Instituto Universitário de Lisboa

Department of Finance

Valuation of Financial Derivatives through Transmutation Operator Methods

A thesis presented in partial fulfillment of the requirements for the degree of Doctor in Finance

by

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September, 2018

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Resume

Nowadays there is a fast development of the methods based on transmutation operators (TO) theory for solving differential equations. The possibility to construct the images of solutions for TO in certain cases allowed the construction of accurate numerical solutions to several problems that appear in different applied fields. In the present work, for the first time, it is shown that these methods can be effectively applied to the optimal stopping problems that appear in mathematical finance.

The first part of the thesis (Chapter 2) consists of an application of the method to the valuation of European-style double-barrier knock-out options (DBKO). This is done by using the efficient computation of eigenvalues for the Shrödinger equation and a representation of solutions in terms of Neumann series of Bessel functions. This knowledge was used in the construction of a novel analytically tractable method for pricing (and hedging) DBKO, which can be applied to the whole class of one-dimensional time-homogeneous diffusions even for the cases where the corresponding transition density is not known. The proposed numerical method is shown to be efficient and simple to implement. To illustrate the flexibility and computational power of the algorithm it is constructed an extended jump to default model that is able to capture several empirical regularities commonly observed in the literature.

The second part of the thesis (Chapters 3 and 4) is dedicated to the study of the more complicated problems: the free boundary problems. For this purpose, the method was first (in some certain sense) generalized and tested on the Stefan-like problem. The method consists in efficiently constructing a complete system of solutions for parabolic equation from known solutions for the heat equation, heat polynomials (HP). This way it was possible to extend the numerical method that existed only for the heat equation to the large class of parabolic equations. However, for the selected financial problem, Russian option with finite horizon (ROFH), the numerical computation from the method based on HP revealed to be non-efficient. This is due to the more complex structure of the problem, specifically the non-consistent boundary conditions. Hence, it was developed another variation of the method that uses different systems of solutions for the heat equation: the generalized exponential basis. The constructed method proved to be accurate, relatively easy to implement and can it can be applied to the large class of the free boundary problems. The value of the ROFH has been an important theme of discussion in the last decades. The application of the method to this problem confirmed several results that have appeared recently in the literature and shred some light on the differences that were present.

The constructed methods have a large scope of applications not only in financial field, but also in other disciplines. Both studies also open a variety of future research and applications that are discussed in the text.

JEL Classification: G13, C60, G33.

Keywords: Finance, Double barrier options, Russian Options, Transmutation operators, Free boundary problems, Sturm-Liouville equations, Neumann series of Bessel functions.

Resumo

Actualmente estamos a assistir a um rápido desenvolvimento de métodos baseados nos operadores de transmutação (OT) para a resolução de equações diferenciais. Em certos casos, é possível calcular as imagens de soluções para OT, o que permite construir soluções numéricas com um elevado grau de precisão para diversos problemas aplicados. No presente trabalho, pela primeira vez, é desenvolvida e ilustrada uma aplicação eficiente destes métodos aos problemas de paragem óptima que surgem na matemática financeira.

A primeira parte da tese (Capítulo 2) consiste na aplicação do método ao problema de avaliação de opção com dupla barreira knock-out (DBKO) de estilo europeu. A construção do método passa por um apurado cálculo de valores próprios do respectivo problema de Schrödinger e a representação de soluções em termos de séries de Neumann de funções de Bessel. Esse conhecimento foi utilizado para construir um novo método de expressão analítica para definição de preço (e cobertura) de DBKO. O método pode ser aplicado a toda uma classe de difusões uni-dimensionais homogéneas no tempo, mesmo para os casos em que não é conhecida a função de densidade de transição. Neste capítulo é demonstrado que o método proposto é eficiente e simples de implementar. Para ilustrar a flexibilidade e a robustez computacional do respectivo algoritmo é construído um modelo estendido de salto para o incumprimento que oferece a possibilidade de captar certos efeitos empíricos presentes na literatura.

