Journal of Engineering Mathematics **24**: 213–236 1990.

On the large-time asymptotics of the diffusion equation on infinite domains

R.C. KLOOSTERZIEL

*Institute of Meteorology and Oceanography, University of Utrecht, Princetonplein 5, 3584 CC Utrecht, The Netherlands**

Received 10 October 1989; accepted 27 November 1989

Abstract. It is shown that expansions in similarity solutions provide a quick and economical method for assessing the large-time asymptotics of the diffusion equation on infinite and certain semi-infinite domains if Dirichlet or Neumann conditions are imposed. The similarity solutions are shown to form a basis for the Hilbert space $L^2(\mathbf{R}^n, e^{\frac{1}{4}|x|^2})$. This implies that initial conditions for the diffusion equation that are square integrable with respect to the exponentially-growing weight function $e^{\frac{1}{4}|x|^2}$ can be expanded in a discrete, infinite sum of mutually orthogonal similarity solutions, each having a different rate of amplitude decay. This leads to a rapid, almost effortless recognition of the large-time asymptotic behaviour of the solution.

1. Introduction

This paper studies the large-time asymptotic behaviour of solutions of the diffusion equation on infinite and semi-infinite domains. On finite domains of simple geometry, the large-time asymptotic structure of the evolving field is usually determined by the eigenfunctions of the Laplace operator with the smallest eigenvalues that fit in the domain. If initial conditions can be expanded on a basis of such eigenfunctions, it is the slowest-decaying mode in the expansion spectrum, the one with the smallest eigenvalue or largest wavelength, that becomes dominant as time increases. Initial conditions can be classified then by the smallest eigenvalue occurring in the spectrum. Two initial conditions belonging to such a class will asymptotically 'look alike'. On infinite and semi-infinite domains no such 'longest wavelength' exists – a continuous spectrum is found in such cases (if an expansion is sought in eigenfunctions of the Laplace operator) – and it is not clear at all whether in general two different initial conditions can be predicted to evolve towards the same decaying spatial structure or not.

The equation of diffusion in a homogeneous isotropic medium studied here is

$$\frac{\partial C}{\partial t} = D \sum_{i=1}^{n} \frac{\partial^2 C}{\partial x_i^2} \quad (n = 1, 2 \text{ or } 3) \tag{1}$$

where C is the concentration of the diffusing 'substance' at the point $\mathbf{x} = (x_1, \ldots, x_n)$ (in rectangular coordinates) at time t, and D the diffusion coefficient for the particular case considered. In kinetic theory the diffusion equation governs the flow of fluid matter in another medium due to random molecular motion (see [1]), and in fluid mechanics it describes the evolution of the vorticity of certain vortices with D then being the kinematic viscosity of the fluid (see [2]). In a conducting solid the local rate of change of temperature is

* Present address: Institute for Nonlinear Science (INLS), La Jolla, California 92093, U.S.A.

also governed by (1) – in that context it is usually called the heat equation. Several other areas of research in which the diffusion equation has been found important are either listed or referred to by Carslaw and Jaeger [3].

In the theory of heat conduction a typical problem is the following. Let a solid conductor occupy a singly connected closed domain $\Omega \subset \mathbf{R}^n$ that is bounded by a regular surface $\partial\Omega$. For a given initial temperature distribution $C(\mathbf{x}; t=0) \equiv C^0(\mathbf{x})$ the evolution $C(\mathbf{x}; t)$ is asked to be determined for all $t > 0$. Some appropriate boundary conditions necessarily supplement this problem. If the solid is imagined to be surrounded by insulating material say, the boundary condition is that of zero heat flux across the surface $\partial\Omega$, i.e. $\partial C/\partial \mathbf{n} = 0$ where $\mathbf{n}$ denotes the outward normal on $\partial\Omega$ (Neumann condition). Another condition could be that of constant surface temperature, that is $C(\mathbf{x}; t) = \text{constant}$ for all $\mathbf{x} \in \partial\Omega$ (Dirichlet condition). Both types of boundary conditions make the task of solving (1), which is of parabolic type, a well-posed problem with a unique solution (see [4]: in the case of a Neumann problem it is of course unique only up to a constant). The simplest case imaginable concerns a slab of conducting material between $x_1 = 0$ and $x_1 = l$ with no dependence on the other coordinates x_2 and x_3. With some mild restrictions imposed on the allowed initial conditions, a Fourier-series expansion will be sought. Assuming for example both ends to be kept at zero temperature, the initial temperature distribution is expanded in a sine-series (the index 1 is dropped momentarily for convenience)

$$C^0(x) = \sum_{n=1}^{\infty} a_n \sin \lambda_n x$$

where

$$a_n = \frac{2}{l} \int_0^1 C^0(x) \sin \lambda_n x \, dx$$

and

$$\lambda_n = \frac{n\pi}{l} \quad (n = 1, 2, 3, \ldots) .$$

The solution of (1) that satisfies the boundary condition at all times is

$$C(x; t) = \sum_{n=1}^{\infty} a_n \, e^{-\lambda_n^2 D t} \sin \lambda_n x \quad (t > 0)$$

(see [3] for a rigorous discussion of this example and many others). A convenient way of writing this result is

$$C(x; t) = \sum_{n=1}^{\infty} A_n(t) \sin \lambda_n x$$

with

$$A_n(t) = a_n \, e^{-\lambda_n^2 D t} .$$

It is seen that for each n the amplitude $A_n(t)$ in the point-spectrum decays exponentially. Moreover, an ordening is apparent, that is, if $m > n$ then $\lim_{t\to\infty} A_m/A_n = 0$ (assuming

$A_n(0) \neq 0$). The usual norm $\|\cdots\|$, defined by $\|f-g\| = \{\int_0^l |f-g|^2 \, dx\}^{\frac{1}{2}}$, is convenient for expressing the large-time asymptotic behaviour of the solution. If m is the smallest integer for which $a_m \neq 0$, one has

$$\|C(x;t) - a_m \, e^{-\lambda_m^2 Dt} \sin \lambda_m x\| \leq e^{-\lambda_{m+k}^2 Dt} \|C^0(x) - a_m \sin \lambda_m x\| ,$$

where $m + k > m$ (and $\lambda_{m+k}^2 > \lambda_m^2$). If this is multiplied by a factor $e^{\lambda_m^2 Dt}$ one finds

$$\|C(x;t) \, e^{\lambda_m^2 Dt} - a_m \sin \lambda_m x\| \leq e^{-(\lambda_{m+k}^2 - \lambda_m^2)Dt} \|C^0(x) - a_m \sin \lambda_m x\|$$

so,

$$\lim_{t \to \infty} \|C(x;t) \, e^{\lambda_m^2 Dt} - a_m \sin \lambda_m x\| = 0 .$$

It is seen therefore that for increasing time the solution gets closer and closer to an exponentially decaying, single sinusoidal structure. One could put it as

$$\lim_{t \to \infty} C(x;t) = a_m \, e^{-\lambda_m^2 Dt} \sin \lambda_m x ,$$

although this may look a little strange. In order to discover the large-time asymptotic behaviour the solution has to be 'blown up' because it is continuously diminishing in amplitude. Note that from

$$\lim_{t \to \infty} \|C(x;t) - a_m \, e^{-\lambda_m^2 Dt} \sin \lambda_m x\| = 0$$

nothing can be inferred about the large-time structure of the solution: it merely shows that the solution asymptotically has a vanishing amplitude. The ordering in decay rates of the amplitudes in the spectrum corresponds to the well-known feature of diffusive-like processes that small-scale irregularities in the initial state (corresponding to the higher-wavenumber components in the Fourier expansion) are 'ironed out' with increasing time.

Similar results hold for higher-dimensional domains of simple geometry and finite extent if initial conditions can be expanded in eigenfunctions of the Laplace operator. With boundary conditions as mentioned above, due to the finiteness of the domain the eigenvalues that determine the decay-rate of the corresponding mode take discrete values (the λ_n's in the one-dimensional example) and the asymptotic time-dependent structure towards which the initial field will evolve is easily determined. In infinite domains things are different, however. Instead of a discrete spectrum there will be a continuous spectrum of eigenfunctions of the Laplace operator. If, for example, one lets $l \to \infty$ while retaining the boundary condition at $x = 0$, under some mild restrictions imposed on the initial conditions, a Fourier transform can be found (see [3])

$$C(x;t) = \sqrt{\frac{2}{\pi}} \int_0^\infty a(\lambda) \, e^{-\lambda^2 Dt} \sin \lambda x \, dx$$

where

$$a(\lambda) = \sqrt{\frac{2}{\pi}} \int_0^\infty C^0(x) \sin \lambda x \, dx .$$

In this case an exponentially decaying continuous spectrum $A_\lambda(t) = a(\lambda)\,\mathrm{e}^{-\lambda^2 Dt}$ is found. No 'slowest decaying' mode is recognizable with this representation of the time-dependent solution of the diffusion equation.

In this paper it will be shown that, if one slightly restricts the allowed initial conditions, general asymptotics again do exist on infinite domains. One needs a denumerable set of solutions of the diffusion equation $C_n(\mathbf{x}; t)$ that can be ordered according to their rate of decay

$$\lim_{t\to\infty} C_m(\mathbf{x}; t)/C_n(\mathbf{x}; t) = 0$$

for all $m > n$, and such that an initial condition can be expanded in a sum of these solutions, giving the evolution in the form $C(\mathbf{x}; t) = \Sigma_n\, a_n C_n(\mathbf{x}; t)$. Such functions are provided for by a certain class of similarity solutions of the diffusion equation as will be shown below. Before proceeding, however, it will be convenient to non-dimensionalize (1). From hereon $\mathbf{x}$ and t will denote the dimensionless position vector $\mathbf{x} = \mathbf{x}/L$ and time $t = Dt/L^2$ where L is an arbitrary lengthscale. After substitution the following non-dimensional form of the diffusion equation is found

$$\frac{\partial C}{\partial t} = \sum_{i=1}^{n} \frac{\partial^2 C}{\partial x_i^2} \quad (n = 1, 2, \text{ or } 3) \tag{2}$$

where C has been scaled with an amplitude of appropriate dimension. In the sequel the diffusion equation will be studied in this form.

