Numerical solution of the azimuth-dependent Fokker-Planck equation in 1D slab geometry

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Abstract

This paper is devoted to solve the steady monoenergetic Fokker-Planck equation in the 1D slab when the incoming fluxes and the source term are allowed to depend on the azimuth θ. The problem is split into a collection of θ-independent problems for the Fourier coefficients of the full solution. The main difficulty is that, except for the zeroth Fourier coefficient, each of these problems contains an artificial absorption coefficient which is singular at the poles. Two numerical schemes capable of dealing with the singularities are proposed: one that is considered as the main scheme, and a second 'security' scheme which is used to verify that the results obtained by means of the first one are reliable. Numerical experiments showing second order of convergence are conducted and discussed.

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1 Introduction

Consider $Z_{\text{ini}}, Z_{\text{fin}} \in \mathbb{R}$ such that $Z_{\text{ini}} < Z_{\text{fin}}$.

Let $Q_{z,\mu,\theta} \subset \mathbb{R}^3$ be the open set $(Z_{\text{ini}}, Z_{\text{fin}}) \times (-1,1) \times (0, 2\pi)$, and let $\overline{Q}_{z,\mu,\theta}$ be its closure, that is, $[Z_{\text{ini}}, Z_{\text{fin}}] \times [-1,1] \times [0,2\pi]$. Also, let (z,μ,θ) be a generic element of $\overline{Q}_{z,\mu,\theta}$.

These notations provide $Q_{z,\mu}$ and $\overline{Q}_{z,\mu}$ with the natural meanings $Q_{z,\mu} = (Z_{\text{ini}}, Z_{\text{fin}}) \times (-1,1)$ and $\overline{Q}_{z,\mu} = [Z_{\text{ini}}, Z_{\text{fin}}] \times [-1,1]$, and other

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choices of one or two subscripts in the set $\{z, \mu, \theta\}$ must be analogously understood in what follows.

In a quite standard way, an expression like $\alpha = \alpha(z, \mu)$ will mean that α is a function of the two independent variables z and μ.

In order to state that two functions are equal in the intersection of their domains, we will generally place between them the equal symbol '=', but, for the sake of clarity, the notation '$\equiv 0$' will be employed on certain occasions to indicate that a given function is identically zero, so that the function is not confused with the real number 0.

The goal of this paper is to solve for

$$\psi : (z, \mu, \theta) \in \overline{Q}_{z,\mu,\theta} \longrightarrow \psi(z, \mu, \theta) \in \mathbb{R}$$

the partial differential equation (PDE)

$$\mu \frac{\partial \psi}{\partial z} + \alpha \psi = \sigma \left\{ \frac{\partial}{\partial \mu} \left[\left(1 - \mu^2\right) \frac{\partial \psi}{\partial \mu} \right] + \frac{1}{1 - \mu^2} \frac{\partial^2 \psi}{\partial \theta^2} \right\} + W \qquad (1)$$

in $Q_{z,\mu,\theta}$, with $\alpha = \alpha(z, \mu)$, $\sigma = \sigma(z, \mu)$, and $W = W(z, \mu, \theta)$ three given functions, accompanied by the following conditions:

$$\psi_{|\{z=Z_{\text{ini}},\ \mu \in (0,1]\}} = f, \text{ with } f = f(\mu, \theta) \text{ given}, \qquad (2)$$

$$\psi_{|\{z=Z_{\text{fin}},\ \mu \in [-1,0)\}} = g, \text{ with } g = g(\mu, \theta) \text{ given}, \qquad (3)$$

$$\psi_{|\{\theta=0\}} = \psi_{|\{\theta=2\pi\}}, \quad \left(\frac{\partial \psi}{\partial \theta} \right)_{|\{\theta=0\}} = \left(\frac{\partial \psi}{\partial \theta} \right)_{|\{\theta=2\pi\}}. \qquad (4)$$

It must be understood that

$$\{z = Z_{\text{ini}},\ \mu \in (0, 1]\} = \{(z, \mu, \theta) :\ z = Z_{\text{ini}},\ (\mu, \theta) \in (0, 1] \times \overline{Q}_\theta\}, \qquad (5)$$

$$\{\theta = 0\} = \{(z, \mu, \theta) :\ (z, \mu) \in \overline{Q}_{z,\mu},\ \theta = 0\}, \qquad (6)$$

and so on for $\{z = Z_{\text{fin}},\ \mu \in [-1, 0)\}$ and $\{\theta = 2\pi\}$.

It will always be assumed that α is nonnegative and that σ is positive.

Notice that functions f and g must be (2π)-periodic with respect to θ in order that conditions (2)–(4) are compatible, but that W is not obliged in principle to exhibit this periodicity.

From the point of view of the numerical schemes, the main difficulties are associated to the facts that the PDE (1) degenerates for $\mu = 0$, since this choice makes the term $\mu \frac{\partial \psi}{\partial z}$ be null, and also that tends to present another pair of degeneracies in $\frac{\partial}{\partial \mu} \left[\left(1 - \mu^2\right) \frac{\partial \psi}{\partial \mu} \right]$, plus a couple of singularities in $\frac{1}{1-\mu^2} \frac{\partial^2 \psi}{\partial \theta^2}$, as μ approaches 1 or -1.

From the point of view of the computing time, the main issue is that the problem is three-dimensional. We can say, in this regard, that the technique used in this paper allows getting the solution by solving a generally small collection of two-dimensional problems. This technique cannot be applied, however, if any of the coefficients α or σ depends on θ, and the reason will be clear later, in Section 6.

The paper is organized as follows: in Section 2 some words about the significance of the problem are said. The hypotheses on the data are established in Section 3. Section 4 explains some features of the problem that have to do with its physical meaning and fixes what we will understand by 'the physically relevant case'. In Section 5 we prove that functions f, g and W must satisfy some compatibility conditions so that the solution can be regular in $Q_z \times \overline{Q}_{\mu,\theta}$, and that these compatibility conditions are automatically satisfied in the physically relevant case. Section 6 shows how the problem can be split into a collection of θ-independent transport problems for the Fourier coefficients of ψ with respect to θ, and that all of these problems fit in with a general problem that we call 'the core problem'. Upon the basis of certain assumptions, a numerical scheme for solving the core problem is presented in Section 7, and also a security 'assumption-independent' scheme is considered in order to check the results obtained with the first one. Sections 8 and 9 are devoted to show numerical results for the core and the full problem, respectively. Lastly, Section 10 contains the most significant conclusions drawn from this paper.

2 Significance of the problem

Among the nuclear engineering community, the PDE in Equation (1) is known at times as the steady monoenergetic Fokker-Planck equation (FPE) in the 1D slab. The importance of this model comes from the fact that its solution ψ is, under certain hypotheses, an approximation of the solution to the Boltzmann transport equation (see [5] and [8]), which is harder to solve. In such a context,

- Function ψ is representing the angular flux density of charged particles like, for example, electrons, and
- Variable z stands for 1D space, μ for the cosine of the polar angle, and θ for the azimuthal angle.[1] The pair (μ, θ) specifies the direction in which particles travel from a given spatial location. Notice that the values $\mu = \pm 1$ are special ones because they are representing the North and South Poles, where the variation of θ in $[0, 2\pi]$ should not imply a variation in the values of the functions. Concerning this issue, we advance that the presence of the term $\frac{1}{1-\mu^2}\frac{\partial^2 \psi}{\partial \theta^2}$ in the PDE obliges the two functions $\psi(\cdot, \pm 1, \cdot)$ to be independent of θ under rather mild assumptions; this assertion will be properly enunciated in Theorem 1.

We do not consider it necessary to include a comprehensive explanation of the physical meaning of this problem, since it can be found in [6, Section 4], authored by us. In this regard, the only caveat is that the continuous scattering operator in the present paper is

$$\frac{\partial}{\partial \mu}\left[\left(1-\mu^2\right)\frac{\partial \cdot}{\partial \mu}\right] + \frac{1}{1-\mu^2}\frac{\partial^2 \cdot}{\partial \theta^2}, \tag{7}$$

while it is

$$\frac{\partial}{\partial \mu}\left[\left(1-\mu^2\right)\frac{\partial \cdot}{\partial \mu}\right] \tag{8}$$

in reference [6]. This difference is nevertheless coherent because the problem studied in [6] is independent of θ.

We recall that, in mathematical language, the continuous scattering operator is the Laplacian operator on the unit sphere.

It is quite common for the FPE to be found in the literature without a source[2] term, i.e., with $W \equiv 0$. Aside from the intrinsic value of adding a

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[1] The reader must think of the standard spherical coordinate system centred at a generic point $(x_1, x_2, x_3) \in \mathbb{R}^3$. Since in the 1D slab one assumes independency of x_1 and x_2, it suffices to work, from the spatial standpoint, with the x_3-coordinate, which is constantly called in this paper the z-coordinate.

[2] We will employ the generic word 'source' even though W could be negative (hence a 'sink') in part or in the whole of its domain.

new term to the PDE, there are another two reasons why it is important to include W: on the one hand, the transient and the energy dependent FPEs (even if there is no source in them) are reduced, after the corresponding time or energy discretization, to a collection of problems with non-zero source W that fit the framework herein; on the other hand, the presence of W allows for the easy design of problems with known regular exact solution: one simply chooses any regular ψ which is going to be the exact solution and computes W so that the PDE is satisfied. Solutions obtained in such a way are sometimes known as *manufactured solutions*, and they permit one to check, numerically, the order of convergence of the schemes.

We do not forget that the FPE in the 1D slab is usually presented under the additional hypothesis of *planar-geometry symmetry*, which is the expression that nuclear engineers use to indicate that the problem is independent of θ (see for instance [4, page 3]). From this perspective, problem (1)–(4) can be considered as an intermediate model between the typical θ-independent FPE in the 1D slab and more complex models that depend on θ and incorporate the three spatial variables.

3 Hypotheses on the data

Even though our goal is the plain numerical resolution, and not the statement of theoretical results on numerical analysis, existence, uniqueness or regularity issues, it is true that, in order to design numerical schemes, one needs to have in mind some idea about what the involved functions are like. In this spirit, the C^0 and C^1 requirements below have been thought as comfortable working hypotheses under which the mathematical operations have a justification rather than as precise conditions that must be met without fail; we are going to be able to prove some useful results under them, but at the same time we have found out that our numerical schemes also work even in cases where these hypotheses are not satisfied.

Specifically, the data functions are supposed to fulfil the following requirements:

$$f \in \mathrm{C}^1\left([0,1] \times \overline{Q}_\theta\right), \quad f_{|\{\theta=0\}} = f_{|\{\theta=2\pi\}}, \tag{9}$$

$$g \in \mathrm{C}^1\left([-1,0] \times \overline{Q}_\theta\right), \quad g_{|\{\theta=0\}} = g_{|\{\theta=2\pi\}}, \tag{10}$$

$$\alpha,\ \sigma \in \mathrm{C}^0\left(\overline{Q}_{z,\mu}\right), \text{ with } \alpha \geq 0 \text{ and } \sigma > 0, \tag{11}$$

$$(1-\mu^2)W \in \mathrm{C}^1\left(\overline{Q}_{z,\mu,\theta}\right), \quad W_0 \in \mathrm{C}^1\left(\overline{Q}_{z,\mu}\right), \tag{12}$$

where

$$W_0(z,\mu) = \frac{1}{2\pi}\int_0^{2\pi} W(z,\mu,\theta)\ \mathrm{d}\theta \tag{13}$$

is the zeroth Fourier coefficient of W with respect to θ.

