

**REVISITING DIFFUSION:  
SELF-SIMILAR SOLUTIONS AND THE  $t^{-1/2}$  DECAY IN INITIAL  
AND INITIAL-BOUNDARY VALUE PROBLEMS**

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**Abstract.** The diffusion equation is a universal and standard textbook model for partial differential equations (PDEs). In this work, we revisit its solutions, seeking, in particular, self-similar profiles. This problem connects to the classical theory of special functions and, more specifically, to the Hermite as well as the Kummer hypergeometric functions. Reconstructing the solution of the original diffusion model from self-similar solutions of the associated self-similar PDE, we infer that the  $t^{-1/2}$  decay law of the diffusion amplitude is *not necessary*. In particular, it is possible to engineer setups of *both* the Cauchy problem and the initial-boundary value problem in which the solution decays at a *different rate*. Nevertheless, we observe that the  $t^{-1/2}$  rate corresponds to the dominant decay mode among integrable initial data, i.e., ones corresponding to finite mass. Hence, unless the projection to such a mode is eliminated, generically this decay

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will be the slowest one observed. In initial-boundary value problems, an additional issue that arises is whether the boundary data are *consonant* with the initial data; namely, whether the boundary data agree at all times with the solution of the Cauchy problem associated with the same initial data, when this solution is evaluated at the boundary of the domain. In that case, the power law dictated by the solution of the Cauchy problem will be selected. On the other hand, in the non-consonant cases a decomposition of the problem into a self-similar and a non-self-similar one is seen to be beneficial in obtaining a systematic understanding of the resulting solution.

**1. Introduction.** The model of diffusion is a textbook one both at the microscopic level of Brownian motion [1], as well as at the macroscopic PDE level and its mathematical analysis [2, 3], hence it needs no particular introduction. In its one-dimensional form, to which we will restrict our considerations herein, it reads

$$u_t = u_{xx}, \quad (1.1)$$

where  $u = u(x, t)$  represents a physical (dependent) variable such as temperature or concentration, and the subscripts denote partial derivatives with respect to time  $t$  and space  $x$ . This is a model so widely studied that it is hard to envision any elements of novelty in its study at present.

Nevertheless, the 1969 work of [4] identified an apparently previously unknown class of solutions of equation (1.1) using the method of similarity variables. When connecting with the special case of self-similar solutions whose spatial dependence arises in terms of the traditional self-similar variable  $x/t^{1/2}$ , the authors of [4] derive special solutions associated with parabolic cylinder functions (a special case of the confluent hypergeometric series). In this context, they remark that in order to have a solution vanishing (“actually exponentially”, as they point out) as the similarity variable tends to  $\pm\infty$ , these special solutions must be characterized by an integer index. They also remark that if the total mass is constant, then the “standard” solution, namely

$$u(x, t) \propto t^{-1/2} e^{-\frac{x^2}{4t}}, \quad (1.2)$$

must be chosen. The application of the method was subsequently extended to boundary value problems [5], while other authors extended it to a variety of different settings including, e.g., Schrödinger-type equations [6], and the sine-Gordon [7], non-linear diffusion [8], and non-linear Boltzmann equation [9].

The identification of similarity solutions is also by now a textbook subject [10, 11]; see also the Appendix of [12] for a discussion of relevant solutions in the context of density distributions of domain walls in the Potts model in the limit of an infinite number of states. Nevertheless, a recent methodology, occasionally referred to as MN-dynamics [13] (see also [14, 15], as well as [16], where a general formulation thereof was presented for non-linear PDE problems) offers a simple and systematic alternative to deriving such waveforms and the corresponding scaling properties. It is worthwhile to note in passing that there is a considerable volume of literature in the study of such problems in dispersive equations; see, e.g., [17, 18]. It is this MN-dynamics methodology that we will adopt here, in a prototypical problem such as the diffusion equation.

What we first obtain is in fact the self-similar solutions of [4], but now for *arbitrary* real values of the relevant index as opposed to just integer values of this index. From this, we infer that scaling laws including but certainly not limited by the standard  $t^{-1/2}$  law of equation (1.2) are not only feasible, but actually entirely realizable in both the initial value (Cauchy) problem and the initial-boundary value problem setting (in the case of finite domain considerations). These decay laws can bear an *arbitrary* negative exponent in the (temporal) scaling of the solution amplitude. It is shown on the basis of a general class of initial conditions and of the (full) solution of the MN-dynamics problem that the  $t^{-1/2}$  decay is the slowest one (for integrable initial data of finite mass), and it is explained under what conditions a different decay rate is observed.

Similar considerations are relevant to examine when boundary conditions are present. Furthermore, it is now important to also discuss the role of conservation laws. In this case, we introduce the notions of *compatible* and *consonant* boundary conditions. The former ones are identified as boundary conditions that agree with the initial condition at the endpoints of the spatial domain and at time  $t = 0$  (but not necessarily at all times), while the latter ones correspond to boundary conditions that match at all times the solution of the associated Cauchy problem, when this solution is evaluated at the boundary of the domain of the initial-boundary value problem.

As we will see below, in the case of the Cauchy problem there exist initial data for which there are “eigenfunctions” that lead to self-similar evolution with a specific decay rate. On the other hand, there are initial conditions that do not project solely on one such eigenfunction but have a finite projection on multiple modes, decaying at different rates and resulting in non-self-similar evolution with a single rate of decay.

Similarly, in the case of initial-boundary value problems there are choices of boundary conditions that are conducive to self-similar dynamics, and others that are not. The latter category includes typical examples taught in undergraduate courses, such as homogeneous Dirichlet, homogeneous Neumann, and constant coefficient Robin conditions (cf., e.g., Chapter 4 in [2]). These case examples, which are solvable by different forms of Fourier series and bear the associated exponential time dependence, are not inherently self-similar. In the conducive category, there are time-dependent boundary conditions that are consonant with self-similar evolution. For instance, let us consider an exact eigenfunction of the self-similar MN diffusion problem discussed above, and boundary conditions that are consonant with it (i.e., in agreement with the value of the relevant eigenfunction at the boundaries of the domain over all times). It is clear that in this case the solution is “transparent” to the presence of the boundary conditions. In this setting, we can still engineer solutions with various kinds of decay rates (different from  $t^{-1/2}$ ).