The similarity solutions that hold the key to a quick assessment of the large-time asymptotics, are all of the form (see Section 2)

$$(2t+1)^{-\frac{1}{2}m} F(\mathbf{x}/\sqrt{2t+1}) \tag{3}$$

for some $m > 0$. If this expression is substituted in (2), an ordinary differential equation is found for the (yet) unknown function F in terms of the similarity variable $\mathbf{x}/\sqrt{2t+1}$. There are several ways to recognize this reduction possibility. For instance, dimensional analysis of (1) (see [9]) as well as invariance of (2) under the scaling transformations $(\mathbf{x}, t, C) \to (\lambda\mathbf{x}, \lambda^2 t, \lambda^m C)$ for any $\lambda > 0$ (see [5], [6]), shows the existence of a similarity variable. Once having reached this point, one customarily looks for solutions of the form

$$t^{-\frac{1}{2}m} F(\mathbf{x}/\sqrt{t})\,. \tag{4}$$

An important solution of this kind is the so called 'source' solution which on $\mathbf{R}^n$ takes the canonical form

$$C_s(\mathbf{x}; t) = \frac{1}{(2\sqrt{\pi t})^n} \exp\left\{-\frac{|\mathbf{x}|^2}{4t}\right\}. \tag{5}$$

The source solution has the property that for all $t > 0$

$$\int_{\mathbf{R}^n} C_s(\mathbf{x}; t)\,\mathrm{d}x_1 \cdots \mathrm{d}x_n = 1$$

and

$$\lim_{t\to 0^+} C_s(\mathbf{x}; t) = 0$$

for all $\mathbf{x} \neq 0$. It can therefore be interpreted as the field due to an instantaneous 'point' source at $\mathbf{x} = 0$. It does solve (see [4])

$$\nabla^2 C - \frac{\partial C}{\partial t} = -\delta(|\mathbf{x}|)\delta(t)\,,$$

so it is in fact Green's function for the diffusion equation on $\mathbf{R}^n$. For a given arbitrary initial condition $C^0(\mathbf{x})$, the evolution can be expressed in the following concise form:

$$C(\mathbf{x}; t) = \frac{1}{(2\sqrt{\pi t})^n} \int_{\mathbf{R}^n} C^0(\mathbf{x}') \exp\left\{-\frac{|\mathbf{x}-\mathbf{x}'|^2}{4t}\right\} \mathrm{d}x'_1 \cdots \mathrm{d}x'_n\,.$$

This highly useful solution is only one of an infinite set of similarity solutions. Most others do not allow for such a simple interpretation as the source solution does, if one lets $\lim t \to 0^+$ (their integral vanishes for example, they have no net content). If time is shifted a little however, these solutions will have 'spread out' at the shifted time $t = 0$, and are ordinary functions by then. The similarity solutions indicated by (3) thus are the same as the ones given by (4) where in the latter t has been replaced by $t + \frac{1}{2}$. The similarity solutions of Section 2, that have the form given by (3), have the nice property of being regular functions $F(\mathbf{x})$ at $t = 0$. Moreover, these functions will be shown to form a basis for the Hilbert space $L^2(\mathbf{R}^n, e^{\frac{1}{2}|\mathbf{x}|^2})$, with inner product $(f, g) = \int_{\mathbf{R}^n} fg^* \, e^{\frac{1}{2}|\mathbf{x}|^2} \, dx_1 \cdots dx_n$ (an asterisk denotes complex conjugate). This means that at $t = 0$ any initial condition $C^0(\mathbf{x})$ in $L^2(\mathbf{R}^n, e^{\frac{1}{2}|\mathbf{x}|^2})$ can be expanded in the set of similarity solutions. It is found that the basis consists of a denumerable set for which the m's in (3) take discrete values. Since each function, if it serves as an initial condition for the diffusion equation, has its own unique decay-rate (the factor $(2t+1)^{-\frac{1}{2}m}$), as soon as one knows the smallest m occurring in the expansion, the large-time asymptotic structure can be predicted. Or, in other words, as on finite domains point spectra are found that allow for an ordering in decay-rates: this makes it possible to pin-point a slowest decaying mode.

In Section 2 the one-dimensional similarity solutions of the diffusion equation are derived that prove to be the key to an assessment of the large-time behaviour, as is shown in Section 3, where expansions in these similarity solutions are shown to be possible in the above mentioned weighted L^2-space with $n = 1$. Generalizations to higher-dimensional problems and several examples are finally given in Section 4. The properties of the one-dimensional similarity solutions that are of interest, are discussed at some length in Section 2 since they prove to be basic also in all higher-dimensional cases. Instead of directly substituting (3) in (2) in order to determine the possible F's, a geometrical approach has been chosen for, in which the idea of self-similarity is extended to be the property of solutions that remain a mere copy of themselves as time increases, that is, any solution that simply scales in amplitude, in spatial extent, or both (the last being of the form given by (3)). This approach was inspired by the observational evidence of self-similarity of certain vortices in a rotating fluid (see [7]). The observations described in this reference initiated the present study. It is for this reason too that the examples in Section 4 have a distinct fluid-mechanical character, but all results are general results concerning just the diffusion equation, irrespective of the diffusing property.

2. One-dimensional similarity solutions

In this section an important set of solutions of (2) is constructed for the one-dimensional case ($n = 1$) on $\mathbf{R}$ and $\mathbf{R}^+$ (or $\mathbf{R}^-$) that consists of the so-called similarity solutions of the diffusion equation. These particular solutions form a subset of the set of solutions generated by the general symmetry group of the diffusion equation, but for our purposes here there is no need to go into this in any detail (as extensive treatment on how to exploit local Lie groups of symmetries for finding solutions of particular partial or ordinary differential equations is given by Bluman and Cole [5] and Olver [6]). It is merely noted that similarity solutions will be called those solutions that have the property of being at all times a scaled version of themselves, that is for all $t > 0$ one has

$$C(x;t) = \frac{1}{a(t)}\, C^0\!\left(\frac{x}{b(t)}\right)$$

with $a(0) = b(0) = 1$ and $C^0(x) \equiv C(x; t = 0)$. The trigonometric functions discussed in the previous section are a special case of self-similar solutions with $b(t) = \text{constant}$. Without invoking the machinery explained in the above mentioned treatises, the ansatz of self-similarity is directly used in (2) in order to determine what possible $C^0(x)$, $a(t)$ and $b(t)$ one can have. After some algebraic manipulations, one finds

$$\frac{\mathrm{d}^2C^0}{\mathrm{d}s^2} + b\,\frac{\mathrm{d}b}{\mathrm{d}t}\,s\,\frac{\mathrm{d}C^0}{\mathrm{d}s} + \frac{b^2}{a}\,\frac{\mathrm{d}a}{\mathrm{d}t}\,C^0 = 0 \tag{6}$$

where $s \equiv x/b(t)$ is the similarity variable. This equation can only be identically satisfied for all t and s if

$$\frac{b^2}{a}\,\frac{\mathrm{d}a}{\mathrm{d}t} = \alpha\,; \qquad b\,\frac{\mathrm{d}b}{\mathrm{d}t} = \beta \tag{7}$$

where α and β are constants, and

$$\frac{\mathrm{d}^2C^0}{\mathrm{d}s^2} + \beta s\,\frac{\mathrm{d}C^0}{\mathrm{d}s} + \alpha C^0 = 0\,. \tag{8}$$

It is illuminating to discern the following three possibilities: A) $\alpha \neq 0$, $\beta = 0$, B) $\alpha = 0$, $\beta \neq 0$, C) $\alpha \neq 0$, $\beta \neq 0$. In the first case (A), for $\alpha > 0$ the exponentially-decaying trigonometric functions are recovered with, as alternative, for $\alpha < 0$, exponentially-exploding cosh and sinh functions. In the second case (B) a solution of constant amplitude is found ($a(t) = \text{constant}$) that can be expressed in terms of the error function for $\beta > 0$, $C^0(s) = \int^s \mathrm{e}^{-\frac{1}{2}\beta u^2}\,du$, whereas for $\beta < 0$ unbounded solutions are found. The third possibility provides us with the similarity solutions that do have both a time-dependent amplitude as well as shifting maxima and minima, as opposed to the trigonometric functions that have $b(t) = \text{constant}$. The solutions of (7) with $a(0) = b(0) = 1$ are

$$a(t) = b^{\alpha/\beta}(t)\,; \qquad b(t) = (2\beta t + 1)^{1/2}\,. \tag{9}$$

It is seen that for $\beta < 0$ singular behaviour of the solutions occurs at $t = \frac{1}{2}|\beta|$. Such solutions are of no interest here and attention is focused on solutions of equation (8) with $\beta > 0$ only. Without loss of generality β can be put equal to one in (8). Therefore, if $C_\alpha(x)$ solves

$$\frac{d^2C}{dx^2} + x\frac{dC}{dx} + \alpha C = 0 \tag{10}$$

and one has as initial condition, at time $t = 0$, $C^0(x) = C_\alpha(x)$, then the subsequent evolution is simply

$$C(x;t) = \frac{1}{b^\alpha(t)}\, C_\alpha\left(\frac{x}{b(t)}\right). \tag{11}$$

Note that – since $b'(t) \neq 0$ – these solutions cannot solve any initial-value problem on a finite interval with fixed boundary conditions at both ends. The only fixed point under the stretching $x \to x/b(t)$ is $x = 0$, so either the whole $\mathbf{R}$ or $\mathbf{R}^+$(or $\mathbf{R}^-$) axis has to be considered as domain for solutions of this type with appropriate boundary conditions for $x \to \pm\infty$ and, if semi-infinite intervals are considered, at $x = 0$. It may also be noted that solutions of (10) decay algebraically for $\alpha > 0$, which is in marked contrast with the exponential decay of the trigonometric functions that are found if β is put equal to zero in (8).