The regularity which is imposed by conditions (9), (10) and (12) guarantees convergence of the Fourier series with respect to θ of functions f, g and W, a fact which is important in this paper.

Following the line of (9) and (10), one could have expected, instead of (12), the stronger hypothesis $W \in \mathrm{C}^1\left(\overline{Q}_{z,\mu,\theta}\right)$. This is indeed reasonable in the physically relevant case, because, as we will see, the Physics of problem (1)–(4) obliges W to be defined at $\mu = \pm 1$. However, we notice that, due to the presence of the coefficient $\frac{1}{1-\mu^2}$ in the PDE (1), sources W which are not defined at $\mu = \pm 1$ easily occur when building manufactured solutions. This explains why we have imposed $(1-\mu^2)W \in \mathrm{C}^1\left(\overline{Q}_{z,\mu,\theta}\right)$. The second condition, $W_0 \in \mathrm{C}^1\left(\overline{Q}_{z,\mu}\right)$, is reflecting the fact that W_0 acts as the source of a problem which does not have any singularity at $\mu = \pm 1$; this assertion will be clarified later. When W is not defined at $\mu = \pm 1$, one must understand in hypothesis (12) that functions $(1-\mu^2)W$ and W_0 admit of C^1 extensions to $\overline{Q}_{z,\mu,\theta}$ and $\overline{Q}_{z,\mu}$, respectively, and that the same notations are being used for the extended functions.

We state in the following lemma a useful characterization of the functions satisfying (12); its proof is a simple exercise. The notation $(\mathcal{H}_W)_0$ will stand, as in Equation (13), for the zeroth Fourier coefficient of $\mathcal{H}_W$ with respect to θ.

Lemma 1 (Representation of the source W)**.** *W satisfies (12) if, and only if, it admits of the representation*

$$W(z,\mu,\theta) = \widehat{W}(z,\mu) + \frac{\mathcal{H}_W(z,\mu,\theta)}{1-\mu^2} \ \forall (z,\mu,\theta) \in \overline{Q}_z \times Q_\mu \times \overline{Q}_\theta, \qquad (14)$$

being, on the one hand, $\widehat{W}$ a function in $\mathrm{C}^1\left(\overline{Q}_{z,\mu}\right)$ and, on the other hand, $\mathcal{H}_W$ a function in $\mathrm{C}^1\left(\overline{Q}_{z,\mu,\theta}\right)$ such that $(\mathcal{H}_W)_0 \equiv 0$ in $\overline{Q}_{z,\mu}$.

Necessarily, $\widehat{W} = W_0$ and $\mathcal{H}_W = (1-\mu^2)(W - W_0)$, and so the representation (14) is unique.

One of the consequences of Lemma 1 is that W can be extended with continuity to the whole $\overline{Q}_{z,\mu,\theta}$ if $\mathcal{H}_W(\cdot,\pm 1,\cdot) \equiv 0$, because this condition permits defining

$$W(z,\pm 1,\theta) = \widehat{W}(z,\pm 1) \mp \frac{1}{2}\frac{\partial \mathcal{H}_W}{\partial \mu}(z,\pm 1,\theta) \ \forall (z,\theta) \in \overline{Q}_{z,\theta} \qquad (15)$$

by means of the L'Hôpital's rule. In other words, if we assume that (12) holds, then $W \in \mathrm{C}^0\left(\overline{Q}_{z,\mu,\theta}\right)$ if, and only if, $\mathcal{H}_W(\cdot,\pm 1,\cdot) \equiv 0$ (one can easily prove separate continuity with respect to each variable, but in fact one has continuity; see Lemma 4 in the Appendix).

4 The physically relevant case

Problem (1)–(4) can be solved without further considerations, from a pure mathematical viewpoint, or can be solved within its physical context. In the last case, we will say that the 'physically relevant case' of the problem is being solved. In this section we are going to explain those aspects affected by physical considerations and to precisely define what the expression 'physically relevant case' will mean in this paper.

The physical meaning of this problem demands the fulfilment of the following conditions:

1. The angular flux density ψ must be nonnegative. Hence, the incoming fluxes f and g must be nonnegative, while the internal source W, which has not got sign restrictions, could be negative only up to a point that still rendered $\psi \geq 0$.
2. All functions involved in this problem must be:
    (a) (2π)-periodic with respect to θ, and
    (b) Independent of θ when they are restricted to the intersection of their domains with the affine hyperplanes $\mu = \pm 1$. Not only $W(\cdot,\pm 1,\cdot)$ (if W is defined at $\mu = \pm 1$), $f(1,\cdot)$ and $g(-1,\cdot)$ must be independent of θ, but also the restrictions of the solution to $\mu = \pm 1$, i.e. $\psi(\cdot,\pm 1,\cdot)$, must result in two θ-independent functions.

The features in points (2a) and (2b) above are trivial consequences of the geometrical meaning of μ and θ in the spherical coordinate system.

Giving necessary and sufficient conditions for $\psi(\cdot,\pm1,\cdot)$ to be independent of θ is not difficult if one makes the following assumptions:

$$\psi \in \mathrm{C}^0(\overline{Q}_{z,\mu,\theta}), \tag{16}$$

$$\frac{\partial\psi}{\partial z},\ \frac{\partial^2\psi}{\partial\mu^2} \in \mathrm{C}^0\left(Q_z \times \overline{Q}_{\mu,\theta}\right), \tag{17}$$

$$\frac{\partial^2\psi}{\partial\theta^2} \in \mathrm{C}^0\left(Q_z \times \overline{Q}_{\mu,\theta}\right). \tag{18}$$

We notice that (18) is meaning that both $\frac{\partial\psi}{\partial\theta}$ and $\frac{\partial^2\psi}{\partial\theta^2}$ are assumed to exist as continuous functions defined on $Q_z \times \overline{Q}_{\mu,\theta}$, and an analogous comment is valid for $\frac{\partial^2\psi}{\partial\mu^2}$ in (17). We have not put the assumption (18) within (17) because, occasionally, we will make reference to each of them separately.

Lemma 2. *Under the hypotheses (9)–(12), any function ψ satisfying the PDE (1) and the assumptions (16)–(18) also satisfies the following equality:*

$$\sigma(z,\pm1)\frac{\partial^2\psi}{\partial\theta^2}(z,\pm1,\theta) = -\mathcal{H}_W(z,\pm1,\theta)\ \forall(z,\theta)\in Q_z\times\overline{Q}_\theta. \tag{19}$$

Proof. The existence of $\frac{\partial^2\psi}{\partial\mu^2}$ guarantees that

$$\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\frac{\partial\psi}{\partial\mu}\right] = -2\mu\frac{\partial\psi}{\partial\mu} + \left(1-\mu^2\right)\frac{\partial^2\psi}{\partial\mu^2}. \tag{20}$$

Now, using (14), the PDE (1) can be written as follows:

$$\mu\frac{\partial\psi}{\partial z} + \alpha\psi = \sigma\left\{-2\mu\frac{\partial\psi}{\partial\mu} + \left(1-\mu^2\right)\frac{\partial^2\psi}{\partial\mu^2} + \frac{1}{1-\mu^2}\frac{\partial^2\psi}{\partial\theta^2}\right\} + \widehat{W} + \frac{\mathcal{H}_W}{1-\mu^2}, \tag{21}$$

which holds in $Q_{z,\mu,\theta}$ and hence in $Q_{z,\mu}\times\overline{Q}_\theta$ by continuity.

Multiplying Equation (21) by $1-\mu^2$ one gets an equality that holds in $Q_z\times\overline{Q}_{\mu,\theta}$, and evaluating the terms of this new equality at $\mu=\pm1$ one obtains (19). ∎

Theorem 1. *Let ψ be the solution to the problem (1)–(4). Under the hypotheses (9)–(12) and the assumptions (16)–(18), functions $\psi(\cdot,\pm1,\cdot)$ are independent of θ if, and only if,*

Functions $f(1,\cdot)$ and $g(-1,\cdot)$ do not depend on θ
(i.e., they are constant), and (22)

Functions $\mathcal{H}_W(\cdot,\pm1,\cdot)$ are identically 0. (23)

Proof. The proof follows easily by taking into account the identity (19), the positivity of σ (really only the fact that σ is never zero), and conditions (2)–(4). ∎

Remark 1. *From the mathematical viewpoint, it is interesting to notice that for $\psi(\cdot,\pm1,\cdot)$ to be independent of θ it is not necessary that $W(\cdot,\pm1,\cdot)$ be independent of θ; take for instance $W(z,\mu,\theta)=z\mu+\sin\theta$.*

To properly understand the following definition, recall that, under the hypothesis (12), the source W is continuous if, and only if, (23) holds (see Equation (15)).

Definition 1 (Physically relevant case)**.** *Under the hypotheses (9)–(12), the physically relevant case of problem (1)–(4) is the one we have when*

- *Functions f and g are nonnegative,*
- *Condition (22) holds,*
- *$W \in \mathrm{C}^0\left(\overline{Q}_{z,\mu,\theta}\right)$ (equivalently, condition (23) holds),*
- *$W_{|\{\theta=0\}} = W_{|\{\theta=2\pi\}}$, and*
- *Functions $W(\cdot, \pm 1, \cdot)$ are independent of θ.*

To the authors' knowledge, there is no theoretical result guaranteeing that assumptions (16)–(18) will always hold,[3] either under the hypotheses (9)–(12) or under any other set of conditions. Nevertheless, it is obvious that they will easily hold for manufactured solutions. It can be added that these assumptions are in accordance with the available numerical results, which suggest that ψ is continuous on $\overline{Q}_{z,\mu,\theta}$ and smooth on $Q_z \times \overline{Q}_{\mu,\theta}$ for the problems of interest. The spatial domain Q_z in (17) is open since there is strong numerical evidence that, even for constant data functions, $\frac{\partial\psi}{\partial z}$ can be infinity and $\frac{\partial\psi}{\partial\mu}$ can fail to exist at (z, μ, θ) when $(z, \mu) \in \{(Z_{\text{ini}}, 0), (Z_{\text{fin}}, 0)\}$ (see [3], [6], [9], and also some plots within the numerical results of this paper). In other words, changing (17) by $\frac{\partial\psi}{\partial z}, \frac{\partial^2\psi}{\partial\mu^2} \in \mathrm{C}^0(\overline{Q}_{z,\mu,\theta})$ would be inadequate.

All mathematical operations involving ψ in this paper are valid under assumptions (16)–(18).