Another intriguing possibility is that of boundary conditions that are compatible with the initial condition (e.g. continuous so as to avoid Gibbs-type phenomena [2]), yet not consonant. In this scenario, we will advocate the decomposition of the problem into (i) an initial-boundary value problem which is both consonant and compatible, takes care of the boundary conditions, and (ii) a complementary problem with homogeneous boundary data that does not have a self-similar solution. In what follows, we will restrict our considerations to the above cases and will not examine the definitively non-self-similar

evolutions of general boundary conditions that are neither consonant, nor compatible with any self-similar waveform.

Our presentation is structured as follows. In Section 2, we present the MN-dynamics approach for the diffusion equation and its basic conclusions. In Section 3, we consider a number of select numerical experiments in the initial-boundary value problem setting. Finally, in Section 4 we summarize our findings and provide a discussion of future perspectives.

**2. Theoretical analysis: Self-similar solutions.** As discussed in [13–15] (see also the recent exposition in the Appendix of [16]), the scaling ansatz for seeking a self-similar solution of equation (1.1) via the MN-dynamics approach is of the form

$$u(x, t) = A(\tau)w(\xi, \tau), \quad \xi = \frac{x}{L(\tau)}, \quad \tau = \tau(t), \tag{2.1}$$

where  $\xi$  is the similarity variable and the functions  $\tau$ ,  $A$  and  $L$  are to be determined.

Direct substitution and division by  $A$  yields

$$\left( w_\tau + \frac{A_\tau}{A}w - G\xi w_\xi \right) \tau_t = \frac{1}{L^2}w_{\xi\xi}. \tag{2.2}$$

In the above equation, we have set

$$\frac{L_\tau}{L} \doteq G = \text{const.} > 0, \tag{2.3}$$

assuming that in the  $(\xi, \tau)$  frame the solution has a constant rate of expansion of its width during its self-similar evolution. From this, it is immediate to infer that

$$L(\tau) = L_0 e^{G\tau}. \tag{2.4}$$

To obtain solutions that are steady in the self-similar frame, the explicit time dependence must be eliminated by necessitating that

$$\tau_t = \frac{1}{L^2}. \tag{2.5}$$

Substitution of  $L$  given by equation (2.4) into equation (2.5) yields the relation between the old and new time frames as

$$e^\tau = \left[ \frac{2G}{L_0^2} (t - t^*) \right]^{\frac{1}{2G}}. \tag{2.6}$$

As will be evident below, the positive constant  $G$  can be scaled out of the equations. Hence, upon manifesting this scaling, we will select  $G = 1$  for simplicity. Moreover, evaluating equation (2.6) at  $t = 0$  naturally reveals that  $t^* < 0$ , suggesting the well-known feature that diffusion processes blow up in reverse time. Note that in the rescaled temporal variable, this time corresponds to  $\tau \rightarrow -\infty$ .

A key observation that distinguishes the present problem from other ones where the above method has been applied (such as, e.g., [15, 16]) is that now the amplitude scaling is *not* fixed by the PDE dynamics (self-similarity of the first kind [13]), but rather it

has to be obtained from the solution of an eigenvalue problem (see below; this is the self-similarity of the second kind [13]). In particular, we have the freedom to select

$$\frac{A_\tau}{A} \doteq b = \text{const.}, \tag{2.7}$$

which in turn leads to

$$A(\tau) = A_0 e^{b\tau}, \tag{2.8}$$

or, in the original frame via equation (2.6),

$$A(t) = A_0 \left[ \frac{2}{L_0^2} (t - t^*) \right]^{\frac{b}{2}}. \tag{2.9}$$

Upon the above scaling choices, the original PDE in the renormalized frame, i.e., equation (2.2), can be expressed as

$$w_\tau = w_{\xi\xi} + \xi w_\xi - bw. \tag{2.10}$$

Making the additional explicit transformation

$$w = e^{-\xi^2/2} W, \tag{2.11}$$

as well as slightly modifying the  $(\xi, \tau)$  frame according to the change of variables

$$\xi \rightarrow \tilde{\xi} = \frac{\xi}{\sqrt{2}}, \quad \tau \rightarrow \tilde{\tau} = \frac{\tau}{2}, \tag{2.12}$$

we obtain in the new  $(\tilde{\xi}, \tilde{\tau})$  frame the equation

$$W_{\tilde{\tau}} = W_{\tilde{\xi}\tilde{\xi}} - 2\tilde{\xi}W_{\tilde{\xi}} + 2\nu W, \tag{2.13}$$

where

$$\nu = -(b + 1). \tag{2.14}$$

The steady state problem of equation (2.13) (i.e., the one obtained by setting the right hand side equal to zero) is *precisely* the Hermite differential equation.

From this reduction, we can infer the self-similar solutions, thereby connecting the results with the earlier work of [4]. If we assume, in particular, that in the renormalized frame the motion is self-similar in the original variables (i.e., steady in the new frame), then the resulting solutions are of the form

$$w = e^{-\frac{\xi^2}{2}} \left[ c_1(\nu) H_\nu \left( \frac{\xi}{\sqrt{2}} \right) + c_2(\nu) {}_1F_1 \left( -\frac{\nu}{2}, \frac{1}{2}, \frac{\xi^2}{2} \right) \right], \tag{2.15}$$

where  $H_\nu$  denote the Hermite functions and  ${}_1F_1$  denote the so-called Kummer confluent hypergeometric series functions. These solutions are also related to the so-called Weber or parabolic cylinder functions (see [19] for more details).

It is now important to clarify some points regarding the solutions (2.15). First, the Kummer functions are *even* for any value of  $\nu$ . On the other hand, the Hermite functions have definite parity only in the case of *integer*  $\nu$ . Actually, in that case they reduce to the well-known Hermite polynomials, which are even for  $\nu$  even and odd for  $\nu$  odd. Furthermore, importantly, and *differently* from what was suggested in [4],  $\nu$  does *not* have to be an integer. Indeed, the solutions of equation (2.10) are still well-defined functions for any  $\nu$  (equivalently,  $b$ ) real. However, as may be evident when interpolating

between, e.g., an even and an odd value of  $\nu$ , the Hermite solution  $H_\nu$  for general  $\nu$  is an *asymmetric* one.