A segunda parte da tese (Capítulos 3 e 4) é dedicada ao estudo de problemas mais complexos: problemas de fronteira livre. Para esse propósito, o método foi (em certo sentido) generalizado e testado no problema do tipo de Stefan. O método consiste numa construção eficiente de um sistema completo de soluções para uma equação diferencial parabólica a partir de um sistema completo de soluções para a equação de calor, os polinómios de calor (PC). Deste modo, foi possível estender o método numérico que existia apenas par a equação de calor para uma larga classe de equações parabólicas. No entanto, para o problema financeiro seleccionado, a opção russa com horizonte finito (ORHF), o método baseado nos PCs revelou-se computacionalmente ineficiente. Isso deve-se a uma estrutura mais complicada do problema, nomeadamente as não-consistentes condições de fronteira. Como tal, foi desenvolvida uma outra variação do método que usa um sistema de soluções diferente de PCs: uma base exponencial generalizada. O método construído provou ser preciso, de relativamente fácil implementação e pode ser aplicado a uma larga classe de problemas de fronteira livre. O valor de ORHF foi e continua a ser um importante tema de discussão nas últimas décadas. A aplicação do método a esse problema confirmou vários resultados que surgiram recentemente na literatura e revelou o porquê de algumas diferenças.

Os métodos construídos têm uma larga gama de aplicações, tanto no âmbito de matemática financeira como em outras disciplinas. Ambos os estudos abrem várias possibilidades para futuras investigações e aplicações, as discussão das quais se encontram no texto.

JEL Classification: G13, C60, G33.

Palavras chave: Finanças, Opções barreira, Opções russas, Operadores de trasmutação, Problemas de fronteira livre, Equações de Sturm-Liouville, Séries de Neumann de funções de Bessel

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Contents

1. Introduction

1.1 Thesis structure

The thesis focuses on the application of the numerical methods derived from transmutation operators theory to problems in mathematical finance. The three main chapters 2-4 are the following independent articles:

- *Pricing double barrier options on homogeneous diffusions: a Neumann series of Bessel functions representation*
  This paper is a joint work with Vladislav V. Kravchenko, Sergii M. Torba and José Carlos Dias, it was submitted to Quantitative Finance and is available at *arXiv:1712.08247*.
  The article was accepted and presented at *INFORMS Annual Meeting 2017, Houston*.

- *Solution of parabolic free boundary problems using transmuted heat polynomials*
  This paper is a joint work with Vladislav V. Kravchenko and Sergii M. Torba. It was submitted to Computational Mathematics and Mathematical Physics and is available at *arXiv:1706.07100*.
  The exposition based on this article was accepted and presented at *Bachelier Finance Society, 10th World Congress 2018, Dublin*.

- *Generalized exponential basis for efficient solving of homogeneous diffusion free boundary problems: Russian option pricing*

  This paper is a joint work with Vladislav V. Kravchenko, Sergii M. Torba and José Carlos Dias, in preparation to be submitted and is available at *arXiv:1808.08290*. The article was accepted and presented at *Bachelier Finance Society, 10th World Congress 2018, Dublin*.

Each of the chapters is a self contained article the repetition of the concepts is unavoidable. It is also to be expected that the notation might differ between the chapters. Besides the present introduction and the chapters described above, in the final chapter are presented final comments and expected directions for future research.

1.2 Motivation and outline of the thesis

One of the modern problems in mathematical finance is the valuation of exotic options. The introduction of the Black-Scholes-Merton formula for valuing European-type options triggered the development of mathematical models assuming a given stochastic behaviour of the underlying asset. Under some general assumption, exotic option valuation problems often lead to optimal stopping problems, which is an exciting field of mathematics, transversal to many applications, not only financial, but also in physics, biology, etc.

To the best of my knowledge, this thesis focuses for the first time on the application of the numerical methods derived from the transmutation operators (TO) theory for solving the optimal stopping problems that appear in mathematical finance. An additional challenge for the practical applications is the ability of the method to be numerically executable, i.e. to actually be implemented. This way for each separate problem the two objectives have to be fulfilled:

- Construct the method for solving the proposed problem;
- Show that the method can be numerically implemented.