Remark 2. *The reader can easily check that Theorem 1 is still valid if, maintaining assumption (18), assumptions (16) and (17) are weakened as follows:*

$$\psi \in \mathrm{C}^0(Q_{z,\mu,\theta}), \tag{24}$$

$$\frac{\partial\psi}{\partial z}, \ \frac{\partial^2\psi}{\partial\mu^2} \ \textit{exist in } \mathbb{R} \textit{ at every point of } Q_{z,\mu,\theta}, \tag{25}$$

provided that $(1-\mu^2)\psi$, $(1-\mu^2)\frac{\partial\psi}{\partial z}$, $(1-\mu^2)\frac{\partial\psi}{\partial\mu}$ and $(1-\mu^2)^2\frac{\partial^2\psi}{\partial\mu^2}$ tend to 0 when μ tends to ± 1, for every $(z, \theta) \in Q_{z,\theta}$.

5 Compatibility conditions

As it occurs with other problems, a regular solution cannot exist unless certain compatibility conditions between the data hold. In this case, Equation (19) can be further exploited to state the following result, which makes it clear that there must be certain relationships between functions f, g, and W in order that a solution ψ satisfying (16)–(18) can exist. In the physically relevant case, these relationships are automatically met.

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[3] Even the questions of existence and uniqueness are not treated in the existing literature. The reader is referred, however, to the paper [2], where these two issues are studied for a similar problem.

Theorem 2 (Compatibility conditions)**.** *Under the hypotheses (9)–(12), a necessary condition for the problem (1)–(4) to have got a solution satisfying assumptions (16)–(18) is that the following two equalities be satisfied:*

$$f(1,\theta) = f(1,0) + \frac{1}{\sigma(Z_{\rm ini},1)}\left\{\frac{\theta}{2\pi}\int_0^{2\pi}\left(\int_0^s \mathcal{H}_W(Z_{\rm ini},1,t)\ {\rm d}t\right){\rm d}s - \int_0^\theta\left(\int_0^s \mathcal{H}_W(Z_{\rm ini},1,t)\ {\rm d}t\right){\rm d}s\right\}\ \forall\theta\in\overline{Q}_\theta, \qquad (26)$$

$$g(-1,\theta) = g(-1,0) + \frac{1}{\sigma(Z_{\rm fin},-1)}\left\{\frac{\theta}{2\pi}\int_0^{2\pi}\left(\int_0^s \mathcal{H}_W(Z_{\rm fin},-1,t)\ {\rm d}t\right){\rm d}s - \int_0^\theta\left(\int_0^s \mathcal{H}_W(Z_{\rm fin},-1,t)\ {\rm d}t\right){\rm d}s\right\}\ \forall\theta\in\overline{Q}_\theta. \qquad (27)$$

Proof. Both equalities hold trivially if conditions (22) and (23) are fulfilled, and so their proofs are not an issue in the physically relevant case. In order to prove (26) and (27) otherwise, firstly integrate Equation (19) between 0 and θ to obtain

$$\frac{\partial\psi}{\partial\theta}(z,\pm1,\theta) = \frac{\partial\psi}{\partial\theta}(z,\pm1,0) - \frac{1}{\sigma(z,\pm1)}\int_0^\theta \mathcal{H}_W(z,\pm1,s)\ {\rm d}s. \qquad (28)$$

We can remark here that the equality $\frac{\partial\psi}{\partial\theta}(z,\pm1,0) = \frac{\partial\psi}{\partial\theta}(z,\pm1,2\pi)$, which is entailed by (4), is not in contradiction with Equation (28), because $(\mathcal{H}_W)_0 \equiv 0$ implies $(\mathcal{H}_W(\cdot,\pm1,\cdot))_0 \equiv 0$.

Secondly, integrate Equation (28) between 0 and θ to get

$$\psi(z,\pm1,\theta) = \psi(z,\pm1,0) + \theta\frac{\partial\psi}{\partial\theta}(z,\pm1,0) - \frac{1}{\sigma(z,\pm1)}\int_0^\theta\left(\int_0^s \mathcal{H}_W(z,\pm1,t)\ {\rm d}t\right){\rm d}s. \qquad (29)$$

Evaluating Equation (29) at $\theta = 2\pi$ and taking into account that $\psi(z,\pm1,0) = \psi(z,\pm1,2\pi)$, we obtain

$$\frac{\partial\psi}{\partial\theta}(z,\pm1,0) = \frac{1}{2\pi\sigma(z,\pm1)}\int_0^{2\pi}\left(\int_0^s \mathcal{H}_W(z,\pm1,t)\ {\rm d}t\right){\rm d}s, \qquad (30)$$

what allows rewriting Equation (29) as

$$\psi(z,\pm1,\theta) = \psi(z,\pm1,0) + \frac{1}{\sigma(z,\pm1)}\left\{\frac{\theta}{2\pi}\int_0^{2\pi}\left(\int_0^s \mathcal{H}_W(z,\pm1,t)\ {\rm d}t\right){\rm d}s - \int_0^\theta\left(\int_0^s \mathcal{H}_W(z,\pm1,t)\ {\rm d}t\right){\rm d}s\right\}. \qquad (31)$$

Finally, the compatibility conditions (26) and (27) are easily derived from Equation (31). ■

6 Reduction to a collection of θ-independent problems

Throughout the whole of this section, the letter '*i*' will stand for the imaginary unit.

The idea which will be developed right now for solving the θ-dependent problem (1)–(4) is fairly natural. Applied to a Fokker-Planck problem, we have seen this idea published for the first time in reference [3], although the problem therein solved is only that of the zeroth Fourier coefficient with a zero source term and with coefficients that depend solely on z.

Notice that the periodicity conditions (4) invite one to use Fourier techniques for converting the problem (1)–(4) into a collection of θ-independent problems. Indeed, our intention is to compute ψ from its Fourier series with respect to θ, that is to say, from

$$\psi(z,\mu,\theta) = \sum_{m=-\infty}^{\infty} \psi_m(z,\mu)\ \mathrm{e}^{im\theta}\ \forall (z,\mu,\theta) \in \overline{Q}_{z,\mu,\theta}, \tag{32}$$

where the coefficients ψ_m are given by the well-known formula

$$\psi_m(z,\mu) = \frac{1}{2\pi}\int_0^{2\pi} \psi(z,\mu,\theta)\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta\ \forall (z,\mu) \in \overline{Q}_{z,\mu}. \tag{33}$$

Since ψ is real, Equation (33) immediately implies that $\psi_{-m} = \overline{\psi_m}$ for every $m \in \mathbb{Z}$. As a result, Equation (32) can be rewritten as

$$\psi(z,\mu,\theta) = \psi_0(z,\mu) + 2\sum_{m=1}^{\infty}\left\{ \mathrm{Re}[\psi_m(z,\mu)]\cos(m\theta) - \mathrm{Im}[\psi_m(z,\mu)]\sin(m\theta)\right\}. \tag{34}$$

For numerical purposes, Equation (34) is more appropriate than Equation (32), because it prevents spurious non-real values from appearing. Naturally, one must understand that the series will be truncated at a certain level. If the series converges rapidly, then one can get ψ with high accuracy from the knowledge of only a few coefficients ψ_m. We notice in this regard that, once the commanding harmonics have been reached, rapid convergence occurs if ψ is, for each fixed pair (z,μ), the restriction to $[0,2\pi]$ of a (2π)-periodic function of class $\mathrm{C}^p(\mathbb{R})$; the larger p, the faster rate of convergence (see for instance [10, Chapter 5, Section 8, Theorem 2]). Since there are continuous functions with divergent Fourier series, we must implicitly understand in this paragraph that $p \geq 1$.

The point is that each ψ_m is the solution to a Fokker-Planck equation which is independent of θ, and hence much cheaper to solve than Equation (1). We proceed now to obtain this equation. Hereinafter, G_m will denote the m^{th} Fourier coefficient of a function G with respect to the variable θ.

The first thing to do, according to Equation (33), is to multiply each term in Equation (1) by $\mathrm{e}^{-im\theta}$, then integrate from $\theta = 0$ to $\theta = 2\pi$, and finally divide by 2π. The results are the following:

$$\frac{1}{2\pi}\int_0^{2\pi} \mu\frac{\partial\psi}{\partial z}\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta = \mu\frac{\partial\psi_m}{\partial z}, \tag{35}$$

$$\frac{1}{2\pi}\int_0^{2\pi} \alpha\psi\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta = \alpha\psi_m, \tag{36}$$

$$\frac{1}{2\pi}\int_0^{2\pi} \sigma\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\frac{\partial\psi}{\partial\mu}\right]\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta = \sigma\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\frac{\partial\psi_m}{\partial\mu}\right], \tag{37}$$

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{\sigma}{1-\mu^2}\frac{\partial^2\psi}{\partial\theta^2}\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta = -\frac{m^2\sigma}{1-\mu^2}\psi_m, \tag{38}$$

$$\frac{1}{2\pi}\int_0^{2\pi} W\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta = W_m. \tag{39}$$

Under the hypotheses (9)–(12) and the assumptions (16)–(18), Equations (35)–(39) hold for all $(z, \mu) \in Q_{z,\mu}$. The theorem we are thinking of for differentiating under the integral sign is [1, (8.11.2), p. 177].

Looking at Equations (36), (37) and (38) it is now understood why, as anticipated, neither α nor σ can depend on θ.

Equation (38), the only one which might demand further explanation, is the result of integrating twice by parts and taking into account the periodicity conditions (4):

$$\int_0^{2\pi} \frac{\partial^2 \psi}{\partial \theta^2}\, \mathrm{e}^{-im\theta}\, \mathrm{d}\theta = \left(\frac{\partial \psi}{\partial \theta}\right)_{|\{\theta=2\pi\}} - \left(\frac{\partial \psi}{\partial \theta}\right)_{|\{\theta=0\}} + \\ im\left(\psi_{|\{\theta=2\pi\}} - \psi_{|\{\theta=0\}}\right) - m^2 \int_0^{2\pi} \psi\, \mathrm{e}^{-im\theta}\, \mathrm{d}\theta = \\ -m^2 \int_0^{2\pi} \psi\, \mathrm{e}^{-im\theta}\, \mathrm{d}\theta. \tag{40}$$

Now, adding Equations (35)–(36) on the one hand, Equations (37)–(39) on the other hand, using Equation (1), and defining

$$\mathrm{A}(m) := \alpha + \frac{m^2\sigma}{1-\mu^2} \text{ for } m \in \mathbb{N} \cup \{0\}, \tag{41}$$

one arrives at the problem of solving for

$$\psi_m : (z, \mu) \in \overline{Q}_{z,\mu} \longrightarrow \psi_m(z, \mu) \in \mathbb{C}$$

the PDE

$$\mu \frac{\partial \psi_m}{\partial z} + \mathrm{A}(m)\psi_m = \sigma \frac{\partial}{\partial \mu}\left[\left(1-\mu^2\right)\frac{\partial \psi_m}{\partial \mu}\right] + W_m \tag{42}$$

in $Q_{z,\mu}$, accompanied by the conditions

$$\psi_m(Z_{\mathrm{ini}}, \mu) = f_m(\mu) \text{ for } \mu \in (0, 1], \tag{43}$$

$$\psi_m(Z_{\mathrm{fin}}, \mu) = g_m(\mu) \text{ for } \mu \in [-1, 0). \tag{44}$$

Remark 3 (About the shape and regularity of W_m)**.** *According to Equation (14), one has*

- *When* $m = 0$,

$$W_0(z, \mu) = \widehat{W}(z, \mu)\ \forall (z, \mu) \in \overline{Q}_{z,\mu}, \tag{45}$$

  which belongs to $\mathrm{C}^1(\overline{Q}_{z,\mu})$. *Notice that in this case the PDE (42) has got no singularity at* $\mu = \pm 1$ *since* $\mathrm{A}(0) = \alpha \in \mathrm{C}^0\left(\overline{Q}_{z,\mu}\right)$.