Another key point to make is that bounded solutions exist only for  $b < 0$  (equivalently, for  $\nu > -1$ ), while integrable solutions exist only for  $b < -1$  (equivalently, for  $\nu > 0$ ). These distinctions will be important in what follows, not only for mathematical reasons but also for physical ones, since integrability here is tantamount to finite mass, a requirement of particular physical relevance. Yet another important observation concerns asymptotic properties. In the case of integer  $\nu$ , the standard asymptotic properties that we expect from the Hermite polynomials in connection to  $w$  apply, i.e., asymptotically the solutions decay as  $w \sim \xi^\nu e^{-\xi^2/2}$ ; this is the case referred to in [4]. *However*, in the case where this integer “quantization” of  $\nu$  is absent, the stationary series solution of equation (2.13) does not close as a regular, finite-order polynomial. Instead, it produces a more general function and, in this case, it is known [20] that, e.g., for the Kummer solution the asymptotics as the argument tends to infinity are

$${}_1F_1(\alpha, \beta; z) = e^z z^{\alpha-\beta} \frac{\Gamma(\beta)}{\Gamma(\alpha)}. \tag{2.16}$$

Straightforward substitution reveals that in this general, non-quantized case the asymptotics decay in the form of a power law according to  $w \sim \xi^b$ , once again suggesting that for decay, we need  $b < 0$ , while for integrability we must have  $b < -1$ .

Another important observation concerns the cases where  $\nu$  is an even integer. In this case, the two solutions of equation (2.10) *coincide*. This is natural to expect since for these particular values the Hermite polynomials are even and, as mentioned previously, the Kummer functions are always even. Hence, a second linearly independent solution must be present for  $\nu$  even. This can be found on a case-by-case basis. For example, for  $\nu = 0$  ( $b = -1$ ) this is  $w = e^{-\xi^2/2} \text{Erfi}(\xi/\sqrt{2})$  (where Erfi is the imaginary error function). Similarly, for  $\nu = 2$  ( $b = -3$ ) we have  $w = 2\xi + \sqrt{2\pi} (1 - \xi^2) e^{-\xi^2/2} \text{Erfi}(\xi/\sqrt{2})$ , and so on.

The general features of the Hermite and Kummer components of the steady state, self-similar solution (2.15) of equation (2.10) discussed above are visualized in Fig. 2.1. In the left column of Fig. 2.1, we provide plots of the Hermite component against  $\xi$  for various choices of  $b = -(\nu + 1)$ . The same is done for the Kummer component in the right column of Fig. 2.1. Note that for the cases shown with  $b > -1$ , the non-integrability of the wavefunction is a result of the slow decay in both figures. Moreover, note that for  $b < -1$  the solution also acquires negative values, a feature somewhat atypical for diffusional dynamics when considering the model, e.g., for chemical concentrations.

Armed with the above special (self-similar) solutions, we can actually solve the original problem of equation (1.1) in the basis most naturally tailored to address self-similar evolution profiles, namely the basis of stationary solutions (2.15) of equation (2.10). To do so in a more general form, we separate variables in equation (2.10) using  $w(\xi, \tau) = X(\xi)T(\tau)$ . The temporal part yields directly an exponential decay of the form

$$T(\tau) \sim e^{-\lambda\tau}, \tag{2.17}$$

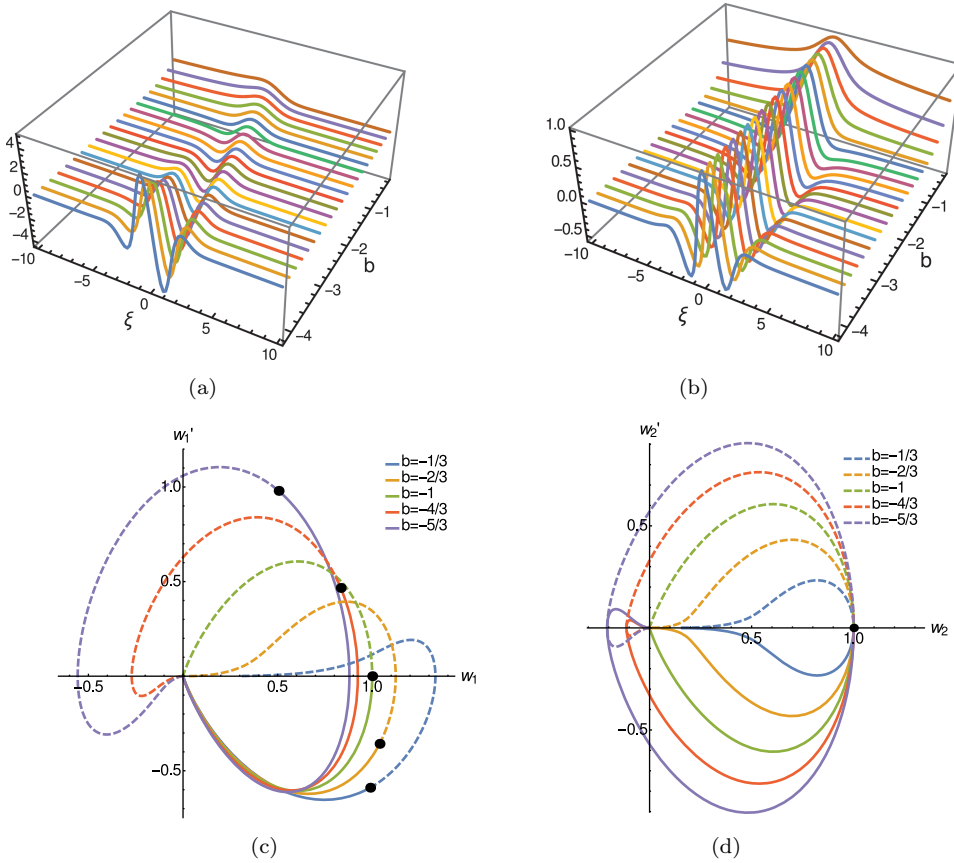


FIG. 2.1. *Left and right columns respectively correspond to the Hermite component  $w_1 = e^{-\xi^2/2} H_\nu(\xi/\sqrt{2})$  and the Kummer component  $w_2 = e^{-\xi^2/2} {}_1F_1(-\nu/2, 1/2, \xi^2/2)$  (recall  $\nu = -b - 1$ ) of the steady state, self-similar solution (2.15). (a) and (b): Plots of  $w_1$  and  $w_2$  against both  $\xi$  and  $b$ . (c) and (d): Phase portraits, i.e. plots of  $w'_{1,2}$  against  $w_{1,2}$ , for  $\xi \in (-\infty, 0]$  (dashed)  $\cup [0, \infty)$  (solid) and various values of  $b$ . The black dots correspond to  $\xi = 0$ .*