A few properties of solutions of (10) can be derived without knowing exact expressions for them. Assuming that C_α has a Fourier-series representation, put

$$C_\alpha(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ikx} F_\alpha(k)\, dk. \tag{12}$$

If this expression is substituted in (10), the following equations for the spectrum of the similarity solutions is obtained,

$$\frac{d}{dk}(kF_\alpha) = (\alpha - k^2)F_\alpha, \tag{13}$$

which is solved by

$$F_\alpha(k) = k^{\alpha-1}\, e^{-\frac{1}{2}k^2} \tag{14}$$

(a multiplicative integration constant that determines the amplitude of the solution has been left out here). With the Fourier-series expansion the evolution can be expressed as

$$C(x;t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ikx}\, e^{-k^2t} F_\alpha(k)\, dk. \tag{15}$$

Substitution of (14) in this expression then shows that, although each Fourier component decays exponentially, indeed algebraically-decaying solutions as in (11) are found,

$$\begin{aligned} C(x;t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ikx}\, e^{-\frac{1}{2}k^2(2t+1)} k^{\alpha-1}\, dk \\ &= \frac{1}{b(t)^\alpha}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ilx/b(t)}\, e^{-\frac{1}{2}l^2} l^{\alpha-1}\, dl \quad (l \equiv b(t)k) \\ &= \frac{1}{b(t)^\alpha}\, C_\alpha\left(\frac{x}{b(t)}\right). \end{aligned} \tag{16}$$

A glance at (12), with $F_\alpha(k)$ given by (14), suffices to infer that if α is an odd integer, C_α is an even function of x, whereas for α an even integer it is an odd function.

By casting (10) in the well-known Sturm–Liouville form

$$\frac{\mathrm{d}}{\mathrm{d}x}\, \mathrm{e}^{\frac{1}{2}x^2}\, \frac{\mathrm{d}C}{\mathrm{d}x} + \alpha\, \mathrm{e}^{\frac{1}{2}x^2} C = 0\,, \tag{17}$$

it is seen that if the C_α's are integrable with respect to the exponentially-growing weight-function $w(x) \equiv \mathrm{e}^{\frac{1}{2}x^2}$, orthogonality follows

$$\int_{-\infty}^{+\infty} C_\nu(x) C_\mu(x) w(x)\, \mathrm{d}x = 0 \quad (\nu \neq \mu)\,. \tag{18}$$

For integer $\alpha(>0)$ exact solutions of (10) are easily found. By putting $C \equiv \mathrm{e}^{-\frac{1}{2}x^2} H(x)$ and introducing a variable $y \equiv x/\sqrt{2}$, after substitution in (10) the standard Hermite equation is found for H

$$\frac{\mathrm{d}^2 H}{\mathrm{d}y^2} - 2y\, \frac{\mathrm{d}H}{\mathrm{d}y} + 2(\alpha - 1)H = 0\,. \tag{19}$$

Solutions of this equation are Hermite polynomials H_n if $\alpha - 1 \equiv n$ is a positive integer or zero (see [4]),

$$H_n(y) \equiv (-1)^n\, \mathrm{e}^{y^2}\, \frac{\mathrm{d}^n}{\mathrm{d}y^n}\, \mathrm{e}^{-y^2}\,.$$

One has $H_0 = 1$, $H_1 = 2y$, $H_2 = 4y^2 - 2$ and so on. A particular set of similarity solutions thus is

$$\Omega_n(x) = H_n\!\left(\frac{x}{\sqrt{2}}\right) \mathrm{e}^{-\frac{1}{2}x^2} \quad (n = 0, 1, 2, \ldots)\,. \tag{20}$$

For general α solutions of (10) can be expressed in terms of parabolic cylinder functions that reduce to the above derived Hermite functions for positive integer α. This is by no means a new result (see [5], [6]), but what seems to have escaped recognition is that this particular set of similarity solutions – given by (20) – holds the clue to the large-time asymptotics of a large class of initial conditions for the diffusion equation on infinite domains.

3. Similarity solutions and large-time asymptotics

It is a well-established fact that the set

$$\phi_n(x) = \frac{H_n(x)\, \mathrm{e}^{-\frac{1}{2}x^2}}{\sqrt{2^n n! \sqrt{\pi}}} \tag{21}$$

with

$$\int_{-\infty}^{+\infty} \phi_n \phi_m\, \mathrm{d}x = \delta_{nm} \quad (n, m = 0, 1, 2, \ldots) \tag{22}$$

is complete in $L^2(\mathbf{R})$ (see [8]). It directly follows that the normalized set of similarity solutions

$$\Omega_n(x) = \frac{H_n\left(\frac{x}{\sqrt{2}}\right) e^{-\frac{1}{4}x^2}}{\sqrt{2^n n! \sqrt{2\pi}}} \tag{23}$$

with

$$\int_{-\infty}^{+\infty} \Omega_n(x)\Omega_m(x)w(x)\,\mathrm{d}x = \delta_{nm} \quad (n, m = 0, 1, 2, \ldots) \tag{24}$$

where $w(x) = e^{\frac{1}{2}x^2}$, is complete in $L^2(\mathbf{R}, w)$. If an initial condition on $\mathbf{R}$ is quadratically integrable with respect to the weight function $w(x)$

$$\int_{-\infty}^{+\infty} |C^0(x)|^2 e^{\frac{1}{2}x^2}\,\mathrm{d}x < \infty , \tag{25}$$

then C^0 can be expanded in a sum of similarity solutions

$$C^0(x) = \sum_{n=0}^{\infty} a_n \Omega_n(x) \tag{26}$$

where

$$a_n = \int_{-\infty}^{+\infty} C^0(x)\Omega_n(x)w(x)\,\mathrm{d}x . \tag{27}$$

The evolution of the field with initial condition $C^0(x)$ then is

$$C(x; t) = \sum_{n=0}^{\infty} \frac{a_n}{b(t)^{n+1}} \Omega_n\left(\frac{x}{b(t)}\right) . \tag{28}$$

The set $\{\Omega_n\}$ thus forms a basis for the Hilbert space $L^2(\mathbf{R}, w)$ that is endowed with an inner product (,) defined by $(f, g) = \int_{\mathbf{R}} fg^* w\,\mathrm{d}x$.

As on a finite interval, discussed in the introduction, a point-spectrum is found that allows for an ordering of decay rates of each contributing 'Fourier mode'. The large-time asymptotic behaviour is determined by the first non-zero amplitude a_n that occurs in the discrete spectrum calculated according to (27). If an initial condition in $L^2(\mathbf{R}, w)$ is an even function of x, an expansion in the subset with $n = 0, 2, 4, \ldots$ is found. This subset suffices also for problems on $\mathbf{R}^+$ or $\mathbf{R}^-$ if at $x = 0$ the boundary condition $\partial C/\partial x = 0$ is imposed. For initial value problems that are anti-symmetric around $x = 0$ or for problems with boundary condition $C = 0$ at $x = 0$, the subset with $n = 1, 3, 5, \ldots$ will do. It may be remarked here that all functions that fall off to zero faster than $|x|^{-\frac{1}{2}} e^{-\frac{1}{4}x^2}$ for $x \to \pm\infty$ are in $L^2(\mathbf{R}, w)$, as well as all functions that are zero outside any finite interval on $\mathbf{R}$. All such initial conditions asymptotically tend to one of the similarity profiles.

As an illustration of the foregoing consider the following initial value problem that is discussed in all treatises on the heat or diffusion equation. Let on $\mathbf{R}$, at $t = 0$, the initial condition be: $C^0(x) = 1$ on the interval $[-1, +1]$ and zero everywhere else. Using Green's function for the diffusion equation on $\mathbf{R}$, the solution can be expressed as

$$C(x;t) = \frac{1}{2}\left\{\operatorname{erf}\frac{1-x}{2\sqrt{t}} + \operatorname{erf}\frac{1+x}{2\sqrt{t}}\right\} \tag{29}$$

or, by means of the Fourier transform, as

$$C(x;t) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\sin k}{k}\, e^{ikx}\, e^{-k^2 t}\, dk\,. \tag{30}$$

This expression, nor (29), is very transparent with regard to the large-time behaviour. An expansion of the initial condition in similarity solutions, however, shows directly towards what structure the field will evolve. With (27) and (23) it follows that the expansion spectrum is calculated as follows

$$a_n = \frac{1}{\sqrt{2^n n!\sqrt{2\pi}}}\int_{-\infty}^{+\infty} C^0(x) H_n\left(\frac{x}{\sqrt{2}}\right) dx\,. \tag{31}$$

In the case considered here one easily calculates

$$a_0 = \frac{2}{\sqrt{\sqrt{2\pi}}}\,; \qquad a_1 = 0\,; \qquad a_2 = -\frac{8}{3}\frac{1}{\sqrt{2^3\sqrt{2\pi}}}\,; \qquad a_3 = 0\,, \tag{32}$$

and so on. Generally, if m is the smallest integer for which $a_m \neq 0$, the similarity solution it is attached to is the slowest decaying one which therefore survives longest. This can be elucidated by considering the norm for the Hilbert space $L^2(\mathbf{R}, e^{\frac{1}{2}x^2})$. The usual norm $\|\cdots\|$ for this weighted L^2-space is (the extension to $\mathbf{R}^n$ is discussed in the next section):

$$\|f-g\| = \left\{\int_{-\infty}^{+\infty} |f-g|^2 e^{\frac{1}{2}x^2}\, dx\right\}^{\frac{1}{2}}. \tag{33}$$