- *When* $m > 0$,

$$W_m(z, \mu) = \frac{(\mathcal{H}_W)_m(z, \mu)}{1-\mu^2}\ \forall (z, \mu) \in \overline{Q}_z \times Q_\mu, \tag{46}$$

  where $(\mathcal{H}_W)_m \in \mathrm{C}^1(\overline{Q}_{z,\mu})$. *In the physically relevant case, after Lemma 4 in the Appendix, one has* $W_m \in \mathrm{C}^0(\overline{Q}_{z,\mu})$ *due to the fact that* $(\mathcal{H}_W)_m(\cdot, \pm 1) \equiv 0$*; however, one never gets rid of the singularities of the artificial absorption coefficient* $A(m)$ *at* $\mu = \pm 1$.

Notice that Equation (34) implies that the functions $\psi(\cdot,\pm1,\cdot)$ are independent of θ (cf. Theorem 1) if, and only if,

$$\psi_m(\cdot,\pm1) \equiv 0 \text{ for all } m > 0. \tag{47}$$

We do not know how to get *a priori* the values $\psi_0(\cdot,\pm1)$, and so they are obtained as a by-product of the resolution process, but, as the following theorem asserts, when $m > 0$ there is an easy way of knowing in advance the values of $\psi_m(\cdot,\pm1)$ under the regularity assumptions (16)–(18). This will be of prime importance in the forthcoming numerical scheme, and moreover furnishes a justification of why the PDE (42) does not need 'boundary' conditions at $\mu = \pm1$.[4] In particular, the theorem asserts that $\psi_m(\cdot,\pm1) \equiv 0$ in the physically relevant case whenever $m > 0$ and assumptions (16)–(18) hold.

Theorem 3 (Formula for $\psi_m(\cdot,\pm1)$ when $m > 0$)**.** *Take $m > 0$ and suppose that the compatibility conditions*

$$f_m(1) = \frac{(\mathcal{H}_W)_m(Z_{\text{ini}},1)}{m^2\sigma(Z_{\text{ini}},1)}, \tag{48}$$

$$g_m(-1) = \frac{(\mathcal{H}_W)_m(Z_{\text{fin}},-1)}{m^2\sigma(Z_{\text{fin}},-1)} \tag{49}$$

hold. Then, under the hypotheses (9)–(12) and the assumptions (16)–(18),

$$\psi_m(z,\pm1) = \frac{(\mathcal{H}_W)_m(z,\pm1)}{m^2\sigma(z,\pm1)} \quad \forall z \in \overline{Q}_z. \tag{50}$$

In particular,

$$\psi_m(\cdot,\pm1) \equiv 0 \tag{51}$$

provided that conditions (22) and (23) are satisfied.

Proof. The proof is similar to that of Theorem 1. Fix $m > 0$ and notice that ψ_m inherits from ψ the regularity which will be demanded by this proof. Specifically, the hypotheses (9)–(12) and the assumptions (16)–(18) imply that

$$f_m \in \mathrm{C}^1([0,1]), \tag{52}$$

$$g_m \in \mathrm{C}^1([-1,0]), \tag{53}$$

$$\alpha,\ \sigma \in \mathrm{C}^0\left(\overline{Q}_{z,\mu}\right), \text{ with } \alpha \geq 0 \text{ and } \sigma > 0, \tag{54}$$

$$W_m(z,\mu) = \frac{(\mathcal{H}_W)_m(z,\mu)}{1-\mu^2}\ \forall (z,\mu) \in \overline{Q}_z \times Q_\mu, \text{ with } (\mathcal{H}_W)_m \in \mathrm{C}^1(\overline{Q}_{z,\mu}), \tag{55}$$

and

$$\psi_m \in \mathrm{C}^0(\overline{Q}_{z,\mu}), \tag{56}$$

$$\frac{\partial\psi_m}{\partial z},\ \frac{\partial^2\psi_m}{\partial\mu^2} \in \mathrm{C}^0\left(Q_z \times \overline{Q}_\mu\right). \tag{57}$$

Now, write the PDE (42) as

$$\mu\frac{\partial\psi_m}{\partial z} + \alpha\psi_m + \frac{m^2\sigma}{1-\mu^2}\psi_m = \sigma\left\{-2\mu\frac{\partial\psi_m}{\partial\mu} + (1-\mu^2)\frac{\partial^2\psi_m}{\partial\mu^2}\right\} + \frac{(\mathcal{H}_W)_m}{1-\mu^2}. \tag{58}$$

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[4] The PDE (42) also does not need 'boundary' conditions at $\mu = \pm1$ when $m = 0$, but giving a justification for this case is beyond the scope of this paper. The reader is referred to the bibliography in [6].

Equation (58) holds in $Q_{z,\mu}$. After multiplying it by $1-\mu^2$ one gets an equation that holds in $Q_z \times \overline{Q}_\mu$, and evaluating the terms of this equation at $\mu = \pm 1$ one obtains

$$m^2 \sigma(z, \pm 1) \psi_m(z, \pm 1) = (\mathcal{H}_W)_m(z, \pm 1) \quad \forall z \in Q_z. \tag{59}$$

By continuity, this equation actually holds in $\overline{Q}_z$, and thus the proof of (50) is done.

In what regards (51), one can either combine Theorem 1 and Equation (47) or observe that $(\mathcal{H}_W)_m(\cdot, \pm 1) \equiv 0$ due to (23) and then use (50). ■

Remark 4. *Theorem 3 can also be proved by combining Equation (19) with the equality*

$$(\mathcal{H}_W)_m(z, \pm 1) = \frac{1}{2\pi} \int_0^{2\pi} \mathcal{H}_W(z, \pm 1, \theta)\ \mathrm{e}^{-im\theta}\ \mathrm{d}\theta \tag{60}$$

and integrating twice by parts.

Remark 5. *The compatibility conditions (48) and (49) are trivially satisfied* ($0 = 0$) *in the physically relevant case.*

Remark 6. *It is clear that Theorem 3 still holds if we weaken* C^1 *into* C^0 *in (52), (53) and (55).*

Since the main problem (1)–(4) can be split into a collection of smaller problems of type (42)–(44), we will call the last one *the core problem.*

7 Scheme for the core problem (42)–(44)

In this section, the letter 'i' will stand for a natural subscript marking the i^{th} node of the μ-mesh, rather than for the imaginary unit. Also, we are going to distinguish the case $m = 0$ from the cases $m > 0$ by calling them the regular and the singular cases, respectively.

In the regular case ($m = 0$) we have a problem like the one studied in [6] and [7], and so we can directly use the odd scheme therein described for solving it.[5] For the sake of completeness, and also because it will be useful in the subsequent writing, we are going to describe here this scheme. Let us consider the uniform meshes

$$\mu_i = -1 + (i-1)h \text{ for } i \in \{1, \dots, I\}, \text{ with } h = \frac{2}{I-1}, \tag{61}$$

where I is odd, and

$$z_n = Z_{\text{ini}} + (n-1)k \text{ for } n \in \{1, \dots, N\}, \text{ with } k = \frac{Z_{\text{fin}} - Z_{\text{ini}}}{N-1}, \tag{62}$$

and consider the following notations: $i^\star = \frac{I+1}{2}$; $\overline{D}_i = D(\mu_i)$ and $\overline{D}_{i \pm \frac{1}{2}} = D(\mu_i \pm \frac{h}{2})$, being $D(\mu) = 1 - \mu^2$; $\overline{\mathrm{A}}_i^n = \mathrm{A}(0)(z_n, \mu_i) = \alpha(z_n, \mu_i)$, $\overline{\sigma}_i^n = \sigma(z_n, \mu_i)$, $\overline{W}_i^n = W_0(z_n, \mu_i)$; $\overline{f}_i = f_0(\mu_i)$, $\overline{g}_i = g_0(\mu_i)$; $\psi_i^n \approx \psi_0(z_n, \mu_i)$.

The scheme, which is well defined whenever $I \geq 5$, I odd, and $N \geq 3$, reads as follows:

---

[5] Two schemes, both of order 2, are described in reference [6]: the even and the odd scheme. Inasmuch as the same reference shows that the second one is better behaved, it is the odd scheme the one to be used.

- For $(i,n) \in \{1\} \times \{1,\dots,N-1\}$,

$$\begin{aligned}
&\left(-\frac{\mu_1}{k}+\frac{\overline{\mathrm{A}}_1^n}{2}+\frac{\overline{\sigma}_1^n\overline{D}_2}{2h^2}\right)\psi_1^n+\left(-\frac{\overline{\sigma}_1^n\overline{D}_3}{8h^2}\right)\psi_2^n+\\
&\qquad+\left(-\frac{\overline{\sigma}_1^n\overline{D}_2}{2h^2}\right)\psi_3^n+\left(\frac{\overline{\sigma}_1^n\overline{D}_3}{8h^2}\right)\psi_4^n+\\
&\qquad+\left(\frac{\mu_1}{k}+\frac{\overline{\mathrm{A}}_1^{n+1}}{2}+\frac{\overline{\sigma}_1^{n+1}\overline{D}_2}{2h^2}\right)\psi_1^{n+1}+\\
&+\left(-\frac{\overline{\sigma}_1^{n+1}\overline{D}_3}{8h^2}\right)\psi_2^{n+1}+\left(-\frac{\overline{\sigma}_1^{n+1}\overline{D}_2}{2h^2}\right)\psi_3^{n+1}+\\
&\qquad+\left(\frac{\overline{\sigma}_1^{n+1}\overline{D}_3}{8h^2}\right)\psi_4^{n+1}=\frac{\overline{W}_1^n+\overline{W}_1^{n+1}}{2}.
\end{aligned}\tag{63}$$