where  $\lambda$  is a suitable eigenvalue, while the (rescaled) spatial part  $X(\xi)$  satisfies the same ODE as the steady state problem of (2.10), but now with the substitution

$$b \rightarrow \tilde{b} = b - \lambda. \quad (2.18)$$

Hence, using the separated variables solutions we can *formally* construct a linear superposition of the solutions of equation (2.10) as

$$w(\xi, \tau) = e^{-\frac{\xi^2}{2}} \int_{\lambda} e^{-\lambda\tau} \left[ c_1(\lambda) H_{\tilde{\nu}} \left( \frac{\xi}{\sqrt{2}} \right) + c_2(\lambda) {}_1F_1 \left( -\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{\xi^2}{2} \right) \right] d\lambda, \quad (2.19)$$

where

$$\tilde{\nu} = -(b - \lambda + 1). \quad (2.20)$$

The superposition (2.19) is done at a formal level, since the range of the relevant parameter  $\lambda$  and the associated decay and smoothness properties of  $c_1(\lambda), c_2(\lambda)$  have not been specified. In fact, for solutions lying in most function spaces it is unclear what the range of integration in (2.19) or the properties of the kernel functions  $c_1(\lambda), c_2(\lambda)$  should be. In the case of e.g.  $\lambda$  spanning over all real numbers, it is not known whether the “component” functions  $H_{\tilde{\nu}}(\xi/\sqrt{2})$  and  ${}_1F_1(-\tilde{\nu}/2, 1/2, \xi^2/2)$  form a well-defined basis (with an appropriate inner product, etc.).

On the other hand, it can be shown [21] (see also [22]) that for exponentially decaying initial data, there exists a Hilbert space such that the superposition equation (2.19) “collapses” in such a way that only the “quantized” modes associated with  $\tilde{\nu} \in \mathbb{Z}$  survive, and that the resulting sum gives a convergent representation of the solution for all times. In that case, spectral projections and decompositions are well defined and the solution of equation (2.10) is indeed given by a variant of equation (2.19) expressed as a sum over these integer indices.

From a function-analytic perspective, an understanding of how to incorporate the continuum of power law decay solutions into the superposition of the quantized, integer-indexed, exponentially decaying ones represents a particularly timely and relevant direction for future work. In our numerical computations presented in the following section, we will focus chiefly on rapidly decaying initial data. Nevertheless, we have confirmed that power law solutions (of the type identified above) can be observed for all times by employing suitable choices of initial conditions and corresponding consonant boundary conditions.

We now return to the frame of the original variables  $(x, t)$  in order to reconstruct the superposition appearing in equation (2.19). Combining equations (2.4), (2.6), (2.8) and (2.19) with equation (2.1), we thereby arrive at the solution formula

$$u(x, t) = e^{-\frac{x^2}{4(t-t^*)}} \int_{\lambda} (t-t^*)^{\frac{b-\lambda}{2}} \left[ c_1(\lambda) H_{\tilde{\nu}} \left( \frac{x}{2\sqrt{t-t^*}} \right) + c_2(\lambda) {}_1F_1 \left( -\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{x^2}{4(t-t^*)} \right) \right] d\lambda. \tag{2.21}$$

The superposition (2.21) sheds some direct light on the selection of the  $t^{-1/2}$  amplitude decay. In particular, recall (see earlier discussion about the behavior of the stationary solution (2.15)) that in order for  $w$  as given by equation (2.19) to manifest decay as  $|\xi| \rightarrow \infty$ , we must have  $\tilde{b} < 0$ , while  $\tilde{b} < -1$  is required in order for  $w$  to be integrable with respect to  $\xi$ . Thus, among all integrable solutions of the form (2.21) (i.e., from a physical perspective, among all solutions of finite mass), the limiting case  $\tilde{b} = -1^- \Leftrightarrow \tilde{\nu} = 0^-$  corresponds to the dominant in time “mode”, since it is the one that has the slowest decay of  $t^{-1/2}$ . It is therefore this slowest mode that we should generically expect to observe in physical measurements. This is analogous, in a way, to the familiar, textbook case from separation of variables of diffusion with homogeneous boundary conditions on a finite interval. For example, in the case of homogeneous Dirichlet conditions on the interval  $[0, D]$ , the solution reads

$$u(x, t) = \sum_{n \in \mathbb{Z}} A_n e^{-\left(\frac{n\pi}{D}\right)^2 t} \sin \left( \frac{n\pi x}{D} \right), \tag{2.22}$$



and for generic initial data bearing a projection to the dominant ( $n = 1$ ) mode of equation (2.22), all additional terms die out (in this latter case exponentially fast) and only the ground state proportional to  $\sin(\pi x/D)$  survives, decaying at the rate of the slowest mode.

However, although our analysis suggests that, generically, in the Cauchy problem the dominant mode will decay like  $t^{-1/2}$ , at the same time we explicitly illustrate that it is possible to prescribe *any* rate of decay at will, provided that a suitable initial condition is prescribed. For instance, in the case of an initial condition for which the coefficient  $c_1(\lambda)$  is a Dirac  $\delta$ -function centered at  $\lambda = b+2$  (thus implying  $\tilde{\nu} = 1$  through equation (2.20)), only the mode  $H_1$  arises, whose decay rate is *different* from  $t^{-1/2}$ . In particular, for  $u(x, 0) = xe^{-x^2/2} = f(x)$ , we obtain the solution

$$u(x, t) = \frac{x}{(2t+1)^{\frac{3}{2}}} e^{-\frac{x^2}{2(2t+1)}} \equiv \frac{1}{2t+1} f(\xi), \quad (2.23)$$

where  $\xi = x/\sqrt{2t+1}$ , which is in full agreement with the prediction of the MN-dynamics approach. Here, the vanishing projection of the initial condition on the lowest-order mode enables the observation of a different rate of decay. One may wonder how this possibility is compatible with the well-known fact [3] that the unique solution of the Cauchy problem of equation (1.1) is given by the formula

$$u(x, t) = \frac{1}{\sqrt{4\pi t}} \int_{y \in \mathbb{R}} e^{-\frac{(x-y)^2}{4t}} f(y) dy. \quad (2.24)$$

Actually, equation (2.24) produces precisely the result of equation (2.23) upon its application to the corresponding initial condition. Hence, although the fundamental solution of diffusion may decay at the  $t^{-1/2}$  rate, this is by no means necessary for all self-similarly decaying solutions of the Cauchy problem (and for the analogous solutions of initial-boundary value problems, as we will see in the following section).

