(t-t')}} \exp\left\{-\frac{x^2}{4D(t-t')}\right\} = \frac{\partial M_1}{\partial x} \tag{85}$$

The equivalence of Eq. (20) and Eq. (49) is then proven thanks to the decisive resort to the square completion method, just as in many gaussian-like integrals found in the path integral approach to Quantum Field Theory.

Appendix A

A few not quite trivial aspects about the Fourier transform require explanation to avoid misunderstanding. Eqs. (3) and (4) represent, respectively, the Fourier transform and the inverse Fourier transform of a function $u(t)$. However, this representation is not unique, as different choices of the coefficients are possible [18] provided that their product is $(2\pi)^{-1}$. In this paper the symmetric representation is used, i.e., both the coefficients are set equal to $(2\pi)^{-1/2}$, but it is also common to find the anti-symmetric convention, where the factor $(2\pi)^{-1}$ only appears in the inverse Fourier transform. On the other hand, this requirement on the coefficients could even be removed, as shown in James [38]. The preface of this book introduces the subject of Fourier's analysis with this witty remark: "Showing a Fourier transform to a physics student generally produces the same reaction as showing a crucifix to Count Dracula". An interesting historical overview of the Fourier Transform is given by Bracewell [39].

Appendix B

Dimensional analysis is probably the easiest way to define the Boltzmann number. Nevertheless, its physical meaning is better understood considering diffusion at a molecular scale and introducing the concept of random walk [40].

Consider a particle of a species A that diffuses through a substance B undergoing a random walk described by a broken line $P_0P_1P_2P_3...$ where points P_0, P_1, P_2, P_3... correspond to the particle random strikes. Neither the location of the points nor the length of the vector paths $\overrightarrow{P_0P_1}, \overrightarrow{P_1P_2}, \overrightarrow{P_2P_3}...$ can be predicted. However, if the random walk is made of a very large number of paths, some general property is statistically inferred. The final position P_N is related to the starting point P_0 by the relation

$$\overrightarrow{P_0P_N} = \sum_{n=1}^{N} \overrightarrow{P_{n-1}P_n} \tag{B1}$$

The absolute value of the overall path length is given by

$$\left|\overrightarrow{P_0P_N}\right|^2 = \overrightarrow{P_0P_N} \cdot \overrightarrow{P_0P_N} \tag{B2}$$

The scalar product in Eq. (B2) is a summation of N^2 terms that comprises two subsets. The first one if formed by N terms referring to the scalar product of a vector by itself. If $N \to +\infty$ the average value

$$\frac{1}{N}\sum_{n=1}^{N}\left|\overrightarrow{P_{n-1}P_n}\right|^2 = L^2 \tag{B3}$$

is interpreted as the square of a random walk characteristic length. Similarly, it is defined an average time interval Δt between two successive strikes such that the final position P_N is reached after the time

$$T(N) = N\Delta t \tag{B4}$$

The second subset contains the remaining $N^2 - N$ terms that are scalar products of couples of vectors $\overrightarrow{P_{n-1}P_n}$ with different indices. Due to the random nature of the particle motion, these vectors are uncorrelated both in direction and in absolute value, thus for $N \to +\infty$ their contribution is negligible. Consequently, from Eqs. (B3) and (B4), Eq. (B2) becomes

$$\left|\overrightarrow{P_0P_N}\right|^2 = NL^2 = T\frac{L^2}{\Delta t} \tag{B5}$$

This result is written in a more interesting form as

$$\frac{\left|\overrightarrow{P_0P_N}\right|^2}{T\,\dfrac{L^2}{\Delta t}} = 1 \tag{B6}$$

where the left hand term shows the same form of the Boltzmann number Eq. (21) through the correspondences between $\left|\overrightarrow{P_0P_N}\right|^2$ and x^2, T and t, $\dfrac{L^2}{\Delta t}$ and D.

This heuristic argument is also useful to understand the microscopic origin of irreversibility: at each interaction of the particle, any information about the previous one is lost, hence diffusion cannot be inverted. A recent paper by Brazzle [41] discusses a pedagogical method to simulate diffusion by means of spreadsheet computation, which is widely available. Actual random walks are built on a variety of lattices. However the easiest method remains the one followed by Gautreau [40].

References

[1] R.P. Feynman, A. R. Hibbs, *Quantum Mechanics and Path Integrals*, Emended Edition by F. D. Styer, Dover Publications Inc., New York, 2010, p. 58 and p. 359.

[2] B. A. Baaquie, *Path Integrals and Hamiltonians: Principles and Methods*, Cambridge University Press, Cambridge, 2014, p. 130.

[3] A. Zee, *Quantum Field Theory in a Nutshell*, Princeton University Press, Princeton, 2010, p. 23.

[4] M. Slutsky, Diffusion in a half - space: From Lord Kelvin to path integrals, *Am. J. Phys.* **73(4)** (2005), 308 - 314.

[5] L. S. Schulman, *Techniques and Applications of Path Integration*, John Wiley & Sons, New York, 2005, p. 332.

[6] S. Carrà, *Struttura e stabilità: introduzione alla Termodinamica dei materiali*, Mondadori, Milano, 1978, p. 214 (in Italian).

[7] B. C. Hall, *Quantum Theory for Mathematicians*, Springer - Verlag, New York, 2013, ch. 20.

[8] S. J. Farlow, *Partial Differential Equations for Scientists and Engineers*, Dover Publications, New York, 1993, p. 11.