It is not hard to derive that the following estimate holds for some $k \geq 1$:

$$\|b(t)^{m+1}C(b(t)x;t) - a_m\Omega_m(x)\| \leq \frac{1}{b(t)^k}\,\|C^0(x) - a_m\Omega_m(x)\|\,. \tag{34}$$

This estimate gives an asymptotic expression for $C(x;t)$,

$$\lim_{t\to\infty}\|b(t)^{m+1}C(b(t)x;t) - a_m\Omega_m(x)\| = 0\,, \tag{35}$$

which will from hereon be expressed in the following – not very apt, but convenient – way

$$\lim_{t\to\infty} C(x;t) = \frac{a_m}{b(t)^{m+1}}\,\Omega_m\left(\frac{x}{b(t)}\right). \tag{36}$$

So in the particular case considered, the large-time asymptotic behaviour is

$$\lim_{t\to\infty} C(x;t) = \frac{2}{\sqrt{2\pi}\sqrt{2t+1}}\exp\left\{-\frac{x^2}{4t+2}\right\}. \tag{37}$$

The large-time asymptotic behaviour of the solution is thus effortlessly deduced, as opposed to the representations like given by (29) or (30) that in more complicated cases are rather cumbersome to work with. In order to reveal the large-time asymptotic behaviour by means of expansions in similarity solutions of the diffusion equation, the solution needs to be rescaled in amplitude but also spatially since it is both continuously diminishing in amplitude as well as spreading out over increasingly larger scales.

The fact that each coefficient a_n is determined by an integral of the product of the initial condition with a polynomial of degree n implies the following rather general result. Consider some initial condition $C^0(x)$ with $\lim_{x\to\pm\infty} C^0(x) = C_\infty$, where C_∞ is a constant. Assume that $C^0(x) - C_\infty$ is in $L^2(\mathbf{R}, e^{\frac{1}{2}x^2})$. Let there be given that

$$\int_{-\infty}^{+\infty} (C^0 - C_\infty)\,dx = 0, \ldots, \qquad \int_{-\infty}^{+\infty} (C^0 - C_\infty)x^{n-1}\,dx = 0$$

and

$$\int_{-\infty}^{+\infty} (C^0 - C_\infty)x^n\,dx \neq 0\,, \tag{38}$$

then

$$\lim_{t\to\infty} C(x;t) = C_\infty + \frac{\text{constant}}{(2t+1)^{\frac{1}{2}(n+1)}} H_n\left(\frac{x}{\sqrt{4t+2}}\right)\exp\left\{-\frac{x^2}{4t+2}\right\}.$$

In the next section a few additional examples will be discussed that do show the power of expansions in similarity solutions if one aims at isolating the large-time asymptotics.

4. Expansions for higher-dimensional problems

The results from the previous section can straightforwardly be generalized to higher dimensions. For $n = 2$, for instance, it is directly inferred that if initial conditions $C^0(x_1, x_2)$ are in $L^2(\mathbf{R}^2, e^{\frac{1}{2}|\mathbf{x}|^2})$, where $|\mathbf{x}|^2 \equiv (x_1^2 + x_2^2)$, a double expansion is possible

$$C^0(x_1, x_2) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} a_{nm}\Omega_n(x_1)\Omega_m(x_2) \tag{39}$$

where the expansion coefficients are calculated according to

$$a_{nm} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} C^0(x_1, x_2)\Omega_n(x_1)\Omega_m(x_2)\,e^{\frac{1}{2}(x_1^2+x_2^2)}\,dx_1\,dx_2\,. \tag{40}$$

The evolution then simply is

$$C(x_1, x_2; t) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{a_{nm}}{b(t)^{2+n+m}}\,\Omega_n\left(\frac{x_1}{b(t)}\right)\Omega_m\left(\frac{x_2}{b(t)}\right). \tag{41}$$

Such expansions are valid on $\mathbf{R}^2$ but with appropriate boundary conditions they will also suffice on domains as $\mathbf{R}\times\mathbf{R}^+$ or $\mathbf{R}^+\times\mathbf{R}^+$. Similar expressions are easily derived for three-dimensional problems. It will be clear that if initial conditions allow for separation of variables, that is $C^0(x_1, x_2) = F(x_1)G(x_2)$, or if boundary conditions like, say,

$C(x_1 = 0, x_2; t) = 0$ $(\forall x_2, t)$ are imposed, this type of decomposition in a double series of one-dimensional similarity solutions is economical for assessing the large-time asymptotic structure of the solution of the initial value problem. In $\mathbf{R}^2$ and $\mathbf{R}^3$ alternative sets of similarity solutions can be found that in certain cases – depending on initial and boundary conditions – will be preferred instead of expansions as given by (39). The number of alternatives is very limited, however, if one restricts attention to solutions in orthogonal coordinate systems that allow for simple separation of the diffusion equation, as is done in the present study. On unbounded multi-dimensional domains there is no real need for other sets of similarity solutions than the direct product sets of one-dimensional similarity solutions (the calculation of expansion coefficients may be less time consuming for certain initial conditions if an alternative set is used). On semi-infinite domains, with Dirichlet or Neumann conditions specified on the boundary $\partial\Omega$, i.e. $C = 0$ or $\partial C/\partial \mathbf{n} = 0$, certain alternatives are available. There is, however, only a limited class of semi-infinite domains on which similarity solutions can be used to express the evolution subjected to one of the two above mentioned types of boundary conditions. This has to do with the fact that the boundary itself has to be invariant under the stretching transformation $\mathbf{x} \rightarrow \mathbf{x}/b(t)$, that is, if $\mathbf{x} \in \partial\Omega$ then also $\mathbf{x}/b(t) \in \partial\Omega$. On $\mathbf{R}^2$ such domains are just the 'wedge'-like domains, i.e. domains bounded by two straight lines emanating from the origin (extending to infinity). A set of similarity solutions in cylinder coordinates is presented below that forms a basis for such domains with such boundary conditions. In $\mathbf{R}^3$ there are infinitely many invariant, semi-infinite domains. Only few remain of these if attention is restricted to domains of which the boundary coincides with coordinate surfaces of some simple separable orthogonal coordinate system. Simple separable similarity solutions of the diffusion equation have been found in even fewer systems, namely only in spherical coordinates and in conical coordinates. These two possibilities are also presented in the sequel (there are also quasi three-dimensional domains on which expansions in similarity solutions are feasible: all domains with the 'wedge'-structure on some plane and which are further translationally invariant in the direction perpendicular to this plane).

As a first example, similarity solutions in cylindrical coordinates will be derived here which provide us with an alternative set of functions that is complete in $L^2(\mathbf{R}^2, e^{\frac{1}{2}|\mathbf{x}|^2})$. The diffusion equation on $\mathbf{R}^2$ in cylinder coordinates (r, θ) reads (see [11] where the Laplace operator on the right hand side of (2) is given for many different coordinate systems)

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2} \tag{42}$$

where $r = \sqrt{x_1^2 + x_2^2}$ $(0 \leq r < \infty)$ and $\tan\theta = x_2/x_1$ $(0 \leq \theta < 2\pi)$. In the sequel it will be convenient to restrict attention to functions with separated angluar dependence, that is of form $C(r)\,e^{ik\theta}$ $(k = 0, \pm 1, \pm 2, \ldots)$. This induces no loss of generality since any reasonable (say square integrable) function can be Fourier-transformed into a sum of functions of this type. Self-similar solutions of the diffusion equations now take the form

$$C(r; t)\,e^{ik\theta} = \frac{1}{a(t)}\,C^0\left(\frac{r}{b(t)}\right)e^{ik\theta} \tag{43}$$

where $C^0(r)$ is the radius dependent part of the initial condition. As before, $a(t)$ and $b(t)$ satisfy $a(0) = b(0) = 1$. It follows by substitution in (42) that C^0 necessarily solves

$$\frac{d^2C^0}{ds^2} + \frac{1}{s}\frac{dC^0}{ds} + \beta s\frac{dC^0}{ds} + \left(\alpha - \frac{k^2}{s^2}\right)C^0 = 0 \tag{44}$$

where α and β are constants ($a(t)$ and $b(t)$ again are solutions of (7)), and s is the similarity variable $s = r/b(t)$. The two possibilities of either α or β being zero will not be considered since they serve no purpose here (for $\beta = 0$ the solutions are Bessel functions). With neither α nor β being zero, $a(t)$ and $b(t)$ are as in (9). It may be noted here that (44) is easily cast in the Sturm–Liouville form, so some set of orthogonal functions can be expected at this point already. Skipping a few intermediate steps, the result is merely stated that if one substitutes $C^0(y) = y^{\frac{1}{2}|k|}\,e^{-y}L(y)$, with $y = \frac{1}{2}s^2$, and β is put equal to one, Laguerre's equation is found for L,

$$y\frac{d^2L}{dy^2} + (|k| + 1 - y)\frac{dL}{dy} + (\tfrac{1}{2}(\alpha - 2 + |k|) - |k|)L = 0\,. \tag{45}$$