- For $(i,n) \in (\{2,\dots,i^\star-1\} \cup \{i^\star+1,\dots,I-1\}) \times \{1,\dots,N-1\}$,

$$\begin{aligned}
&\left(-\frac{\overline{\sigma}_i^n\overline{D}_{i-\frac{1}{2}}}{2h^2}\right)\psi_{i-1}^n+\\
&+\left(-\frac{\mu_i}{k}+\frac{\overline{\mathrm{A}}_i^n}{2}+\frac{\overline{\sigma}_i^n\left(\overline{D}_{i-\frac{1}{2}}+\overline{D}_{i+\frac{1}{2}}\right)}{2h^2}\right)\psi_i^n+\\
&+\left(-\frac{\overline{\sigma}_i^n\overline{D}_{i+\frac{1}{2}}}{2h^2}\right)\psi_{i+1}^n+\left(-\frac{\overline{\sigma}_i^{n+1}\overline{D}_{i-\frac{1}{2}}}{2h^2}\right)\psi_{i-1}^{n+1}+\\
&+\left(\frac{\mu_i}{k}+\frac{\overline{\mathrm{A}}_i^{n+1}}{2}+\frac{\overline{\sigma}_i^{n+1}\left(\overline{D}_{i-\frac{1}{2}}+\overline{D}_{i+\frac{1}{2}}\right)}{2h^2}\right)\psi_i^{n+1}+\\
&+\left(-\frac{\overline{\sigma}_i^{n+1}\overline{D}_{i+\frac{1}{2}}}{2h^2}\right)\psi_{i+1}^{n+1}=\frac{\overline{W}_i^n+\overline{W}_i^{n+1}}{2}.
\end{aligned}\tag{64}$$

- For $(i,n) \in \{i^\star\} \times \{2,\dots,N-1\}$,

$$\begin{aligned}
&\left(-\frac{\overline{\sigma}_{i^\star}^n}{h^2}\right)\psi_{i^\star-1}^n+\left(\overline{\mathrm{A}}_{i^\star}^n+\frac{2\overline{\sigma}_{i^\star}^n}{h^2}\right)\psi_{i^\star}^n+\left(-\frac{\overline{\sigma}_{i^\star}^n}{h^2}\right)\psi_{i^\star+1}^n=\\
&\qquad=\overline{W}_{i^\star}^n.
\end{aligned}\tag{65}$$

- For $(i,n) \in \{I\} \times \{1,\dots,N-1\}$,

$$\begin{aligned}
&\left(\frac{\overline{\sigma}_I^n\overline{D}_{I-2}}{8h^2}\right)\psi_{I-3}^n+\left(-\frac{\overline{\sigma}_I^n\overline{D}_{I-1}}{2h^2}\right)\psi_{I-2}^n+\\
&+\left(-\frac{\overline{\sigma}_I^n\overline{D}_{I-2}}{8h^2}\right)\psi_{I-1}^n+\left(-\frac{\mu_I}{k}+\frac{\overline{\mathrm{A}}_I^n}{2}+\frac{\overline{\sigma}_I^n\overline{D}_{I-1}}{2h^2}\right)\psi_I^n+\\
&+\left(\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-2}}{8h^2}\right)\psi_{I-3}^{n+1}+\left(-\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-1}}{2h^2}\right)\psi_{I-2}^{n+1}+\\
&+\left(-\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-2}}{8h^2}\right)\psi_{I-1}^{n+1}+\\
&+\left(\frac{\mu_I}{k}+\frac{\overline{\mathrm{A}}_I^{n+1}}{2}+\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-1}}{2h^2}\right)\psi_I^{n+1}=\frac{\overline{W}_I^n+\overline{W}_I^{n+1}}{2}.
\end{aligned}\tag{66}$$

- For $(i,n) \in \{i^\star,\dots,I\} \times \{1\}$,

$$\psi_i^1=\overline{f}_i.\tag{67}$$

- For $(i,n) \in \{1,\dots,i^\star\} \times \{N\}$,

$$\psi_i^N = \overline{g}_i. \tag{68}$$

Obviously, this scheme cannot be applied as it stands when $m > 0$, due to the singularities of the 'absorption' coefficient $\mathrm{A}(m)$ at $\mu = \pm 1$. Specifically, we face the problem that $\overline{\mathrm{A}}_1^n$ and $\overline{\mathrm{A}}_1^{n+1}$ in Equations (63) and $\overline{\mathrm{A}}_I^n$ and $\overline{\mathrm{A}}_I^{n+1}$ in Equations (66) are not defined, not to mention that the same could happen for $\overline{W}_1^n$, $\overline{W}_1^{n+1}$, $\overline{W}_I^n$, $\overline{W}_I^{n+1}$ if one is not in the physically relevant case.

In order to solve the singular cases ($m > 0$), we combine the odd scheme with the information given by Theorem 3. This means that Equations (63) are replaced by

$$\psi_1^n = \frac{(\mathcal{H}_W)_m(z_n,-1)}{m^2\overline{\sigma}_1^n}, \quad n \in \{1,\dots,N-1\}, \tag{69}$$

and Equations (66) are replaced by

$$\psi_I^n = \frac{(\mathcal{H}_W)_m(z_n,1)}{m^2\overline{\sigma}_I^n}, \quad n \in \{1,\dots,N-1\}. \tag{70}$$

Naturally, in addition one must understand in Equations (64), (65), (67) and (68) that $\overline{\mathrm{A}}_i^n = \mathrm{A}(m)(z_n,\mu_i)$, $\overline{W}_i^n = W_m(z_n,\mu_i)$; $\overline{f}_i = f_m(\mu_i)$, $\overline{g}_i = g_m(\mu_i)$; $\psi_i^n \approx \psi_m(z_n,\mu_i)$. It is obvious that $\overline{\mathrm{A}}_i^n$, $\overline{W}_i^n$, $\overline{f}_i$, $\overline{g}_i$ and ψ_i^n depend on m, even though our notation is not indicating this fact.

Remark 7. *Talking in terms of the nomenclature used in reference [7], we always use the* direct *algorithm rather than the* iterative *one for implementing the numerical schemes, since it is typically much faster.*

7.1 A security scheme for the cases $m > 0$

The above described scheme for the singular cases $m > 0$ relies upon the assumption that ψ satisfies (16)–(18), because the equalities in Equations (69) and (70) are consequences of Theorem 3. In view of the fact that there is no theoretical result guaranteeing that (16)–(18) always hold, it would be good to have at our disposal an 'assumption-independent' way of solving the singular cases.

Our proposal is the following: every time that it is not possible to evaluate $\mathrm{A}(m)$ or W_m at $\mu = -1$ (respectively, at $\mu = 1$), we take instead their value at $\mu = -1 + h^p$ (respectively, at $\mu = 1 - h^p$). The value of p is chosen as the minimum natural number such that the scheme maintains the order 2 in our numerical experiments, and this number has been proved to be $p = 4$. Recall that order 2 can only be observed when ψ is regular up to the boundary.

In other words, we define, for $n \in \{1,\dots,N\}$,

$$\widetilde{\mathrm{A}}_1^n = \mathrm{A}(m)(z_n,\mu_1 + h^4), \tag{71}$$

$$\widetilde{\mathrm{A}}_I^n = \mathrm{A}(m)(z_n,\mu_I - h^4), \tag{72}$$

$$\widetilde{W}_1^n = \begin{cases} \overline{W}_1^n \text{ if this number exists,} \\ W_m(z_n,\mu_1 + h^4) \text{ if } \overline{W}_1^n \text{ does not exist,} \end{cases} \tag{73}$$

$$\widetilde{W}_I^n = \begin{cases} \overline{W}_I^n \text{ if this number exists,} \\ W_m(z_n,\mu_I - h^4) \text{ if } \overline{W}_I^n \text{ does not exist,} \end{cases} \tag{74}$$

and use scheme (63)–(68) replacing Equations (63) by

$$\begin{aligned}\left(-\frac{\mu_1}{k}+\frac{\widetilde{\mathrm{A}}_1^n}{2}+\frac{\overline{\sigma}_1^n\overline{D}_2}{2h^2}\right)\psi_1^n+\left(-\frac{\overline{\sigma}_1^n\overline{D}_3}{8h^2}\right)\psi_2^n+&\\ +\left(-\frac{\overline{\sigma}_1^n\overline{D}_2}{2h^2}\right)\psi_3^n+\left(\frac{\overline{\sigma}_1^n\overline{D}_3}{8h^2}\right)\psi_4^n+&\\ +\left(\frac{\mu_1}{k}+\frac{\widetilde{\mathrm{A}}_1^{n+1}}{2}+\frac{\overline{\sigma}_1^{n+1}\overline{D}_2}{2h^2}\right)\psi_1^{n+1}+&\\ +\left(-\frac{\overline{\sigma}_1^{n+1}\overline{D}_3}{8h^2}\right)\psi_2^{n+1}+\left(-\frac{\overline{\sigma}_1^{n+1}\overline{D}_2}{2h^2}\right)\psi_3^{n+1}+&\\ +\left(\frac{\overline{\sigma}_1^{n+1}\overline{D}_3}{8h^2}\right)\psi_4^{n+1}=\frac{\widetilde{W}_1^n+\widetilde{W}_1^{n+1}}{2},&\\ n\in\{1,\ldots,N-1\},&\end{aligned}\tag{75}$$

and Equations (66) by

$$\begin{aligned}\left(\frac{\overline{\sigma}_I^n\overline{D}_{I-2}}{8h^2}\right)\psi_{I-3}^n+\left(-\frac{\overline{\sigma}_I^n\overline{D}_{I-1}}{2h^2}\right)\psi_{I-2}^n+&\\ +\left(-\frac{\overline{\sigma}_I^n\overline{D}_{I-2}}{8h^2}\right)\psi_{I-1}^n+\left(-\frac{\mu_I}{k}+\frac{\widetilde{\mathrm{A}}_I^n}{2}+\frac{\overline{\sigma}_I^n\overline{D}_{I-1}}{2h^2}\right)\psi_I^n+&\\ +\left(\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-2}}{8h^2}\right)\psi_{I-3}^{n+1}+\left(-\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-1}}{2h^2}\right)\psi_{I-2}^{n+1}+&\\ +\left(-\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-2}}{8h^2}\right)\psi_{I-1}^{n+1}+&\\ +\left(\frac{\mu_I}{k}+\frac{\widetilde{\mathrm{A}}_I^{n+1}}{2}+\frac{\overline{\sigma}_I^{n+1}\overline{D}_{I-1}}{2h^2}\right)\psi_I^{n+1}=\frac{\widetilde{W}_I^n+\widetilde{W}_I^{n+1}}{2},&\\ n\in\{1,\ldots,N-1\}.&\end{aligned}\tag{76}$$

The point is that the numerical results obtained with this security scheme coincide with the results that we get via Equations (69) and (70).

8 Numerical results for the core problem

Only numerical tests for the singular case are carried out, because the scheme for the regular case has already been tested in [6].

In order to know whether the main scheme for the singular case (i.e. the scheme (63)–(68) with the modifications (69) and (70)) works properly, it is enough to show the results obtained with the security scheme described in Subsection 7.1 and to check that the resulting solution obeys Equation (50).

We will not include, explicitly, results obtained with the main scheme, since they are almost equal to those got with the security scheme. Typically, the main scheme gives slightly better results for coarse meshes, but both solutions are soon indistinguishable as the mesh is getting refined. No difference between the two schemes has been observed in what regards the order of convergence.

When, in the examples below, the exact solution is not known, the numerical solution which is shown does not change in an essential way if the mesh is getting refined, that is to say, the reader will be observing a converged solution.