The first part of the thesis deals with double barrier knock-out options (DBKO)[1]. The standard technique for solving this problem is to use the method of separation of variables and then represent the solution in terms of eigenfunctions, after solving the corresponding Sturm-Liouville problem. The generalization of this approach to more complicated models (where we cannot explicitly calculate eigenvalues) is challenging. With recent results from TO theory it was possible to construct a numerical algorithm that permitted to generalize this construction for any model where the underlying follows time-homogeneous diffusion with certain type of killing rate. This was done by using Neumann series of Bessel functions (NSBF) decomposition for the derived Shrödinger equation, that itself was obtained by transmutation of the solutions of the equation $u_{xx} = 0$. The use of NSBF decomposition in a standard method opened a large scope of avenues for future research, such as its application to the singular problems that arise in mathematical finance, plain-vanilla options (unbounded domains), default cases (singularities in the coefficients) and others, and showed the potential of these numerical methods for the practical applications. I intend to explore this direction in the future research.

The second part of the thesis considers more complex problems: the free boundary problems. The TO's can be used to transmute (the known) solutions of the heat equation into the solution of the parabolic equation under study (PE). It is possible to take

[1]To avoid repetition and the bloating of this introductory section I have decided to keep the bibliography references to the main chapters

a complete system of solutions (CSS) for the heat equation, such as heat polynomials (HP) and transmute it into the CSS for the PE. Recently, this theoretical construction gained a fundamental practical application for the large class of differential operators and for certain CSS. This was possible due to the newly developed method to compute the images of these CSS under the action of TO. These images possess an analytically tractable representation.

The idea for the numerical method based on the transmuted CSS was first tested on a generalization of the classical Stefan-like problem. This experiment and illustration of the method is presented in Chapter 3. For this purpose, the HP were used as a CSS for the heat equation. This method is referred to as transmuted heat polynomials (THP) method. The numerical implementation revealed to be relatively simple and direct.

However, the extension of the THP to the Russian option with finite horizon (ROFH), the financial problem selected, presented an additional difficulty. The constructed THP increase very rapidly and non-consistency of the boundary conditions requires a large number of functions from CSS for the accurate approximation. These requirements turn out to be hard to satisfy in numerical computations. They made THP unfit for computing a precise approximated solution. This issue was circumvented by using a different CSS for the heat equation, the generalized exponential powers.

The ROFH evaluation presents an interesting problem on both theoretical and numerical sides. For the last decade there seems to be no agreement in the literature on a value of the ROFH under different horizons. The application of our method permitted to compute the values of ROFH that have been in discussion. We were able to confirm some of the values obtained previously and (in our opinion) justifying the differences in discussion. In the process, we were also able to present the valuation surface, never illustrated before in the literature.

The constructed method can be applied to the large class of free boundary problems. It does not depend on the knowledge of the density function and can be applied to general time-homogeneous diffusion models. Currently, the author of this thesis is working on its application to the evaluation problem for American options under a general time-homogeneous diffusion model.

2. Pricing double barrier options on homogeneous diffusions: a Neumann series of Bessel functions representation

Abstract: This paper develops a novel analytically tractable Neumann series of Bessel functions representation for pricing (and hedging) European-style double barrier knock-out options, which can be applied to the whole class of one-dimensional time-homogeneous diffusions even for the cases where the corresponding transition density is not known. The proposed numerical method is shown to be efficient and simple to implement. To illustrate the flexibility and computational power of the algorithm, we develop an extended jump to default model that is able to capture several empirical regularities commonly observed in the literature.

JEL Classification: G13.

Keywords: Double barrier options; Default; Neumann series of Bessel functions; Sturm-Liouville equations; Spectral decomposition; Transmutation operators

2.1 Introduction

In this paper we develop a novel option pricing methodology based on an analytically tractable Neumann series of Bessel functions (hereafter, NSBF) representation. The new representation is derived by applying the NSBF expansion to the arising Sturm-Liouville problem. To highlight the potential of our method, we derive a new analytical tractable representation of the price (and Greeks) of double barrier European-style knock-out options (henceforth, DBKO options), though applications to other similar problems may be designed using this conceptual framework.