Since k is always an integer, it follows that if $\frac{1}{2}(\alpha - 2 + |k|) \equiv n = 0, 1, 2, \ldots$, solutions of (45) are associated Laguerre polynomials $L_n^{|k|}(y)$ (see [4]). The associated Laguerre polynomial is defined by

$$L_n^m(y) \equiv \frac{d^m L_n(y)}{dy^m}$$

where L_n is the ordinary Laguerre polynomial of degree n

$$L_n(y) \equiv e^{+y}\frac{d^n}{dy^n}\,y^n\,e^{-y}\,.$$

For instance, $L_0 = 1$, $L_1 = 1 - y$, $L_2 = 2 - 4y + y^2$ and so on (note that for all $m > n$, $L_n^m = 0$). A particular set of similarity solutions is therefore

$$(\tfrac{1}{2}r^2)^{\frac{1}{2}|k|}L_n^{|k|}(\tfrac{1}{2}r^2)\,e^{-\frac{1}{2}r^2}\,e^{ik\theta} \tag{46}$$

for $n = 0, 1, 2, \ldots$ and $k = 0, \pm 1, \pm 2, \ldots, \pm n$. The fact that the angle-independent solutions are ordinary Laguerre polynomials was previously noted by Birkhoff [9]. The set

$$\varphi_{nm}(y) = \sqrt{\frac{(n-m)!}{(n!)^3}}\;y^{\frac{1}{2}m}\,e^{-\frac{1}{2}y}L_n^m(y) \tag{47}$$

with, for fixed m $(0 \leqslant m \leqslant n)$,

$$\int_0^\infty \varphi_{nm}\varphi_{n'm}\,dy = \delta_{nn'} \tag{48}$$

can be proved to be complete in $L^2(\mathbf{R}^+)$ (see [8], for example). Be warned, however, of the intermixing of the terms 'generalized' and 'associated' Laguerre polynomials. Generalized Laguerre polynomials, sometimes denoted in the literature by $L_n^{(k)}$, are related to associated Laguerre polynomials according to $L_n^{(k)} = (-1)^k L_{n+k}^k$, but they are also defined for non-integer k (an expression is given below by (91)). If one combines completeness of the functions given by (47) with completeness of the trigonometric functions in $L^2(0, 2\pi)$, and it is noted that the functions φ_{nm} are proportional to the radius dependent part of the similarity solutions given by (46), it is deduced that the normalized similarity solutions

$$\Phi_{nk}(r,\theta)=\sqrt{\frac{(n-k)!}{2\pi(n!)^3}}\,(\tfrac{1}{2}r^2)^{\frac{1}{2}|k|}\,\mathrm{e}^{-\frac{1}{2}r^2}L_n^{|k|}(\tfrac{1}{2}r^2)\,\mathrm{e}^{ik\theta} \tag{49}$$

with (an asterisk stands for complex conjugate)

$$\int_0^\infty\int_{-\pi}^{+\pi}\Phi_{nk}(\Phi_{n'k'})^*\,\mathrm{e}^{\frac{1}{2}r^2}r\,\mathrm{d}\theta\,\mathrm{d}r=\delta_{nn'}\delta_{kk'} \tag{50}$$

are complete in $L^2(\mathbf{R}^2,\mathrm{e}^{\frac{1}{2}|x|^2})$. If an initial condition $C^0(r,\theta)$ is in $L^2(\mathbf{R}^2,\mathrm{e}^{\frac{1}{2}|x|^2})$, it thus can be expanded according to

$$C^0(r,\theta)=\sum_{n=0}^{\infty}\sum_{k=-n}^{+n}a_{nk}\Phi_{nk}(r,\theta) \tag{51}$$

where the expansion coefficients are calculated with

$$a_{nk}=\int_0^\infty\int_{-\pi}^{+\pi}C^0(r,\theta)\Phi_{nk}^*(r,\theta)\,\mathrm{e}^{\frac{1}{2}r^2}r\,\mathrm{d}\theta\,\mathrm{d}r\,. \tag{52}$$

Noting that $\alpha=2n+2-|k|$, the evolution is given by

$$C(r,\theta;t)=\sum_{n=0}^{\infty}\sum_{k=-n}^{+n}\frac{a_{nk}}{b(t)^{2n+2-|k|}}\,\Phi_{nk}\left(\frac{r}{b(t)},\theta\right). \tag{53}$$

Subsets of (49) can be used to expand initial conditions on 'wedge'-shaped domains $\mathbf{R}^+\times[0,(p/q)\pi]$ with boundary conditions $C=0$ or $\partial C/\partial\theta=0$, if p/q is a rational number.

Consider for the moment the class of initial conditions with no angular dependence, say $C^0(r)$. For such initial conditions the restricted set of similarity solutions

$$C_n(r)\equiv\frac{1}{n!}\,L_n(\tfrac{1}{2}r^2)\,\mathrm{e}^{-\frac{1}{2}r^2} \tag{54}$$

with

$$\int_0^\infty C_n(r)C_m(r)\,\mathrm{e}^{\frac{1}{2}r^2}r\,\mathrm{d}r=\delta_{nm} \tag{55}$$

can be used as an expansion basis. The expansion coefficients are calculated with

$$a_n=\int_0^\infty C^0(r)C_n(r)\,\mathrm{e}^{\frac{1}{2}r^2}r\,\mathrm{d}r=\frac{1}{n!}\int_0^\infty C^0(r)L_n(\tfrac{1}{2}r^2)r\,\mathrm{d}r\,. \tag{56}$$

The corresponding evolution is

$$C(r;t)=\sum_{n=0}^{\infty}\frac{a_n}{b(t)^{2n+2}}\,C_n\left(\frac{r}{b(t)}\right). \tag{57}$$

In fluid mechanics initial conditions of this type can be thought of as describing initial vorticity distributions $w^0(r)$ of radially-symmetric, planar vortices. The vorticity of such a vortex is related to its azimuthal velocity $v(r)$ according to

$$\omega \equiv \frac{1}{r} \frac{\mathrm{d}}{\mathrm{d}r} (rv) . \tag{58}$$

The evolution of vorticity of an unbounded radially-symmetric, planar vortex in a viscous fluid is governed by (see [2])

$$\frac{\partial \omega}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \omega}{\partial r} \right) . \tag{59}$$

By comparing this equation with (42) it is seen that expansions in the restricted set $C_n(r)$ are appropriate for vorticity distributions that are square-integrable

$$\int_0^\infty |\omega|^2 \, \mathrm{e}^{\frac{1}{2}r^2} r \, \mathrm{d}r < \infty . \tag{60}$$

A well-known model vortex often encountered in the literature is the Rankine vortex, which consists of a core in solid body rotation, surrounded by irrotational (potential) flow (see Fig. 1)

$$\begin{aligned} v_{\mathrm{Ra}}(r) &= \tfrac{1}{2} r \qquad (0 \leqslant r \leqslant 1) , \\ &= \frac{1}{2} \frac{1}{r} \qquad (1 \leqslant r < \infty) . \end{aligned} \tag{61}$$

The prefactor $\frac{1}{2}$ is used to get the following simple expression for the vorticity distribution of the Rankine vortex

$$\begin{aligned} \omega_{\mathrm{Ra}}(r) &= 1 \quad (0 < r < 1) , \\ &= 0 \quad (1 < r < \infty) . \end{aligned} \tag{62}$$

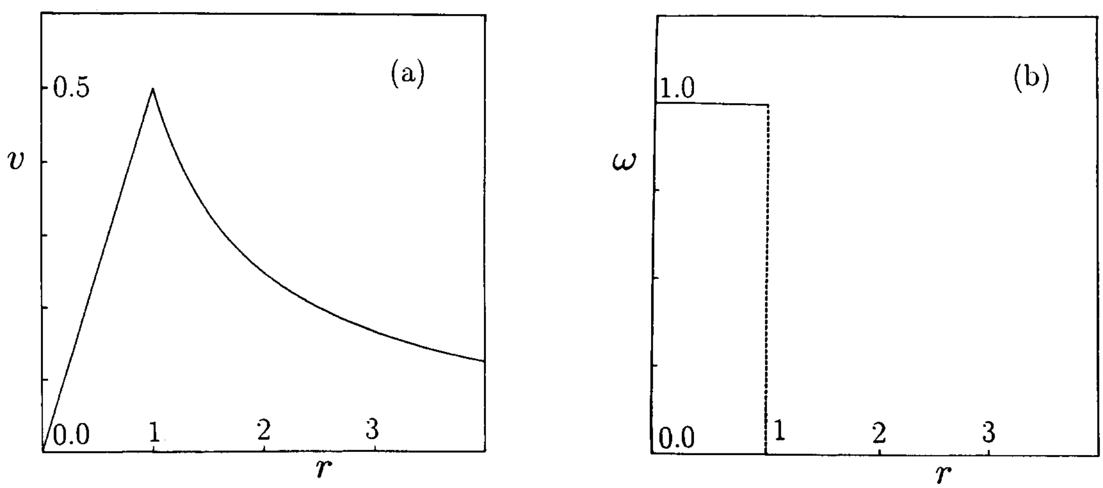

Fig. 1. Velocity (a) and vorticity (b) of a Rankine vortex.