In this subsection, the subscript m is fixed to be $m = 1$, what is not a restriction for the purposes at hand, and the following problem is solved:

$$\mu \frac{\partial \psi}{\partial z} + \mathrm{A}\psi = \sigma \frac{\partial}{\partial \mu} \left[\left(1 - \mu^2\right) \frac{\partial \psi}{\partial \mu} \right] + W \tag{77}$$

in $Q_{z,\mu}$, accompanied by the conditions

$$\psi(Z_{\text{ini}}, \mu) = f(\mu) \text{ for } \mu \in (0, 1], \tag{78}$$

$$\psi(Z_{\text{fin}}, \mu) = g(\mu) \text{ for } \mu \in [-1, 0), \tag{79}$$

where $\mathrm{A} = \alpha + \frac{\sigma}{1-\mu^2}$ and $W = \frac{\mathcal{H}}{1-\mu^2}$. We have been assuming that $\mathcal{H} \in \mathrm{C}^1(\overline{Q}_{z,\mu})$ or at least $\mathcal{H} \in \mathrm{C}^0(\overline{Q}_{z,\mu})$ (see Remark 6), but a good functioning of the scheme will also be observed when $\mathcal{H}$ has got lower regularity as long as it remains bounded; we will include some example where $\mathcal{H}$ is discontinuous.

Let us take

$$Z_{\text{ini}} = 0, \;\; Z_{\text{fin}} = 1, \tag{80}$$

$$\alpha(z, \mu) = |\sin(12z\mu)|, \tag{81}$$

$$\sigma(z, \mu) = 1 + \sin(12z\mu)\cos(12z\mu), \tag{82}$$

and define $E_{\text{abs}} = \max |\psi_{\text{grid}} - \psi|$, where ψ_{grid} is representing the approximate solution and the maximum is taken over the set of all nodes.

The following numerical experiments have been conducted (when an exact *manufactured* solution is given, functions f, g and W are computed so that Equations (77)–(79) are satisfied; when one is not building a manufactured solution, lack of differentiability is observed at points $(z, \mu) \in \{(Z_{\text{ini}}, 0), (Z_{\text{fin}}, 0)\} = \{(0, 0), (1, 0)\}$, as it is typical.):

1. Let us consider the exact solution $\psi(z, \mu) = \ln(2 + \mu^2 + z^3)$. Then, $f(\mu) = \ln(2 + \mu^2)$, $g(\mu) = \ln(3 + \mu^2)$, and

$$W(z, \mu) = \frac{3\mu z^2}{2 + \mu^2 + z^3} + \left(\alpha(z, \mu) + \frac{\sigma(z, \mu)}{1 - \mu^2}\right) \ln(2 + \mu^2 + z^3) + 2\sigma(z, \mu) \frac{(-2 + 7\mu^2 + \mu^4 - z^3 + 3\mu^2 z^3)}{(2 + \mu^2 + z^3)^2}. \tag{83}$$

In this case, W is unbounded and not defined, in an essential way, at $|\mu| = 1$. Results obtained are collected in Table 1.

(I, N)	E_{abs}	order
$(11, 10)$	3.04×10^{-3}	
$(33, 29)$	3.37×10^{-4}	$\frac{2\ln\left(\frac{30.4}{3.37}\right)}{\ln(10)} = 1.91$
$(101, 91)$	3.61×10^{-5}	1.94
$(321, 281)$	3.58×10^{-6}	2.01
$(1001, 901)$	3.67×10^{-7}	1.98

Table 1: Maximum error and order for test 1 (security scheme).

Inasmuch as

$$\mathcal{H}(z, \pm 1) = \sigma(z, \pm 1) \ln(3 + z^3) \tag{84}$$

we should obtain, according to Equation (50),

$$\psi(z,\pm 1) = \frac{\sigma(z,\pm 1)\ln(3+z^3)}{\sigma(z,\pm 1)} = \ln(3+z^3), \tag{85}$$

which is consistent with $\psi(z,\mu) = \ln(2+\mu^2+z^3)$. Since the value of E_{abs} is taking into account comparison at all nodes, including boundary nodes, Table 1 shows that the numerical solution is indeed approaching $\ln(3+z^3)$ when $\mu = \pm 1$.

2. Let us consider the exact solution $\psi(z,\mu) = (1-\mu^2)\ln(2+z^3)$. Then, $f(\mu) = (1-\mu^2)\ln 2$, $g(\mu) = (1-\mu^2)\ln 3$, and

$$W(z,\mu) = \frac{3z^2(\mu-\mu^3)}{2+z^3} + \ln(2+z^3)\left\{\alpha(z,\mu)(1-\mu^2) + \sigma(z,\mu)\left[1+2(1-3\mu^2)\right]\right\}. \tag{86}$$

Now $W \in \mathrm{C}^0(\overline{Q}_{z,\mu})$. Results are shown in Table 2.

(I,N)	E_{abs}	order
$(11,10)$	8.15×10^{-3}	
$(33,29)$	6.32×10^{-4}	$\frac{2\ln(\frac{81.5}{6.32})}{\ln(10)} = 2.22$
$(101,91)$	6.76×10^{-5}	1.94
$(321,281)$	6.71×10^{-6}	2.01
$(1001,901)$	6.90×10^{-7}	1.98

Table 2: Maximum error and order for test 2 (security scheme).

Since

$$\mathcal{H}(\cdot,\pm 1) \equiv 0, \tag{87}$$

we should obtain, according to Equation (50),

$$\psi(\cdot,\pm 1) \equiv 0, \tag{88}$$

which once more is true.

3. For this test, let us take $f(\mu) = 2$, $g(\mu) = \frac{1}{1-\sin(12)\cos(12)}$, and

$$W(z,\mu) = \frac{2+z\mu}{1-\mu^2}. \tag{89}$$

Then, the exact solution is not known, and $\mathcal{H}(z,\mu) = 2+z\mu$. Notice that the compatibility conditions (48) and (49) are satisfied:

$$f(1) = \frac{\mathcal{H}(0,1)}{\sigma(0,1)} = 2, \tag{90}$$

$$g(-1) = \frac{\mathcal{H}(1,-1)}{\sigma(1,-1)} = \frac{1}{1-\sin(12)\cos(12)}. \tag{91}$$

Equation (50) predicts

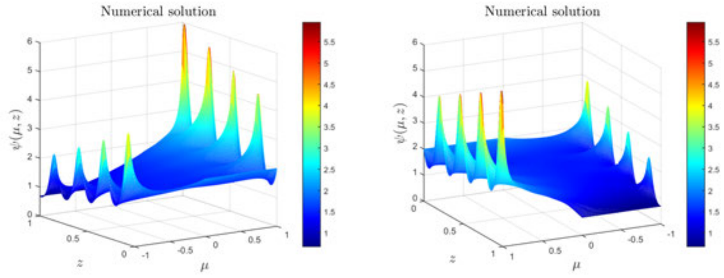
$$\psi(z,\pm 1) = \frac{\mathcal{H}(z,\pm 1)}{\sigma(z,\pm 1)} = \frac{2\pm z}{1\pm\sin(12z)\cos(12z)}, \tag{92}$$

which is shown to be true in Table 3, where the results exhibit convergence to 0, with order about 3.5, of $\left|\psi_{\text{grid}} - \frac{\mathcal{H}}{\sigma}\right|$ restricted to $\mu = \pm 1$.

(I,N)	$\max\left\{\left\lvert\psi_{\text{grid}}-\frac{\mathcal{H}}{\sigma}\right\rvert :\ \mu=\pm1\right\}$	order
$(11,10)$	7.53×10^{-1}	
$(33,29)$	6.07×10^{-3}	$\frac{2\ln(\frac{753}{6.07})}{\ln(10)}=4.18$
$(101,91)$	1.18×10^{-4}	3.43
$(321,281)$	1.99×10^{-6}	3.54
$(1001,901)$	3.64×10^{-8}	3.48

Table 3: Maximum value on $\mu=\pm1$ of $\left\lvert\psi_{\text{grid}}-\frac{\mathcal{H}}{\sigma}\right\rvert$ for different meshes (security scheme). Test 3.

The numerical solution is plotted in Figure 1.



(a) Front.

(b) Back.

Figure 1: Approximate solution for $I=201$, $N=200$ (security scheme). Test 3.

4. Consider now

$$f(\mu)=\begin{cases}\exp[-1/(\mu^2(1-\mu^2))] & \text{if}\quad \mu\in(0,1),\\ 0 & \text{if}\quad \mu\in\{0,1\},\end{cases}\tag{93}$$

$$g(\mu)=0,\tag{94}$$

and

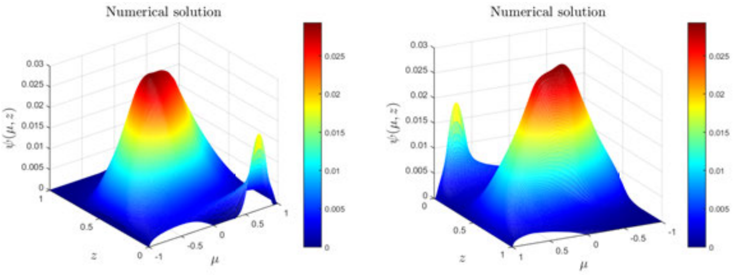
$$W(z,\mu)=\begin{cases}2|z\mu| & \text{if}\quad \|(z,\mu)-(0.5,0)\|_2\leq 0.3,\\ 0 & \text{otherwise.}\end{cases}\tag{95}$$

Again, the exact solution is not known. Although W is discontinuous, the solution ψ, plotted in Figure 2, is continuous due to the effect of the diffusion.

(I,N)	$\max\{\lvert\psi_{\text{grid}}\rvert :\ \mu=\pm1\}$	order
$(11,10)$	6.19×10^{-4}	
$(33,29)$	7.41×10^{-6}	$\frac{2\ln(\frac{619}{7.41})}{\ln(10)}=3.84$
$(101,91)$	8.29×10^{-8}	3.90
$(321,281)$	1.40×10^{-9}	3.54
$(1001,901)$	2.60×10^{-11}	3.46

Table 4: Maximum value on $\mu=\pm1$ of $\lvert\psi_{\text{grid}}\rvert$ for different meshes (security scheme). Test 4.

Notice that $\mathcal{H}(\cdot,\pm1)\equiv0$ and the compatibility conditions (48) and (49) hold. As predicted by Equation (50), one gets $\psi(\cdot,\pm1)\equiv0$.



(a) Front. (b) Back.

Figure 2: Approximate solution for $I = 201$, $N = 200$ (security scheme). Test 4.

   Table 4 shows that the numerical solution restricted to $\mu = \pm 1$ goes to zero with order greater than 3 as the mesh is getting refined.