So far, we have established that the diffusion equation, which is a self-similar PDE, can manifest decay at different power law rates when supplemented with suitable “self-similar” initial data (i.e., data giving rise to self-similar solutions, along the directions of the “eigenfunctions” of the linear operator problem considered above). This is indeed inferred by the explicit solution of the Cauchy problem (2.24). Next, we address the question of how this conclusion is going to be affected by the presence of boundary conditions.

**3. Numerical results: Initial-boundary value problems.** We now turn our attention to the case where boundary conditions are also present. Continuing upon the discussion at the end of the previous section, properties of equation (1.1) such as the maximum principle and the comparison principle, naturally lead to the presence of a unique solution under standard (e.g. Dirichlet, Neumann, etc.) boundary conditions. This immediately suggests how the decay rates (distinct from  $t^{-1/2}$ ) that were identified in the previous section can be observed in initial-boundary value problems (IBVPs). In particular, suppose that we prescribe a self-similar solution among those determined in the previous section and supplement it with *time-dependent* boundary conditions that are consonant with this solution. For instance, continuing our example from the previous

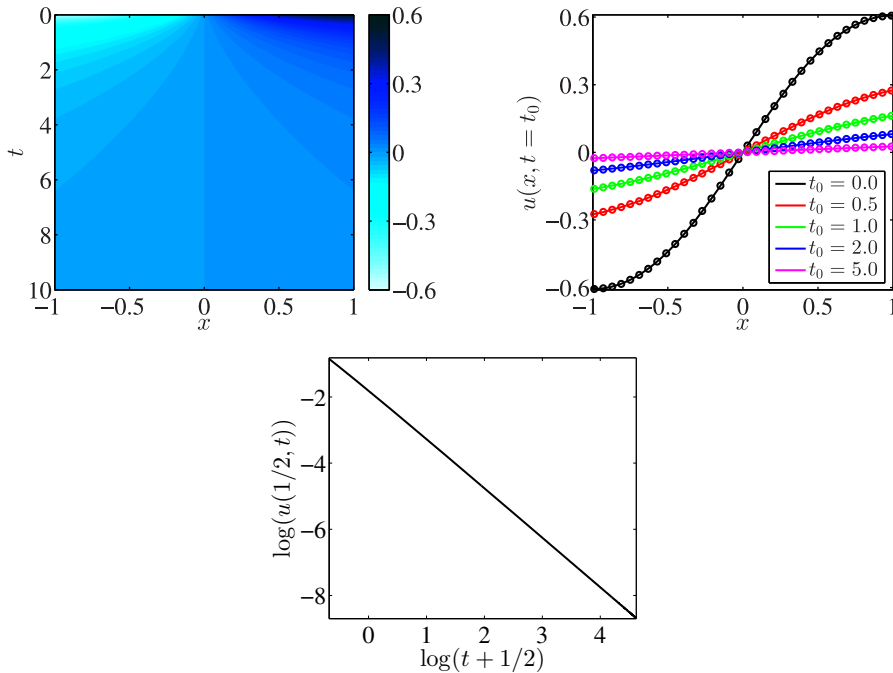


FIG. 3.1. Spatiotemporal evolution (top left panel) and spatial profiles at different times  $t = t_0$  (top right panel) of the solution of the diffusion equation (1.1) on the interval  $[-D, D]$  with initial condition  $u_0(x) = xe^{-x^2/2}$ , boundary conditions  $u(\pm D, t) = \pm \frac{D}{(2t+1)^{3/2}} e^{-\frac{D^2}{2(2t+1)}}$  and  $D = 1$ . The boundary conditions are both compatible and consonant with the initial condition; hence, the solution is simply the self-similar solution associated with the initial condition in the Cauchy problem setting [cf. equation (2.24)], and its (asymptotic for large time) decay rate is  $t^{-3/2}$  as is shown in the bottom panel of the figure.

section, let us prescribe the initial condition  $u(x, 0) = xe^{-x^2/2}$  and boundary conditions in the symmetric domain  $[-D, D]$  of the form  $u(\pm D, t) = \pm \frac{D}{(2t+1)^{3/2}} e^{-\frac{D^2}{2(2t+1)}}$ , which have been chosen to match the solution (2.23) of the Cauchy problem associated with the aforementioned initial condition.<sup>1</sup> Then, the unique solution of this IBVP (i.e., of equation (1.1) supplemented with the above initial and boundary conditions) will obviously once again be given by equation (2.23) (see Fig. 3.1). Similarly to this case example of exponentially decaying self-similar profiles, under suitable initial and boundary conditions we have confirmed (data not shown) the existence of power law solutions of equation (2.13) also for non-integer values of  $\nu$ .

That is to say, we can *engineer* variants of the IBVP for which any rate of decay is possible. In these cases, we can think of the boundary as being effectively “transparent”

<sup>1</sup>Note that in this notion of consonant boundary conditions, one does not necessarily need to prescribe Dirichlet boundary conditions that agree with the solution; other types, including (inhomogeneous) Neumann or Robin conditions, can be engineered in a similarly straightforward manner.

to the profile of the solution, enabling the structure to maintain the decay rate that would be observed in the absence of the boundary i.e., in the Cauchy problem, in the same vein as discussed above.