The expansion coefficients for this case are, according to (56),

$$a_n = \frac{1}{n!}\int_0^1 L_n(\tfrac{1}{2}r^2)r\,\mathrm{d}r\,, \tag{63}$$

which yields $a_0 = \frac{1}{2}$, $a_1 = \frac{3}{8}$, $a_2 = \frac{13}{48}$ and so on. Therefore, asymptotically,

$$\lim_{t\to\infty} \omega_{\mathrm{Ra}}(r;t) = \frac{1}{2}\,\frac{1}{2t+1}\exp\left\{-\frac{1}{2}\,\frac{r^2}{2t+1}\right\}, \tag{64}$$

by which is meant that

$$\lim_{t\to\infty} \|(2t+1)\omega_{\mathrm{Ra}}(\sqrt{2t+1}\,r;t) - \tfrac{1}{2}\,\mathrm{e}^{-\frac{1}{2}r^2}\| = 0\,. \tag{66}$$

The precise details of the evolution can be obtained numerically by either considering the Fourier–Bessel transform or by invoking Green's function for the diffusion equation on $\mathbf{R}^2$. The Fourier–Bessel transform of an initial condition $\omega^0(r)$ is (see [4])

$$\omega^2(r) = \int_0^\infty g(k)J_0(kr)k\,\mathrm{d}k \tag{67}$$

with

$$g(k) = \int_0^\infty \omega^0(r)J_0(kr)r\,\mathrm{d}r\,. \tag{68}$$

Here J_0 is the zero-order ordinary Bessel function. Ordinary square-integrability is sufficient for such a transform to exist (see [4]). Because the Bessel functions are eigenfunctions of the Laplacian on the right-hand side of (59), with eigenvalue $-k^2$, the evolution is simply

$$\omega(r;t) = \int_0^\infty \mathrm{e}^{-k^2t}g(k)J_0(kr)k\,\mathrm{d}k\,. \tag{69}$$

The Fourier–Bessel transforms of the radially-symmetric similarity solutions $C_n(r)$, for instance, are

$$g_n(k) \equiv \int_0^\infty C_n(r)J_0(kr)r\,\mathrm{d}r = \frac{k^{2n}\,\mathrm{e}^{-\frac{1}{2}k^2}}{2^n n!}\,. \tag{70}$$

For the Rankine vortex the Fourier–Bessel transform is quite simple

$$g_{\mathrm{Ra}}(k) = \int_0^1 J_0(kr)r\,\mathrm{d}r = \frac{J_1(k)}{k}\,, \tag{71}$$

where a standard identity for Bessel functions has been used (see [10]), and J_1 is an ordinary Bessel function of order 1. The evolution of the Rankine vortex is therefore in integral form

$$\omega_{\mathrm{Ra}}(r;t) = \int_0^\infty \mathrm{e}^{-k^2t}J_1(k)J_0(kr)\,\mathrm{d}k\,.$$

In order to show the approach to the simple Gaussian shape as given by (64), this integral has been evaluated numerically at three consecutive moments, and the result is compared at each moment with the function $f(R) = e^{-\frac{1}{4}R^2}$ in Fig. 2. Since $\omega_{Ra}(r; t)$ is continuously diminishing in amplitude and spreading out, in order to make this comparison $\omega_{Ra}(r; t)$ is rescaled with scaling factors A and B such that $\omega^*(R; t) \equiv A\omega_{Ra}(BR; t)$ $(R \equiv r/B)$, coincides with $f(R)$ at $R = 0$ and $R = 2$. The latter could have been any point $\neq 0$: it merely serves as an additional point where at any instant the two functions already coincide. It is seen that, with increasing time, the form of the vorticity distribution of the diffusing Rankine vortex rapidly approaches the Gaussian function as predicted by the analysis in terms of similarity solutions: for $t > 1$ the difference is hardly discernable. In the case of a Rankine vortex with a core radius of 10 cm in water with a temperature of about 20 degrees Celsius, for which the kinematic viscosity is approximately 1.10^{-2} cm^2/s, dimensionally $t = 1$ corresponds to $L^2/D = 10000$ seconds (so it may take a while!).

In general, since $L_0 = 1$, the first expansion coefficient a_0 of a vorticity distribution is proportional to the circulation $\Gamma(\infty)$ of the vortex at infinity. The velocity circulation $\Gamma(C)$

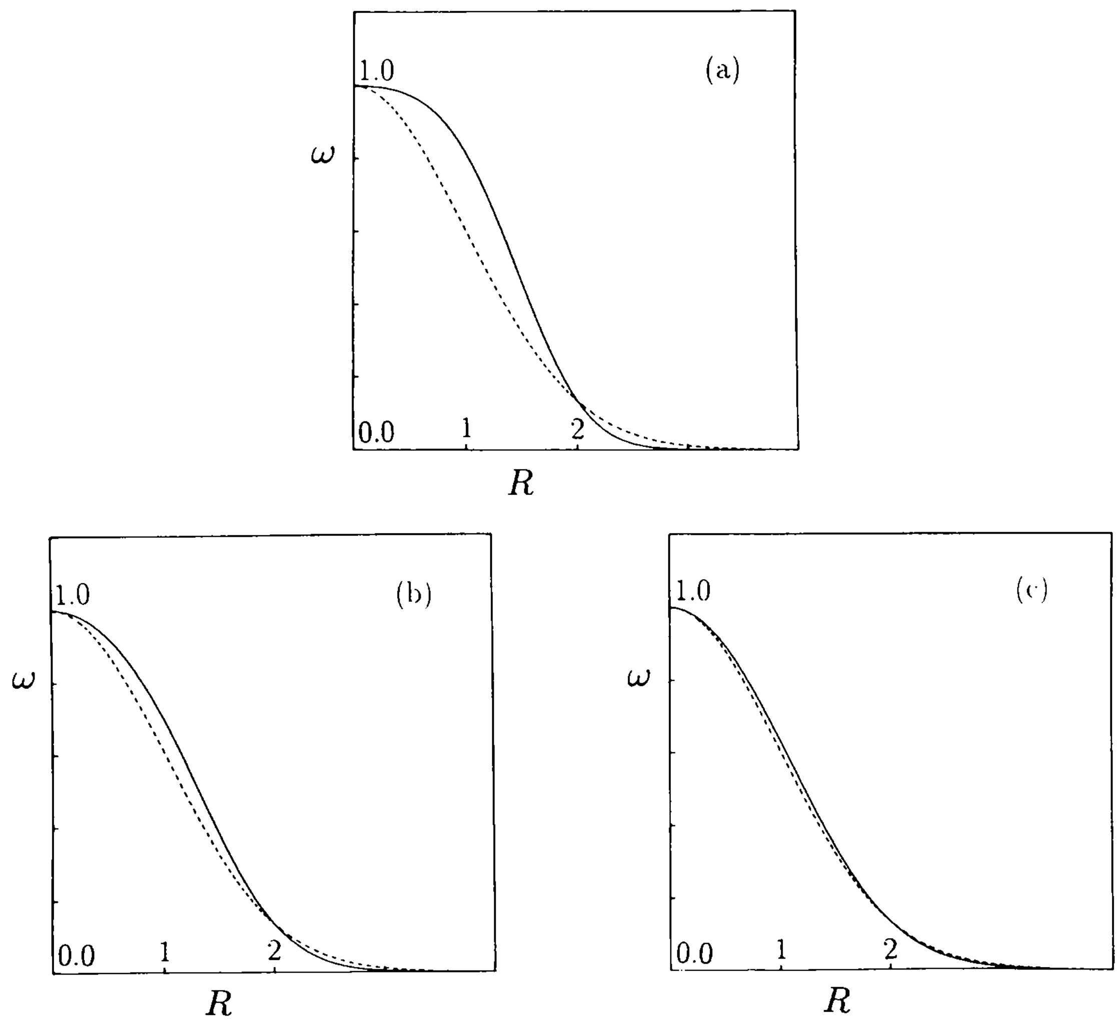

Fig. 2. Graphs showing the evolution of the diffusing vorticity distribution of a Rankine vortex (solid line) towards the similarity solution given by (54), with $n = 0$ (dashed line). Times are (a) $t = 0.1$, (b) $t = 0.5$ and (c) $t = 1.0$.

round a closed contour C is defined by (see [2])

$$\Gamma(C) \equiv \oint_C \mathbf{u} \cdot \mathrm{d}\mathbf{l}$$

where $\mathbf{u}$ denotes the two-dimensional velocity field. If Stokes' theorem is invoked here, the circulation is seen to be equal to the area integral of vorticity

$$\Gamma(C) = \oint_A \omega \, \mathrm{d}A$$

where A is the area bounded by the closed contour C. The circulation round a circle of radius r, of which the centre coincides with that of a radially-symmetric vortex, is

$$\Gamma(r) = 2\pi r v ,$$

and therefore

$$a_0 = \lim_{r\to\infty} \int_0^r \omega^0(s) s \, \mathrm{d}s = \lim_{r\to\infty} rv = \lim_{r\to\infty} \frac{\Gamma(r)}{2\pi} . \tag{72}$$

It can therefore be concluded that any radially-symmetric vortex that has non-zero net vorticity, which means non-vanishing circulation, with increasing time will asymptotically 'look like' the simple two-dimensional source solution, irrespective of the finer details of the initial distribution. Vortices on $\mathbf{R}^2$ with non-zero circulation are from a physical point of view often less interesting since asymptotically, that is, for $\lim_{r\to\infty}$, $v(r) \to 1/r$, which makes important integrals as energy $E = 2\pi \int_0^\infty \frac{1}{2} v^2 r \, \mathrm{d}r$ diverge. A simple model of an isolated vortex, i.e. a vortex with vanishing circulation and finite energy, is the following. Let the vorticity initially be given by (see Fig. 3a)

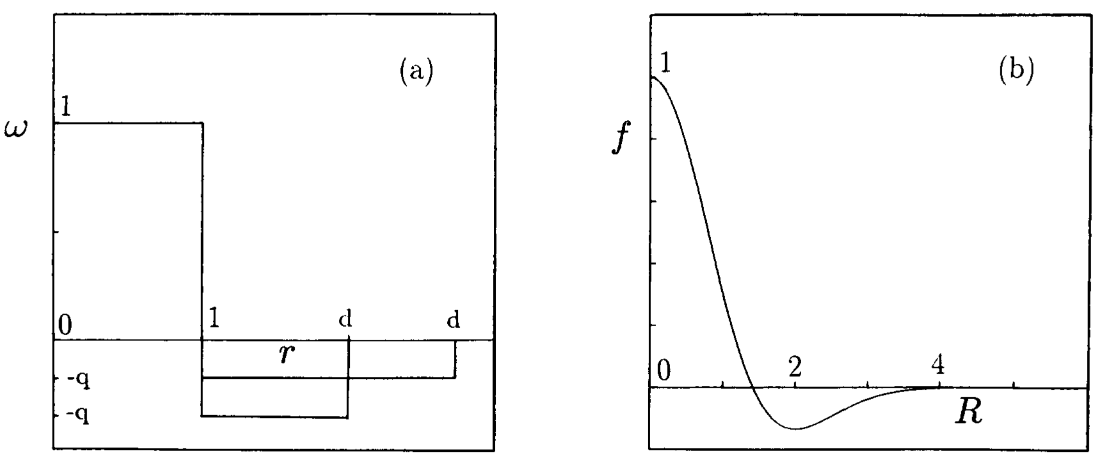

Fig. 3. Any initial vorticity distribution that has vanishing circulation, like the two profiles shown in (a), will asymptotically tend to a scaled version of the function $f(R) = (1 - \frac{1}{2}R^2)\exp(-\frac{1}{2}R^2)$ that is shown in (b).