[9] J. B. J. Fourier, *Théorie Analytique de la Chaleur*, Firmin Didot & Garçons, Paris, 1822, reprinted from the original by Editions Jacques Gabay, Scéaux (1988); the English translation, entitled “The Analytical Theory of Heat”, first appeared in 1878, has been reprinted in 2009 by Cambridge University Press.

[10] D. Kondepudi, Prigogine I, *Modern Thermodynamics: From Heat Engines to Dissipative Structures*, John Wiley and Sons, West Sussex, 1988, p. 270.

[11] B. Liščić, *Steel Heat Treatment in Steel Heat Treatment Metallurgy and Technologies* edited by G.E. Totten, CRC Press, Boca Raton, 2006, ch 6.

[12] M. S. Weston, *Nuclear Reactor Physics*, Wiley - VCH, Weinheim, 2007, p. 43.

[13] L. D. Landau, E.M. Lifsits, *Course of Theoretical Physics: Volume 10*, Pergamon Press, Oxford, 1981, p. 89.

[14] E. Haven, A. Khrennikov, *Quantum Social Science*, Cambridge University Press, Cambridge, 2013, p. 40.

[15] M. R. Spiegel, *Fourier Analysis with Applications to Boundary Value Problems*, McGraw - Hill, New York, 1974, p. 81.

[16] H. J. Pain, *The Physics of Vibrations and Waves*, 5th Edition, John Wiley and Sons, West Sussex, 2005, p. 120.

[17] A. Salazar, Energy Propagation of Thermal Waves, *Eur. J. Phys.*, **27** (2006), 1349 - 1355.

[18] E. Prestini, *The Evolution of Applied Harmonic Analysis: Models of the Real World*, Birkhauser, Boston, 2004.

[19] H. S. Carslaw, J.C Jaeger., *Conduction of Heat in Solids*, Clarendon Press, Oxford, 1959, p. 51.

[20] M. N. Ozisik, D.W. Hahn, *Heat Conduction*, 3rd Edition, John Wiley and Sons, New Jersey, 2012, p. 236.

[21] L. M. Jiji, *Heat Conduction*, Jaico Pubishing House, Mumbai, 2003, p. 104.

[22] M. Moares, Time Varying Heat Conduction in Solids, in *Heat Condution: Basic Research*, edited by V. S. Vikhrenko, InTech, Croazia, 2011.

[23] W. M. Rohsenow, J. R. Hartnett, Y.I. Cho, *Handbook of Heat Transfer*, McGraw - Hill, New York, 1998.

[24] F. Kreith, R. M. Manglik, M.S. Bohn, *Principles of Heat Transfer*, 7th Edition, Cengage Learning, Australia, 2011.

[25] T. L. Bergmann, A. S. Lavine, F.P. Incropera, D. P. Dewitt, *Introduction to Heat Transfer*, 7th Edition, John Wiley and Sons, West Sussex, 2011, p. 327.

[26] A. Bejan, *Heat Transfer*, John Wiley and Sons, 1993, p.148.

[27] J. F. Ritt, *Integration in Finite Terms: Liouville's Theory of Elementary Methods*, Columbia University Press, New York, 1948, p. 49.

[28] A. N. Smith, P.M. Norris, Microscale Heat Transfer, in *Heat Transfer Handbook*, edited by A. Bejan and A. D. Kraus, John Wiley and Sons, Hoboken, 2003, p. 1331.

[29] P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th Edition, Oxford University Press, Oxford, 1968.

[30] B. R. Kusse, *Mathematical Physics: Applied Mathematics for Scientists and Engineers*, Wiley-VCH, 2006, ch. 5.

[31] F. Mandl, Quantum Mechanics, in *The Manchester Physics Series*, John Wiley and Sons, West Sussex, 1997.

[32] V. I. Smirnov, *A Course of Higher Mathematics: Advanced calculus*, Pergamon Press, Oxford, 1964.

[33] M. Ferenc, Can a Lorentz Invariant Equation Describe Thermal Energy Propagation Problems?, in *Heat Condution: Basic Research*, edited by V. S. Vikhrenko, InTech, Croazia, 2011.

[34] L. D. Landau and E. M. Lifshits, *Course of Theoretical Physics: Volume 9*, Pergamon Press, Oxford, 1981, p. 28.

[35] J. E. Kaufmann, K. L. Schwitters, *Elementary Algebra*, 8th Edition, Thomson Brooks/Cole, Canada, 2007, p. 433.

[36] S. Weinberg, *The Quantum Theory of Fields*, Cambridge University Press, Cambridge, 1995, vol. 1, p. 421.

[37] U. C. Merzbach and C. B. Boyer, *A History of Mathematics*, 3rd edition, John Wiley and Sons, New Jersey, 2011, p. 374.

[38] J. F. James, *A Student's Guide to Fourier Transforms With Applications in Physics and Engineering*, Cambridge University Press, Cambridge, 2002, p. 9.

[39] R. N. Bracewell, The Fourier's Transform, *Sci. Am.*, **6** (1989), 62.

[40] R. Gautreau, W. Savin, *Modern Physics*, 2nd Edition, McGraw-Hill, New York, 1999, p. 263.

[41] B. Brazzle, A Random Walk to Stochastic Diffusion through Spreadsheet Analysis, *Am. J. Phys.*, **81(11)** (2013), 823 - 828.

Received: September 11, 2014; Published: November 3, 2014