A question related to the presence of the boundaries, also touched upon in [4], is that of conservation laws (and, more generally, of moment equations for moments of the PDE solution). Arguably, this is especially important for a model such as diffusion, for which the mass  $M = \int_{-D}^D u dx$  obeys the conservation law

$$\frac{dM}{dt} = u_x(D, t) - u_x(-D, t). \quad (3.1)$$

Bearing in mind that the flux in this case is proportional to the (opposite of the) gradient, this suggests that the rate at which mass changes in the domain depends on how much influx (or outflux) occurs from the boundaries (at  $x = \pm D$ ). Here, again, a non-trivial difference with the work of [4] arises. In particular, for an anti-symmetric solution such as that of equation (2.23), the derivative  $u_x$  will be symmetric, hence  $dM/dt = 0$  by construction. Thus, if consonant boundary data of the Neumann type i.e., data that are obtained from the derivative of the solution evaluated at  $x = \pm D$  are considered, the mass will be *conserved*. Nevertheless, the solution will not decay with  $\tilde{\nu} = 0$  (cf. equation (2.20)), contrary to what is suggested in [4].

Hence, two important remarks so far are that (i) arbitrary decay rates of the solution *can* be prescribed even for IBVPs, yet (ii) they do not necessarily conflict with conservation of mass. It may well be that there is a mass inflow and outflow and yet the balance thereof enables the conservation of the mass within the bounded domain. Nevertheless, it is clear that the MN-dynamics solutions, and the initial conditions consonant with them, will necessitate *time-dependent* boundary conditions and hence require a time-dependent flux of mass through each one of the domain boundaries (even if this does not lead to a net flux).

In light of these remarks, Neumann conditions will control the mass flow in the system via equation (3.1). Nevertheless, any type of boundary conditions can be made to be consonant with self-similar evolution. This includes Dirichlet boundary conditions, enforcing e.g.  $u(\pm D, t) = A(t)w(\pm D/L(t))$ , or Robin boundary conditions, in which case consonance (with an exact solution  $w$ ) requires

$$u_x(\pm D, t) = \frac{w' \left( \frac{\pm D}{\sqrt{2}(t-t^*)} \right)}{w \left( \frac{\pm D}{\sqrt{2}(t-t^*)} \right)} \frac{u(\pm D, t)}{\sqrt{2}(t-t^*)}. \quad (3.2)$$

However, we now turn to a more intriguing scenario. In particular, while we can envision initial and boundary conditions consonant with the standard type of decay (i.e.,  $t^{-1/2}$ ), as well as consonant with non-standard types of decay (i.e., with a different exponent), it is also possible to consider non-consonant scenarios. In particular, it is possible to initialize Gaussian data along with boundary conditions that are compatible with it (i.e., time-dependent in a way that is continuous between initial and boundary conditions at  $t = 0$ ), yet inducing flux at a rate associated with a different power law decay.

It is also possible to initialize, e.g., in accordance with the solution of equation (2.23), initial data that are consonant with the  $t^{-1}$  decay and yet use boundary data that are consonant with  $t^{-1/2}$  decay. It is then a natural question to inquire what happens in such cases, i.e., which rate of self-similar decay is observed (if any). It should be noted again here that we choose the initial data to be compatible in order to avoid pathologies such as Gibbs-type phenomena.

Thus, we next examine the scenario of boundary conditions that are compatible but non-consonant with the initial condition. More specifically, let us consider equation (1.1) with initial condition  $u(x, 0) = e^{-x^2/2}$ , which are associated with the standard decay rate of  $t^{-1/2}$ , and boundary conditions

$$u(\pm D, t) = \frac{c^*}{t + 1} {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}, \frac{D^2}{4(t+1)}\right) e^{-\frac{D^2}{4(t+1)}}, \tag{3.3}$$

which are associated with a self-similar decay at a rate of  $t^{-1}$ . Importantly, the value of the constant  $c^*$  is chosen to enforce compatibility at  $x = \pm D$  and  $t = 0$ , namely we have

$$e^{-\frac{D^2}{2}} = c^* {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}, \frac{D^2}{4}\right) e^{-\frac{D^2}{4}}. \tag{3.4}$$

Our approach in solving this broad class of compatible yet non-consonant problems is to exploit linearity in order to decompose them into two sub-problems: one which is *both* consonant and compatible, and thus exhibits the self-similar decay imposed by the boundary conditions, and one with homogeneous boundary data (and appropriately modified initial data) which do *not* feature self-similar decay. In this way, we suggest that the solution at all times maintains a self-similar and a non-self-similar part, with the latter being described by an appropriate Fourier series solution.

More specifically, we begin by writing

$$e^{-\frac{x^2}{2}} = u_0^{(1)}(x) + u_0^{(2)}(x), \tag{3.5}$$

where

$$u_0^{(1)}(x) \doteq e^{-\frac{x^2}{2}} - u_0^{(2)}(x), \tag{3.6}$$

$$u_0^{(2)}(x) \doteq c^* {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}, \frac{x^2}{4}\right) e^{-\frac{x^2}{4}}. \tag{3.7}$$

Exploiting linearity, we then have

$$u(x, t) = u^{(1)}(x, t) + u^{(2)}(x, t), \tag{3.8}$$

where  $u^{(1)}(x, t)$  satisfies the *homogeneous Dirichlet* IBVP

$$u_t^{(1)} = u_{xx}^{(1)}, \quad x \in (-D, D), \quad t > 0, \tag{3.9a}$$

$$u^{(1)}(x, 0) = u_0^{(1)}(x), \quad x \in [-D, D], \tag{3.9b}$$

$$u^{(1)}(\pm D, t) = 0, \quad t \in [0, \infty), \tag{3.9c}$$

and  $u^{(2)}(x, t)$  is the solution of the (self-similar, i.e., both consonant and compatible) *non-homogeneous Dirichlet IBVP*

$$u_t^{(2)} = u_{xx}^{(2)}, \quad x \in (-D, D), \quad t > 0, \tag{3.10a}$$

$$u^{(2)}(x, 0) = u_0^{(2)}(x), \quad x \in [-D, D], \tag{3.10b}$$

$$u^{(2)}(\pm D, t) = u(\pm D, t), \quad t \in [0, \infty). \tag{3.10c}$$

The choice of initial and boundary conditions in IBVP (3.10) implies that the solution of this problem, due to uniqueness, must be the self-similar solution with decay rate  $t^{-1}$ , i.e.

$$u^{(2)}(x, t) = \frac{c^*}{t+1} {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}, \frac{x^2}{4(t+1)}\right) e^{-\frac{x^2}{4(t+1)}}. \tag{3.11}$$