$$\begin{aligned}\omega^0(r) &= 1 \quad (0 \leq r < 1)\,,\\ &= -q \quad (1 < r < d)\,,\\ &= 0 \quad (d < r < \infty)\,.\end{aligned} \tag{73}$$

It can be pictured as a vortex consisting of a constant vorticity core surrounded by a ring of oppositely-signed vorticity. Integration shows that the first expansion coefficient, which is equal to the circulation, has the value

$$a_0 = \int_0^d \omega^0(s)s\,\mathrm{d}s = \tfrac{1}{2}(1+q) - \tfrac{1}{2}qd^2\,. \tag{74}$$

So if one chooses

$$d = \sqrt{\frac{1+q}{q}} \quad \text{or} \quad q = \frac{1}{d^2-1}\,, \tag{75}$$

the circulation is zero. The second coefficient is non-zero for any choice of a pair (q, d) that satisfies this relation. It is given by (note that $L_1(x) = 1 - x$)

$$a_1 = \frac{1}{1!}\int_0^d (1 - \tfrac{1}{2}s^2)\omega^0(s)s\,\mathrm{d}s = a_0 + \tfrac{1}{8}qd^4 - \tfrac{1}{8}(1+q) = \tfrac{1}{8}d^4\,. \tag{76}$$

Therefore, any vortex initially of this type asymptotically tends to

$$\begin{aligned}\lim_{t\to\infty} \omega(r;t) &= \frac{a_1}{b(t)^4}\,C_1\!\left(\frac{r}{b(t)}\right)\\ &= \frac{a_1}{(2t+1)^2}\left(1 - \frac{r^2}{4t+2}\right)\exp\!\left\{-\frac{r^2}{4t+2}\right\}\end{aligned} \tag{77}$$

or, in other words, asymptotically becomes a scaled version of the function $f(R) = (1 - \frac{1}{2}R^2)\exp(-\frac{1}{2}R^2)$ (see Fig. 3b). From the fact that the L_n's in (56) are simple polynomials of degree n, the following general result is inferred. Let some initial vorticity distribution be in $L^2(\mathbf{R}^2, \mathrm{e}^{\frac{1}{2}|\mathbf{x}|^2})$ and have the property

$$\int_0^\infty \omega^0(r)r\,\mathrm{d}r = 0, \ldots, \qquad \int_0^\infty \omega^0(r)r^{2n-1}\,\mathrm{d}r = 0, \qquad \int_0^\infty \omega^0(r)r^{2n+1}\,\mathrm{d}r \neq 0\,,$$

then

$$\lim_{t\to\infty} \omega(r;t) = \frac{\text{constant}}{n!(2t+1)^{n+1}}\,L_n\!\left(\frac{r^2}{4t+2}\right)\exp\!\left\{-\frac{r^2}{4t+2}\right\}. \tag{78}$$

A double expansion in one-dimensional similarity solutions should also work on $\mathbf{R}^2$ and one may wonder therefore at this point how expansions based on similarity solutions in cylindrical coordinates are related to the double expansions presented earlier in this section (both should yield the same results of course). The easiest way to find out is as follows. Any initial condition in $L^2(\mathbf{R}^2, \mathrm{e}^{\frac{1}{2}|\mathbf{x}|^2})$ can either be expanded according to (39) or (51). By equating the expressions for the evolution in these two different forms, given by (41) and

(53) respectively,

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{a'_{nm}}{b(t)^{2+n+m}}\,\Omega_n\left(\frac{x_1}{b(t)}\right)\Omega_m\left(\frac{x_2}{b(t)}\right)=\sum_{l=0}^{\infty}\sum_{k=-l}^{+l}\frac{a_{lk}}{b(t)^{2l+2-|k|}}\,\Phi_{lk}\left(\frac{r}{b(t)},\theta\right), \tag{79}$$

terms on the left-hand side can be identified with terms on the right-hand side by equating powers of $b(t)$. For instance, in the case of the Rankine vortex discussed above, the lowest power is $b(t)^{-2}$ ($l=k=0$). This implies that the first term in the expansion derived for the Rankine vortex should be equal to the term in the double expansion with $n=m=0$. Therefore one necessarily has

$$a'_{00}\Omega_0\left(\frac{x_1}{b(t)}\right)\Omega_0\left(\frac{x_2}{b(t)}\right)=\frac{1}{2}\exp\left\{-\frac{1}{2}\frac{x_1^2+x_2^2}{b(t)^2}\right\}$$

(remember, the first expansion coefficient was $a_{00}=a_0=\frac{1}{2}$ and $r^2=x_1^2+x_2^2$). With (23) one sees

$$a'_{00}\Omega_0\left(\frac{x_1}{b(t)}\right)\Omega_0\left(\frac{x_2}{b(t)}\right)=\frac{a'_{00}}{\sqrt{2\pi}}\exp\left\{-\frac{1}{2}\frac{x_1^2}{b(t)^2}\right\}\exp\left\{-\frac{1}{2}\frac{x_2^2}{b(t)^2}\right\},$$

where use has been made of the fact that $H_0(x)=1$. So all that remains to be checked is whether $a'_{00}=\sqrt{\pi/2}$. This indeed is verified with the elementary calculation of a'_{00} according to (40)

$$\begin{aligned}a'_{00}&=\int_{-1}^{+1}\int_{-\sqrt{1-x_2^2}}^{+\sqrt{1-x_2^2}}\frac{H_0(x_1/\sqrt{2})}{\sqrt{\sqrt{2\pi}}}\,\frac{H_0(x_2/\sqrt{2})}{\sqrt{\sqrt{2\pi}}}\,\mathrm{d}x_1\,\mathrm{d}x_2\\&=\frac{1}{\sqrt{2\pi}}\int_{-1}^{+1}2\sqrt{1-x_2^2}\,\mathrm{d}x_2=\frac{\pi}{\sqrt{2\pi}}\,.\end{aligned}$$

Compatibility of the higher-order terms can also be checked, with considerable more effort however. One has, for instance,

$$H_0\left(\frac{x_1}{\sqrt{2}}\right)H_2\left(\frac{x_2}{\sqrt{2}}\right)+H_2\left(\frac{x_1}{\sqrt{2}}\right)H_0\left(\frac{x_2}{\sqrt{2}}\right)\propto L_1\left(\frac{1}{2}r^2\right)$$

and

$$H_1\left(\frac{x_1}{\sqrt{2}}\right)H_0\left(\frac{x_2}{\sqrt{2}}\right)\propto rL_1^1\left(\frac{1}{2}r^2\right)\cos\theta\,,$$

$$H_0\left(\frac{x_1}{\sqrt{2}}\right)H_1\left(\frac{x_2}{\sqrt{2}}\right)\propto rL_1^1\left(\frac{1}{2}r^2\right)\sin\theta\,,$$

and so on. An interesting set of relations between products of Hermite polynomials and functions of type $r^mL_n^m(\frac{1}{2}r^2)\cdot(\cos m\theta, \sin m\theta)$ can be based on the correspondence expressed by (79).

As a second example, similarity solutions in spherical coordinates will briefly be discussed here. The set of orthogonal functions derived below is complete in $L^2(\mathbf{R}^3, e^{\frac{1}{2}|\mathbf{x}|^2})$ and will therefore be useful for problems in which the initial conditions or the particular geometry of the domain have simple expressions in spherical coordinates. First of all it is noted that the diffusion equation in spherical coordinates is given by

$$\frac{\partial C}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C}{\partial r}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial C}{\partial\vartheta}\right) + \frac{1}{\sin\vartheta^2}\frac{\partial^2 C}{\partial\varphi^2}\right\}, \tag{80}$$

where the spherical coordinates (r, ϑ, φ) are related to the rectangular coordinates (x_1, x_2, x_3) according to:

$$\begin{aligned} r^2 &= x_1^2 + x_2^2 + x_3^2 \qquad &(0 \leq r < \infty)\,, \\ \tan\vartheta &= (x_1^2 + x_2^2)^{\frac{1}{2}}/x_3 \qquad &(0 \leq \vartheta \leq \pi)\,, \\ \tan\varphi &= x_2/x_1 \qquad &(0 \leq \vartheta < 2\pi)\,. \end{aligned} \tag{81}$$