5. For the last test in this subsection, let us take

$$f(\mu) = 0, \tag{96}$$

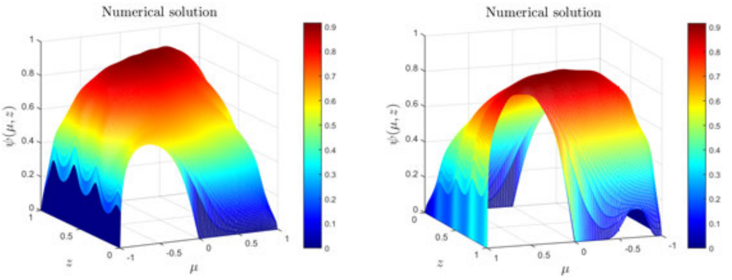
$$g(\mu) = \begin{cases} 10 \exp[-1/(\mu^2(1-\mu^2))] & \text{if} \quad \mu \in (-1, 0), \\ 0 & \text{if} \quad \mu \in \{-1, 0\}, \end{cases} \tag{97}$$

   and

$$W(z, \mu) = \frac{1+z}{\sqrt{1-\mu^2}}. \tag{98}$$

   This is another example with unknown exact solution. Notice that the observed solution ψ, plotted in Figure 3, is zero at $|\mu| = 1$, despite being the source W unbounded. Once more, we have coincidence with the value predicted by Equation (50), since $\mathcal{H}(\cdot, \pm 1) \equiv 0$ and the compatibility conditions (48) and (49) hold.

   Table 5 shows that the numerical solution restricted to $\mu = \pm 1$ goes to zero with order around 2 as the mesh is getting refined.



(a) Front. (b) Back.

Figure 3: Approximate solution for $I = 201$, $N = 200$ (security scheme). Test 5.

(I,N)	$\max\{\lvert\psi_{\text{grid}}\rvert :\ \mu=\pm 1\}$	order
$(11,10)$	3.10×10^{-1}	
$(33,29)$	3.61×10^{-2}	$\frac{2\ln(\frac{31}{3.61})}{\ln(10)}=1.87$
$(101,91)$	4.34×10^{-3}	1.84
$(321,281)$	4.25×10^{-4}	2.02
$(1001,901)$	4.36×10^{-5}	1.98

Table 5: Maximum value on $\mu=\pm 1$ of $|\psi_{\text{grid}}|$ for different meshes (security scheme). Test 5.

9 Numerical results for the full problem

The solution of problem (1)–(4) ψ is approximated from Equation (34) via a truncation of the Fourier series, that is to say,

$$\psi(z,\mu,\theta)\approx\psi_0(z,\mu)+$$
$$2\sum_{m=1}^{M}\left\{\operatorname{Re}[\psi_m(z,\mu)]\cos(m\theta)\ -\operatorname{Im}[\psi_m(z,\mu)]\sin(m\theta)\right\}. \tag{99}$$

Each ψ_m, $m=0,\dots,M$, is computed as the solution of the problem (42)–(44). The case $M=0$ must be understood as $\psi(z,\mu,\theta)\approx\psi_0(z,\mu)$.

The representation (99) implies that ψ will be approximated by a function which is of class C^∞ with respect to the variable θ, and assures that the approximation satisfies the periodicity conditions (4).

When f, g and W do not depend on θ, then the solution ψ is θ-independent as well and the problem is actually the one which is solved in reference [6]; taking $M=0$ is enough in this case. When the exact solution has got the form $\psi(z,\mu,\theta)=\psi_0(z,\mu)+\psi_{\cos}(z,\mu)\cos(p\theta)+\psi_{\sin}(z,\mu)\sin(q\theta)$, with $p,q\in\mathbb{N}$, it is enough to solve for the three values $m=0,p,q$ in order to have exactness with respect to the variable θ.

Following the line of the previous section, when the exact solution is not known, the numerical solution which is shown is a converged one.

Notice that Equation (99) allows computing approximations of the values $\psi(z_n,\mu_i,\theta)$ on grid nodes (z_n,μ_i), for every $\theta\in[0,2\pi)$. In subsequent tables, we will use the notation $E_{\text{abs}}^{\text{full}}=\max|\psi_{\text{grid}}-\psi|$, where ψ_{grid} is representing the approximate solution and the maximum is taken over the set

$$\{(z_n,\mu_i,\theta_j):\ 1\le n\le N,\ 1\le i\le I,\ 1\le j\le J\}, \tag{100}$$

being $\theta_1=0<\theta_2<\cdots<\theta_{J-1}<\theta_J=2\pi$ a uniform mesh of $[0,2\pi]$ with $J=100$.

We will always take $Z_{\text{ini}}=0,\ Z_{\text{fin}}=1$.

9.1 Test 1

Let us consider

$$\alpha(z,\mu)=|\sin(12\mu z)|, \tag{101}$$
$$\sigma(z,\mu)=1+\sin(12\mu z)\cos(12\mu z). \tag{102}$$

The function $\psi(z,\mu,\theta)=\ln(2+\sin(3\mu z))+(1-\mu^2)\mathrm{e}^{\sin\theta}$ is the exact solution of problem (1)–(4) if

$$f(\mu,\theta)=\ln(2)+(1-\mu^2)\mathrm{e}^{\sin\theta}, \tag{103}$$
$$g(\mu,\theta)=\ln(2+\sin(3\mu))+(1-\mu^2)\mathrm{e}^{\sin\theta}, \tag{104}$$

and

$$\begin{aligned} W(z,\mu,\theta) = \frac{3\mu^2\cos(3\mu z)}{2+\sin(3\mu z)} + \alpha(z,\mu)\psi(z,\mu,\theta) - \\ \sigma(z,\mu)\left\{-2\mu\left(\frac{3z\cos(3\mu z)}{2+\sin(3\mu z)} - 2\mu \mathrm{e}^{\sin\theta}\right) + \right. \\ (1-\mu^2)\left(\frac{-18z^2\sin(3\mu z) - 9z^2}{(2+\sin(3\mu z))^2} - 2\mathrm{e}^{\sin\theta}\right) + \\ \left. \left(-\sin\theta + \cos^2\theta\right)\mathrm{e}^{\sin\theta}\right\}. \end{aligned} \tag{105}$$

This is an example where functions $\psi(\cdot,\pm1,\cdot)$ do not depend on θ despite $W(\cdot,\pm1,\cdot)$ do.

Since the Fourier series of $\mathrm{e}^{\sin\theta}$ is infinite, there is no expectancy that Equation (99) can be exact for any value of M. However, the high regularity of this function make the series converge fast, and so a small value of M is enough to capture the solution. Tables 6, 7 and 8 show the results obtained for $M = 5, 6, 7$. One can compare the results for two successive values of M and consider that the solution is good when there is no significant difference between them, but the criterion for not going beyond $M = 7$ in this case is simply that, for the meshes we are using, this value of M preserves for the full problem the order 2 of the core scheme; in other words, it is not worth taking $M > 7$ because the error due to the series truncation at level $M = 7$ is negligible when compared with the error due to discretization of the (z,μ)-domain.

(I,N)	$E_{\mathrm{abs}}^{\mathrm{full}}$	order
$(11,10)$	1.24×10^{-1}	
$(33,29)$	3.74×10^{-3}	$\frac{2\ln(\frac{124}{3.74})}{\ln(10)} = 3.04$
$(101,91)$	4.04×10^{-4}	1.93
$(321,281)$	8.17×10^{-5}	1.38
$(1001,901)$	5.11×10^{-5}	0.41

Table 6: Numerical results for test 1 with $M = 5$.

(I,N)	$E_{\mathrm{abs}}^{\mathrm{full}}$	order
$(11,10)$	1.24×10^{-1}	
$(33,29)$	3.74×10^{-3}	$\frac{2\ln(\frac{124}{3.74})}{\ln(10)} = 3.04$
$(101,91)$	3.77×10^{-4}	1.99
$(321,281)$	4.09×10^{-5}	1.93
$(1001,901)$	6.99×10^{-6}	1.53

Table 7: Numerical results for test 1 with $M = 6$.

(I,N)	$E_{\mathrm{abs}}^{\mathrm{full}}$	order
$(11,10)$	1.24×10^{-1}	
$(33,29)$	3.74×10^{-3}	$\frac{2\ln(\frac{124}{3.74})}{\ln(10)} = 3.04$
$(101,91)$	3.79×10^{-4}	1.99
$(321,281)$	3.92×10^{-5}	1.97
$(1001,901)$	4.18×10^{-6}	1.94

Table 8: Numerical results for test 1 with $M = 7$.

9.2 Test 2

In this test, we take the following data functions:

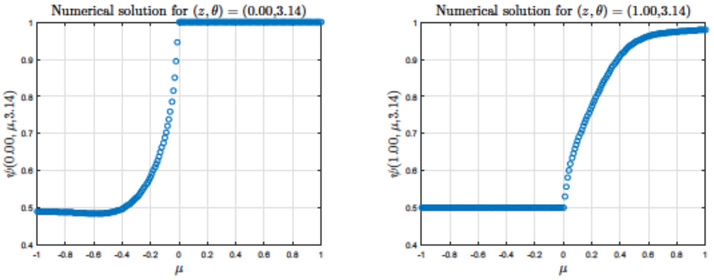
$$\alpha(z,\mu) = 0.02, \tag{106}$$

$$\sigma(z,\mu) = 0.01, \tag{107}$$

$$f(\mu,\theta) = 1, \tag{108}$$

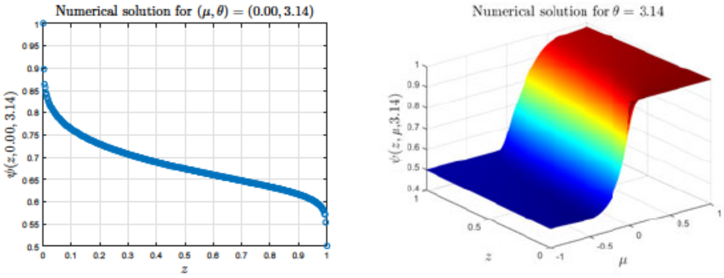
$$g(\mu,\theta) = 0.5 + 0.1(1+\mu)\sin(3\theta), \tag{109}$$

$$W(z,\mu,\theta) = 0. \tag{110}$$



(a) $z = 0$, $\theta = \pi$, and μ varies. (b) $z = 1$, $\theta = \pi$, and μ varies.

Figure 4: Approximate solution for $I = 201$, $N = 400$. Test 9.2.



(a) $\mu = 0$, $\theta = \pi$, and z varies. (b) $\theta = \pi$, and z and μ vary.

Figure 5: Approximate solution for $I = 201$, $N = 400$. Test 9.2.

It is easy to check that

$$f_0(\mu) = 1,\ f_m \equiv 0 \text{ if } m > 0, \tag{111}$$

$$g_0(\mu) = 0.5,\ g_3(\mu) = -\frac{i}{2}\,0.1(1+\mu), \tag{112}$$

$$g_m \equiv 0 \text{ if } m \in \{1,2\} \text{ or } m > 3. \tag{113}$$

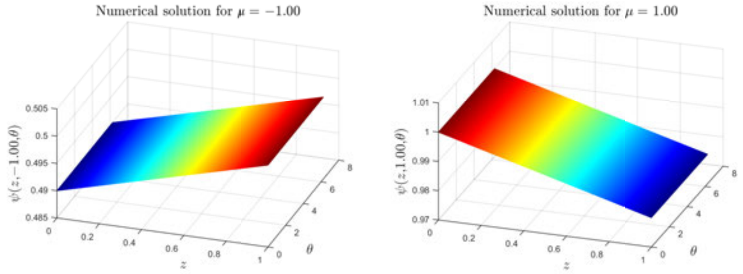
When the three Fourier coefficients f_m, g_m, and W_m are zero, the solution ψ_m to the problem (42)–(44) is zero as well, and consequently the numerical method is exact with respect to θ if we take $M = 3$.