On the other hand, in the case of the homogeneous Dirichlet IBVP (3.9) we expect the solution to decay exponentially as  $t \rightarrow \infty$ . This can be corroborated in two ways: first, by numerically solving the problem directly; and second, by evaluating the first few modes of the general “classical” sine series solution representation

$$\begin{aligned} u(x, t) = & \frac{1}{D} \sum_{n=1}^{\infty} e^{-(\frac{n\pi}{2D})^2 t} \hat{u}_0^s\left(\frac{n\pi}{2D}\right) \sin\left(\frac{n\pi(x+D)}{2D}\right) \\ & + \frac{1}{D} \sum_{n=1}^{\infty} e^{-(\frac{n\pi}{2D})^2 t} \left\{ \frac{n\pi}{2D} \left[ \tilde{g}_0\left(\left(\frac{n\pi}{2D}\right)^2, t\right) - e^{in\pi} \tilde{h}_0\left(\left(\frac{n\pi}{2D}\right)^2, t\right) \right] \right\} \sin\left(\frac{n\pi(x+D)}{2D}\right), \end{aligned} \tag{3.12}$$

where  $\hat{u}_0^s$  denotes the sine transform of  $u_0$  on  $[-D, D]$  defined by

$$\hat{u}_0^s(k) = \int_{-D}^D \sin(k(x+D)) u_0(x) dx, \tag{3.13}$$

and the vanishing – in this case – terms involving  $\tilde{g}_0$  and  $\tilde{h}_0$  are defined via equation (4.2b). The outcome of this analysis is presented in Fig. 3.2, which clearly showcases the exponential decay of the solution of this problem.

Previously, in Fig. 3.1, we verified that the transparency induced by consonant and compatible problems enables arbitrary power law decays for IBVPs. Now, in Fig. 3.3, through the accuracy of the comparison of the numerical solution with the decomposition (into problems (3.9) and (3.10)) of compatible but non-consonant IBVPs, we confirm that the solution of those problems is not genuinely self-similar, yet it can be decomposed in a self-similar power law decay and an exponential one associated with homogeneous boundary conditions.

As a final side remark and a note of caution stemming from direct numerical observations, we should point out that the case of boundary conditions that are both compatible and consonant with the initial condition can be sensitive to the choice of the size of the spatial domain  $[-D, D]$ . Indeed, although in this case one would normally expect to observe the solution decaying at the *algebraic* rate imposed by the initial data and “preserved” by the boundary data (cf. Fig. 3.1), if the choice of  $D$  is such that the size of the boundary data is smaller than machine precision, then one is effectively solving a *homogeneous* Dirichlet problem. In this scenario, one will therefore observe *exponential*,

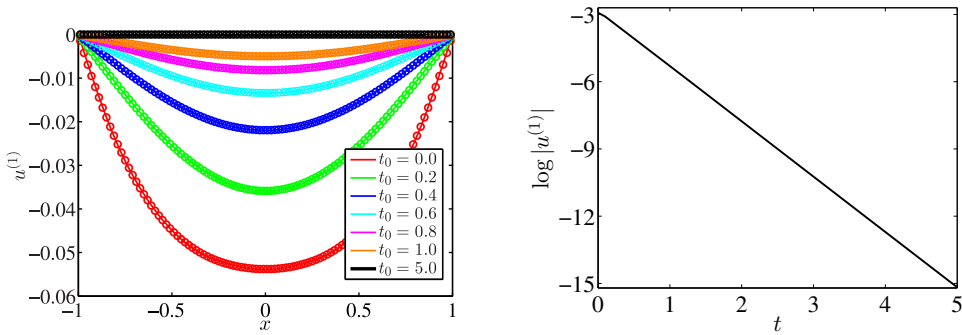


FIG. 3.2. *Left panel:* Spatial profiles of the solution  $u^{(1)}$  of the homogeneous Dirichlet IBVP (3.9) at various times  $t = t_0$ , obtained in two ways: (i) by using the first ten modes of the series representation (3.12) (solid lines); and (ii) by directly solving the IBVP numerically (open circles). *Right panel:* Plot of  $\log|u^{(1)}(0, t)|$ . As expected, the solution decays exponentially to zero with  $t$ .

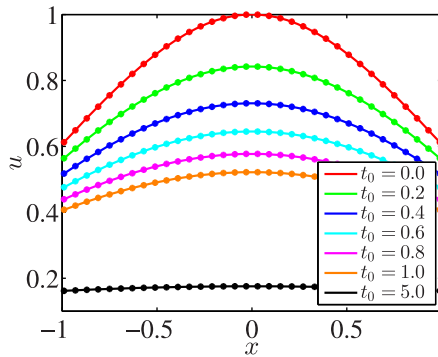


FIG. 3.3. Spatial profiles of the solution  $u$  of the IBVP with initial condition  $u(x, 0) = e^{-x^2/2}$  and boundary conditions given by equation (3.3) at various times  $t = t_0$ . The circles denote the solution  $u$  obtained by direct numerical computation, while the solid lines the corresponding semi-analytical approximation. In the latter, the decomposition (3.8) has been used with the component  $u^{(2)}$  given by the exact formula (3.11) and the component  $u^{(1)}$  obtained by using the first ten modes of the series representation (3.12).

as opposed to algebraic, decay. For example, revisiting the IBVP of Fig. 3.1 but now with  $D = 200$  instead of  $D = 1$  makes the boundary conditions  $u(\pm D, t) = \pm \frac{D}{(2t+1)^{3/2}} e^{-\frac{D^2}{2(2t+1)}}$  effectively zero. Hence, the decay rate observed for the solution is exponential instead of algebraic, as shown in Fig. 3.4.

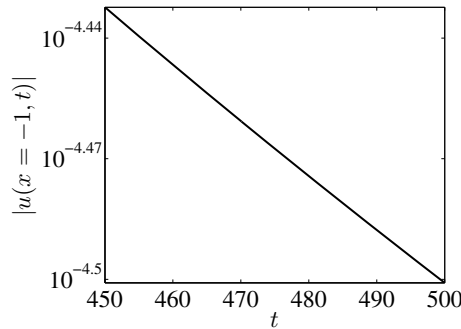


FIG. 3.4. Semi-logarithmic plot of  $|u(-1, t)|$ , where  $u(x, t)$  is the solution of the diffusion equation (1.1) on the interval  $[-D, D]$  with initial condition  $u_0(x) = xe^{-x^2/2}$ , boundary conditions  $u(\pm D, t) = \pm \frac{D}{(2t+1)^{3/2}} e^{-\frac{D^2}{2(2t+1)}}$  and  $D = 200$ . Since the boundary conditions are smaller than machine precision, the solution decays exponentially rather than algebraically.