The similarity ansatz is

$$C(r, \vartheta, \varphi; t) = \frac{1}{a(t)} C^0\left(\frac{r}{b(t)}\right)\Theta_{lk}(\vartheta)\Phi_k(\varphi) \tag{82}$$

where $\Phi_k(\varphi)$ is a normalized trigonometric function

$$\Phi_k(\varphi) = \frac{1}{\sqrt{2\pi}} e^{ik\varphi} \quad (k = 0, \pm 1, \pm 2, \ldots) \tag{83}$$

and $\Theta_{lk}(\vartheta)$ a normalized associated Legendre polynomial (for a definition, see [4])

$$\Theta_{lk}(\vartheta) = \left\{\frac{2l+1}{2}\frac{(l-|k|)!}{(l+|k|)!}\right\}^{\frac{1}{2}} P_l^{|k|}(\cos\vartheta) \quad (l = |k|, |k|+1, \ldots) \tag{84}$$

which has the property

$$\int_0^\pi \Theta_{lk}(\vartheta)\Theta_{l'k}(\vartheta)\sin\vartheta \, d\vartheta = \int_{-1}^{+1} \Theta_{lk}(z)\Theta_{l'k}(z)\, dz = \delta_{ll'} \tag{85}$$

where $z \equiv \cos\vartheta$. The set $\Theta_{lk}(z)$ (with fixed k) is known to be complete in $L^2(-1, +1)$ (see [8]). In conjunction with completeness of the trigonometric functions, it follows that the product set

$$\psi_{lk}(\vartheta, \varphi) = \Theta_{lk}(\vartheta)\Phi_k(\varphi) \tag{86}$$

with

$$\int_0^{2\pi}\int_0^\pi \psi_{lk}(\psi_{l'k'})^* \sin\vartheta \, d\vartheta \, d\varphi = \delta_{ll'}\delta_{kk'} \tag{87}$$

is complete for functions that are square-integrable on a sphere (remember that a surface element on a sphere is equal to $r^2 \sin\vartheta \, d\vartheta \, d\varphi$). One may also use 'spherical harmonics' instead of these functions, in which case the notation slightly simplifies but by which nothing is gained here. No generality has been lost therefore by putting possible similarity solutions in the form given by (82) since any square-integrable function can be written as a sum of functions with separated dependence on the angular coordinates ϑ and φ is this way. Since in most standard text books on mathematical physics or quantum mechanics the properties of associated Legendre polynomials are discussed, it will merely be noted here that if (82) is substituted in (80), and if $a(t)$ and $b(t)$ are again as in (9) (with $\beta = 1$), after separation the following equation for C^0 is obtained

$$\frac{d^2C^0}{ds^2} + \frac{2}{s}\frac{dC^0}{ds} + \left\{\alpha - \frac{l(l+1)}{s^2}\right\}C^0 + s\frac{dC^0}{ds} = 0 \tag{88}$$

where the similarity variable $s \equiv r/b(t)$ has been introduced. The factor $l(l+1)$ is the separation constant that comes from the separated equation for the associated Legendre polynomial. By putting

$$C^0 = y^{\frac{1}{2}l}\,e^{-y}L(y) \tag{89}$$

with $y \equiv \frac{1}{2}s^2$, again, as in the cylindrical case, a Laguerre equation is found for the remaining unknown part of the possible similarity solutions

$$y\frac{d^2L}{dy^2} + \left(l + \frac{1}{2} + 1 - y\right)\frac{dL}{dy} + \frac{1}{2}(\alpha - 3 - l)L = 0\,. \tag{90}$$

This equation has polynomial solutions only for $\frac{1}{2}(\alpha - 3 - l) = m = 0, 1, 2, \ldots$, in which case L is a generalised Laguerre polynomial (see [4])

$$L(y) = L_m^{(l+\frac{1}{2})}(y) = \frac{e^y}{m!\,y^{l+\frac{1}{2}}}\frac{d^m}{dy^m}\left(y^{m+l+\frac{1}{2}}e^{-y}\right). \tag{91}$$

A particular set of similarity solutions in spherical coordinates thus has a radial structure given by (remember that (89) was substituted)

$$(\tfrac{1}{2}r^2)^{\frac{1}{2}l}\,e^{-\frac{1}{2}r^2}L_m^{(l+\frac{1}{2})}(\tfrac{1}{2}r^2)\,.$$

Completeness of the set

$$\Upsilon_n^{(\mu)}(y) = \sqrt{\frac{\Gamma(n+1)}{\Gamma(n+\mu+1)}}\,y^{\frac{1}{2}\mu}\,e^{-\frac{1}{2}y}L_n^{(\mu)}(y)$$

with

$$\int_0^\infty \Upsilon_n^{(\mu)}\Upsilon_m^{(\mu)}\,dy = \delta_{nm}$$

in $L^2(\mathbf{R}^+)$ (see [8]), together with completeness of the set given by (86) on surfaces $r =$ constant, proves that the normalized similarity solutions

$$\Psi_{mlk} = \frac{1}{\sqrt{\sqrt{2}}}\sqrt{\frac{\Gamma(m+1)}{\Gamma(m+l+1+\frac{1}{2})}}\,(\tfrac{1}{2}r^2)^{\frac{1}{2}l}\,e^{-\frac{1}{2}r^2}L_m^{(l+\frac{1}{2})}(\tfrac{1}{2}r^2)\Theta_{lk}(\vartheta)\Phi_k(\varphi) \tag{92}$$

with

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi_{mlk}(\Psi_{m'l'k'})^* \, e^{\frac{1}{2}r^2} r^2 \sin\vartheta \, d\varphi \, d\vartheta \, dr = \delta_{mm'}\delta_{ll'}\delta_{kk'} \tag{93}$$

are complete in $L^2(\mathbf{R}^3, e^{\frac{1}{2}|x|^2})$ and thus form a basis. If an initial condition $C^0(r, \vartheta, \varphi)$ is in $L^2(\mathbf{R}^3, e^{\frac{1}{2}|x|^2})$, it can be expanded in a sum of similarity solutions

$$C^0(r, \vartheta, \varphi) = \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \sum_{k=-l}^{+l} a_{mlk} \Psi_{mlk}(r, \vartheta, \varphi) \,. \tag{94}$$

The expansion coefficients are calculated with

$$a_{mlk} = \int_0^\infty \int_0^\pi \int_0^{2\pi} C^0 \Psi^*_{mlk} \, e^{\frac{1}{2}r^2} r^2 \sin\vartheta \, d\varphi \, d\vartheta \, dr \,. \tag{95}$$

By definition one has $\alpha = 2m + 3 + l$, so the evolution is given by

$$C(r, \vartheta, \varphi; t) = \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \sum_{k=-l}^{+l} \frac{a_{mlk}}{b(t)^{2m+3+l}} \Psi_{mlk}\left(\frac{r}{b(t)}, \vartheta, \varphi\right) . \tag{96}$$

An alternative set that forms a basis for $L^2(\mathbf{R}^3, e^{\frac{1}{2}|x|^2})$ is, of course, the product set of the one-dimensional similarity solutions Ω_n – of Section 3 – with the cylindrical similarity solutions Φ_{nk} of this section.

All possibilities encountered so far have been solutions in coordinate systems that allow for simple separation of the equation that is derived by substituting the similarity ansatz in the diffusion equation. A necessary condition for such simple separable solutions to exist, is that the Helmholtz equation in the particular coordinates can be separated. The list of coordinate systems with this property is quite impressive (see [11]), but of all these very few remain if additionally separability of similarity solutions is imposed. The author has found one more possibility, in addition to the examples already discussed, namely in conical coordinates (r, θ, λ) (see [11] for an extensive discussion of this probably unfamiliar coordinate system). In these coordinates similarity solutions are products of generalized Laguerre polynomials (in the similarity variable $r/b(t)$) with Lamé polynomials in θ and λ. Completeness etc. can straightforwardly be deduced from classical results concerning these polynomials. These similarity solutions form a basis too for semi-infinite domains that are bounded by elliptic cones. With this briefly-mentioned final example, all simple separable possibilities seem to have been touched upon. It may be possible that other highly exotic ones can be found, but for most practical purposes the sets of orthogonal similarity solutions presented will suffice.

5. Discussion

It has been shown that the similarity solutions of the diffusion equation form a basis for the Hilbert space $L^2(\mathbf{R}^n, e^{\frac{1}{2}|x|^2})$. As a consequence, the large-time asymptotic behaviour of initial value problems on infinite and certain semi-infinite domains could be uncovered without much effort. This result could prove to be quite useful, since for many practical purposes it is often of considerable interest to have a knowledge of the large-time structure of the evolving field. The examples discussed in this paper, i.e. sets of similarity solutions in rectangular, cylindrical, spherical and conical coordinates, appear to cover all possible coordinate systems that allow for expansions on semi-infinite domains if Dirichlet or Neumann conditions are imposed on coordinate surfaces. In a more general context these orthogonal functions are of quite some interest too. For instance, computational strain may considerably be lessened if they are used for discrete spectral representations of fields where otherwise some continuous Fourier transform would be calculated. As a final remark it is noted here that the one-dimensional similarity solutions as well as the angle-independent cylindrical similarity solutions have been known for a while, whereas all other ones appear not to have been reported thus far.

Acknowledgement

The author gratefully acknowledges financial support from the working group on Meteorology and Physical Oceanography (MFO) of the Netherlands Organization of Scientific Research (NWO).

References

1. J. Crank, *The mathematics of diffusion*, Clarendon Press, Oxford (1975).
2. G.K. Batchelor, *An introduction to fluid dynamics*, Cambridge University Press, Cambridge (1967).
3. H.S. Carslaw and J.C. Jaeger, *Conduction of heat in solids*, Clarendon Press, Oxford (1959).
4. P.M. Morse and H. Feshbach, *Methods of theoretical physics*, McGraw-Hill, New York (1953).
5. G.W. Bluman and J.D. Cole, *Similarity methods for differential equations*, Appl. Math. Sci., No 13, Springer-Verlag, New York (1974).
6. P.J. Olver, *Applications of Lie groups to differential equations*, Springer-Verlag, New York (1986).
7. R.C. Kloosterziel and G.J.F. van Heijst, The evolution of stable barotropic vortices in a rotating free-surface fluid, submitted to *J. Fluid Mech.* (1990).
8. J.R. Higgins, *Completeness and basic properties of sets of special functions*, Cambridge University Press, Cambridge (1977).
9. G. Birkhoff, *Hydrodynamics – a study in logic, fact and similitude*, Princeton University Press, Princeton (1950).
10. M. Abramowitz and I.A. Stegun (ed.), *Handbook of mathematical functions*, Dover, New York (1965).
11. P. Moon and D.E. Spencer, *Field theory handbook*, Springer-Verlag, New York (1988).