The significance of this example lies in that it allows one to observe a typical behaviour of the solution in problems of interest, where the exact solution shows signs of being singular at points (z,μ,θ) with $\mu = 0$ and

$z \in \{Z_{\text{ini}}, Z_{\text{fin}}\} = \{0, 1\}$, even when all data functions are of class C^∞. To specify, one gets numerical results which seem to indicate that $\frac{\partial \psi}{\partial \mu}(0, 0, \theta)$ and $\frac{\partial \psi}{\partial \mu}(1, 0, \theta)$ do not exist and that $\left|\frac{\partial \psi}{\partial z}(z, 0, \theta)\right| \to \infty$ when $z \to 0$ or $z \to 1$. We show in Figures 4 and 5 some results for $\theta = \pi$; plots for other values of θ are similar.

Notice that this example fits in with the physically relevant case (see Definition 1), and so one would expect that $\psi(\cdot, \pm 1, \cdot)$ were independent of θ (recall Theorem 1), while of course there is no need for $\psi(\cdot, \mu, \cdot)$ to be independent of θ when $|\mu| \neq 1$. Both features can be observed in Figures 6 and 7. The security scheme has been used to solve the core problems, and so we have not forced the scheme to provide us with θ-independent functions $\psi(\cdot, \pm 1, \cdot)$.

Remark 8. *We do not know whether assumptions (16)–(18) are satisfied or not, but nonetheless the results are in agreement with Theorem 1.*



(a) $\mu = -1$, and z and θ vary.

(b) $\mu = 1$, and z and θ vary.

Figure 6: Approximate solution for $I = 201$, $N = 400$, showing that functions $\psi(\cdot, \pm 1, \cdot)$ are independent of θ. Test 9.2.

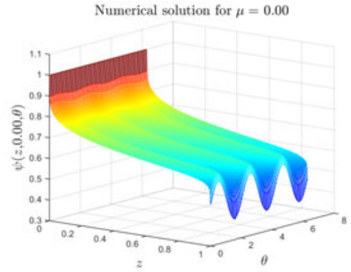


Figure 7: $\mu = 0$, and z and θ vary. Approximate solution for $I = 201$, $N = 400$, showing that $\psi(\cdot, 0, \cdot)$ depends on θ. Test 9.2.

We have taken $N = 400$ only to have at our disposal more points for the graphs, specifically for the plot (a) in Figure 5 showing that $\left|\frac{\partial \psi}{\partial z}(z, 0, \theta)\right| \to \infty$ when $z \to 0$ or $z \to 1$. Nonetheless, a good converged solution is also obtained by taking $N = 200$, as in previous examples.

10 Conclusions and final thoughts

The main conclusion drawn from this paper is that the 3D problem (1)–(4) can be reduced to a collection of θ-independent 2D problems. These core problems contain singularities which can be treated with the aid of several different ideas; the ones we have chosen rely on computing, *a priori*, the values of the solution at the singularities by means of analytical methods or on employing numerical schemes that avoid function evaluations at the conflictive points.

The methods herein described exhibit order 2 of convergence, but this characteristic becomes less important for real problems where the solution is not regular, because the order ceases to be observed as soon as the solution loses regularity.

It is an open problem to prove existence and uniqueness of solution for the problem (1)–(4), and also to prove the amount of regularity that this solution could have. Results in these directions would have great interest from the mathematical standpoint.

Finally, it could be of interest to explore the potential relationship that our problem has got with the field of surface PDEs. This is because the continuous scattering operator (7) is the Laplace-Beltrami operator or, simply, the Laplacian over the sphere, which in turn means that the PDE (1) can be seen, with respect to the angular variables, as a PDE over the unit sphere.

11 Appendix

The result of interest in this appendix will be Lemma 4, the proof of which will require the use of the following lemma.

Lemma 3. *Let p and n be two natural numbers and consider a function*

$$f : \boldsymbol{x} = (x_1, \dots, x_p) \in [0,1]^p \to f(\boldsymbol{x}) \in \mathbb{R} \tag{114}$$

in $\mathrm{C}^n([0,1]^p)$. *Fix* $j \in \{1, \dots, p\}$.

Then, the function $g : [0,1]^p \to \mathbb{R}$ *defined by*

$$g(\boldsymbol{x}) = \begin{cases} \dfrac{f(\boldsymbol{x})}{x_j} & \text{if} \quad x_j \in (0,1], \\ \dfrac{\partial f}{\partial x_j}(\boldsymbol{x}) & \text{if} \quad x_j = 0 \end{cases} \tag{115}$$

belongs to $\mathrm{C}^{n-1}([0,1]^p)$ *if, and only if,* $f(\boldsymbol{x}) = 0$ *whenever* $x_j = 0$, *that is to say, if, and only if,*

$$f(\boldsymbol{x}_{(j,0)}) = 0 \quad \forall (x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_p) \in [0,1]^{p-1}, \tag{116}$$

where $\boldsymbol{x}_{(j,0)} = (x_1, \dots, x_{j-1}, 0, x_{j+1}, \dots, x_p)$. *When* $p = 1$, *Equation (116) must be understood as* $f(0) = 0$.

A proof of Lemma 3 can be done by using rather elementary concepts of Mathematical Analysis.

Remark 9. *In the context of Lemma 3, one has that* $g \in \mathrm{C}^\infty([0,1]^p)$ *when* $f \in \mathrm{C}^\infty([0,1]^p)$ *and satisfies condition (116).*

Remark 10. *The corresponding adaptation of Lemma 3 is true when the domain of* f *is* $K_1 \times \cdots \times K_p$ *for compact intervals* $K_1, \dots, K_p \subset \mathbb{R}$, *with the proviso that they have got nonvoid interior and that* $0 \in K_j$.

Lemma 4 (Regularity of the source W in the physically relevant case)**.** *Suppose that (12) holds. Then, the following assertions are equivalent:*

1. *Condition (23) holds.*
2. $W \in \mathrm{C}^0(\overline{Q}_{z,\mu,\theta})$.

Proof. It suffices to prove that '1 ⇒ 2', as the other implication is clear. So, assume that (12) and (23) hold. Thanks to Lemma 1, we can limit ourselves to demonstrate that the function $\mathcal{G} : \overline{Q}_{z,\mu,\theta} \to \mathbb{R}$ defined by

$$\mathcal{G}(z,\mu,\theta) = \begin{cases} \dfrac{\mathcal{H}_W(z,\mu,\theta)}{1-\mu^2} & \text{if } (z,\mu,\theta) \in \overline{Q}_z \times Q_\mu \times \overline{Q}_\theta, \\[2ex] \dfrac{1}{2}\dfrac{\partial \mathcal{H}_W}{\partial \mu}(z,-1,\theta) & \text{if } (z,\mu,\theta) \in \overline{Q}_z \times \{-1\} \times \overline{Q}_\theta, \\[2ex] -\dfrac{1}{2}\dfrac{\partial \mathcal{H}_W}{\partial \mu}(z,1,\theta) & \text{if } (z,\mu,\theta) \in \overline{Q}_z \times \{1\} \times \overline{Q}_\theta \end{cases} \tag{117}$$

belongs to $\mathrm{C}^0(\overline{Q}_{z,\mu,\theta})$, which in turn amounts to prove C^0 regularity of $\mathcal{G}$ at points of $\overline{Q}_{z,\mu,\theta}$ with $\mu = \pm 1$ (briefly, 'at $\mu = \pm 1$').

- C^0 regularity of $\mathcal{G}$ at $\mu = -1$. Define $\widehat{\mathcal{H}} : \overline{Q}_z \times [0,1] \times \overline{Q}_\theta \to \mathbb{R}$ as follows:

  $$\widehat{\mathcal{H}}(z,t,\theta) = \mathcal{H}_W(z,t-1,\theta). \tag{118}$$

  Now notice that the function $\widehat{\mathcal{G}} : \overline{Q}_z \times [0,1] \times \overline{Q}_\theta \to \mathbb{R}$ defined by

  $$\widehat{\mathcal{G}}(z,t,\theta) = \begin{cases} \dfrac{\widehat{\mathcal{H}}(z,t,\theta)}{t} & \text{if } (z,t,\theta) \in \overline{Q}_z \times (0,1] \times \overline{Q}_\theta, \\[2ex] \dfrac{\partial \widehat{\mathcal{H}}}{\partial t}(z,0,\theta) & \text{if } (z,t,\theta) \in \overline{Q}_z \times \{0\} \times \overline{Q}_\theta \end{cases} \tag{119}$$

  belongs to $\mathrm{C}^0(\overline{Q}_z \times [0,1] \times \overline{Q}_\theta)$, according to Lemma 3 (see Remark 10). Finally, simply observe that

  $$\mathcal{G}(z,\mu,\theta) = \frac{\widehat{\mathcal{G}}(z,1+\mu,\theta)}{1-\mu} \ \forall (z,\mu,\theta) \in \overline{Q}_z \times [-1,0] \times \overline{Q}_\theta. \tag{120}$$

- C^0 regularity of $\mathcal{G}$ at $\mu = 1$. Similarly, if $\mathcal{H}^\star : \overline{Q}_z \times [0,1] \times \overline{Q}_\theta \to \mathbb{R}$ is given by

  $$\mathcal{H}^\star(z,t,\theta) = \mathcal{H}_W(z,1-t,\theta), \tag{121}$$

  then, the function $\mathcal{G}^\star : \overline{Q}_z \times [0,1] \times \overline{Q}_\theta \to \mathbb{R}$ defined by

  $$\mathcal{G}^\star(z,t,\theta) = \begin{cases} \dfrac{\mathcal{H}^\star(z,t,\theta)}{t} & \text{if } (z,t,\theta) \in \overline{Q}_z \times (0,1] \times \overline{Q}_\theta, \\[2ex] \dfrac{\partial \mathcal{H}^\star}{\partial t}(z,0,\theta) & \text{if } (z,t,\theta) \in \overline{Q}_z \times \{0\} \times \overline{Q}_\theta \end{cases} \tag{122}$$

  belongs to $\mathrm{C}^0(\overline{Q}_z \times [0,1] \times \overline{Q}_\theta)$, according again to Lemma 3. Finally, observe that

  $$\mathcal{G}(z,\mu,\theta) = \frac{\mathcal{G}^\star(z,1-\mu,\theta)}{1+\mu} \ \forall (z,\mu,\theta) \in \overline{Q}_z \times [0,1] \times \overline{Q}_\theta. \tag{123}$$

■

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