**4. Conclusions and future work.** In the present work, we have revisited the topic of self-similar solutions of one of the most fundamental models of applied mathematics, namely the linear diffusion equation. Employing the MN-dynamics approach, we have justified the existence of a broad class of self-similar solutions and have developed a superposition of the relevant eigenfunctions upon performing a separation of variables in the MN-frame. This has enabled us to identify solutions that decay exponentially as well as solutions that decay with power laws in the self-similar spatial variable. It has also provided us with eigenfunctions that are bounded, as well as others that are integrable under suitable power law decay conditions (and even ones that are non-integrable). Among the ones that are integrable (and hence physically correspond to finite mass), the slowest one identified has been the customary  $t^{-1/2}$  decay law. This is suggestive concerning the observability of this type of decay in physical experiments. Nevertheless, we showcased explicit examples featuring a different type of decay, arising from initial data with vanishing projection on the corresponding eigenfunction. In this way, we effectively showed that arbitrary power laws in regard to the temporal decay are possible to realize in the context of the linear diffusion model.

On the other hand, we also revisited initial-boundary value problems (IBVPs) associated with the diffusion equation and identified different possibilities. We discussed the case of consonant boundary conditions, for which a self-similar solution remains at all times transparent to the presence of the boundaries and preserves its corresponding rate of decay. This, in turn, illustrates that the associated IBVP can also feature arbitrary temporal power law decay rates. On the other hand, compatible, yet non-consonant IBVPs were formulated with different decay rates prompted by their initial and boundary

data. In this case, we established that the general solution is not self-similar, but instead can be decomposed in a self-similar part and a part with exponential decay due to its satisfying homogeneous boundary conditions (this is the typical, widely explored case considered in the context of Fourier series).

These considerations pave the way to a number of directions for future studies. In the context of the diffusion model, it is well known (see Appendix A for details ) that an analytical solution exists either in the form of the *unified transform method* of Fokas [23,24], or in the form of an infinite series representation (in fact, the former representation can be easily converted into the latter one). Such formulae already encompass a decomposition of the solution into a component that stems from the initial condition and a component that arises from the boundary contributions. In this context, it would be especially interesting to reconstruct from these analytical expressions the parts of the solution that may feature self-similarity, as well as to identify the ones that do not, and to formulate more precise conditions under which we should expect the solution to be self-similar. On the other hand, a far more open-ended problem stems from the introduction of non-linearity in the system. Here, a principal question concerns the potential persistence, as well as the (appropriately adapted notion of) stability of the self-similar solutions over the time evolution. An example in this direction is, for instance, given in the piecewise linear model of [25]. Lastly, an especially important technical question even for the linear diffusion case concerns the properties of the operator (2.13) and potential decompositions of general solutions of this PDE on a basis of associated eigenfunctions. Such questions are presently under investigation and will be reported in future publications.

**Appendix A: Analytical solution of the diffusion IBVP using the unified transform method of Fokas.** In connection with the question of compatible, yet non-consonant boundary data for IBVPs, it is useful to recall that the diffusion equation (1.1) formulated on the interval with any admissible combination of boundary conditions can be solved analytically via the *unified transform method* (UTM), also known as the *Fokas method* [23,24]. For example, in the case of Dirichlet boundary conditions  $u(-D, t) = g_0(t)$  and  $u(D, t) = h_0(t)$  with initial condition  $u(x, 0) = u_0(x)$ , the UTM yields the solution formula

$$\begin{aligned}
 u(x, t) = & \frac{1}{2\pi} \int_{k \in \mathbb{R}} e^{ikx - k^2 t} \hat{u}_0(k) dk & (4.1) \\
 & - \frac{1}{2\pi} \int_{k \in \partial \mathcal{D}^+} \frac{e^{ik(x+D) - k^2 t}}{e^{2ikD} - e^{-2ikD}} \left[ -2ik e^{-2ikD} \tilde{g}_0(k^2, t) \right. \\
 & \qquad \qquad \qquad \left. + 2ik \tilde{h}_0(k^2, t) + e^{ikD} \hat{u}_0(k) - e^{-ikD} \hat{u}_0(-k) \right] dk \\
 & - \frac{1}{2\pi} \int_{k \in \partial \mathcal{D}^-} \frac{e^{ik(x-D) - k^2 t}}{e^{2ikD} - e^{-2ikD}} \left[ -2ik \tilde{g}_0(k^2, t) + 2ike^{2ikD} \tilde{h}_0(k^2, t) \right. \\
 & \qquad \qquad \qquad \left. + e^{-ikD} \hat{u}_0(k) - e^{ikD} \hat{u}_0(-k) \right] dk,
 \end{aligned}$$



where the transforms  $\widehat{u}_0, \tilde{g}_0, \tilde{h}_0$  of the prescribed initial and boundary data are defined by

$$\widehat{u}_0(k) = \int_{-D}^D e^{-ikx} u_0(x) dx, \tag{4.2a}$$

$$(\tilde{g}_0, \tilde{h}_0)(k^2, t) = \int_0^t e^{k^2 t'} (g_0, h_0)(t') dt', \tag{4.2b}$$

and the complex contours of integration  $\partial\mathcal{D}^\pm$  are the positively oriented boundaries of the regions  $\mathcal{D}^\pm$  shown in Fig. 4.1.

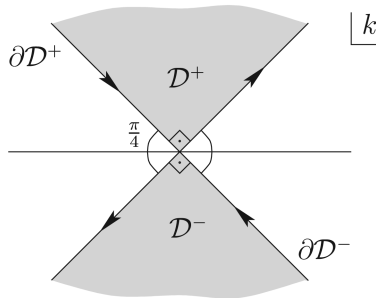


FIG. 4.1. The regions  $\mathcal{D}^+$  and  $\mathcal{D}^-$  and the associated boundaries  $\partial\mathcal{D}^+$  and  $\partial\mathcal{D}^-$ .

Furthermore, the UTM solution of any IBVP for the diffusion equation on the interval can always be reduced to the corresponding “classical” infinite series solution representation (3.12).

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