Barrier option contracts are path-dependent exotic options traded at over-the-counter markets on several underlying assets, e.g., stocks, stock indexes, currencies, commodities, and interest rates. They have been actively traded mainly because they are cheaper than the corresponding vanilla options and offer an important tool for risk managers and traders to better express their market views without paying for outcomes that they may find unlikely. Moreover, they are also used as building blocks of many structured products.

Given their popularity in the market, a vast literature dedicated to their valuation has been developed. For instance, alternative pricing (and hedging) schemes for DBKO options under the classic *geometric Brownian motion* (hereafter, GBM) assumption have been proposed by Kunitomo and Ikeda (1992), Geman and Yor (1996), Sidenius (1998), Pelsser (2000), Schröder (2000), Poulsen (2006), or Buchen and Konstandatos (2009). Given that such modeling framework assumes the volatility is constant throughout the option's life, several attempts have been made to overcome this unrealistic assumption implicit in the GBM diffusion.

It is well-known that the *constant elasticity of variance* (hereafter, CEV) diffusion model of Cox (1975), where the volatility is a function of the underlying asset price, is able to better reproduce two empirical regularities commonly observed in the literature, namely the existence of a negative correlation between stock returns and realized volatility (*leverage effect*) and the inverse relation between the implied volatility and the strike price of an option contract (*implied volatility skew*). To accommodate these observations, the valuation of DBKO options under the CEV model have been performed by Boyle and Tian (1999) through a trinomial scheme, by Davydov and Linetsky (2001) using a pricing framework based on the numerical inversion of Laplace transforms, by Davydov and Linetsky (2003) via an eigenfunction expansion approach, and by Mijatović and Pistorius (2013) whose approach rests on the construction of an approximation based on continuous-time Markov chains, amongst others.

More recently, Dias et al. (2015) tackle the valuation of DBKO options (using the stopping time approach as well as the static hedging approach) under the so-called *jump to default CEV* (hereafter, JDCEV) model proposed by Carr and Linetsky (2006), which is known to be able to capture the empirical evidence of a positive correlation between default probabilities (or credit default swap spreads) and equity volatility.[2.1] Moreover, it nests the GBM and CEV models as special cases and, therefore, it also accommodates the aforementioned leverage effect and implied volatility skew stylized facts. The importance of linking equity derivatives markets and credit markets has thus generated a new class of hybrid credit-equity models with the aim of pricing derivatives subject to the risk of default—for other applications of jump to default models, see, for instance, Nunes (2009), Mendoza-Arriaga et al. (2010), Linetsky and Mendoza-Arriaga (2011), Ruas et al. (2013), Nunes et al. (2015), Nunes et al. (2018), and the references contained therein.

The main purpose of this paper is the development of a new analytically tractable NSBF

[2.1] See, for example, Campbell and Taksler (2003), Zhang et al. (2009), and Carr and Wu (2010).

representation for pricing (and hedging) European-style DBKO options which can be applied to the whole class of one-dimensional time-homogeneous diffusions, independently of knowing the corresponding transition density. Similarly to Davydov and Linetsky (2003), we solve the boundary value problem for the parabolic partial differential equation using a classical separation of the variables method. This technique reduces the problem to the determination of the eigenvalues and eigenfunctions of the associated Sturm-Liouville problem. The approach based on the NSBF representation allows one to compute large sets of eigendata with non-deteriorating accuracy. Hence, we are able to calculate the prices for the general time homogeneous diffusion models, not relying on the knowledge of the exact solutions as for example is done in Davydov and Linetsky (2003) for the CEV model and Carr and Linetsky (2006) and Dias et al. (2015) for the JDCEV model. Therefore, the novel NSBF representation permits the construction of a fast and accurate algorithm for pricing DBKO options and opens its application to other similar problems.[2.2]

We note that Carr and Linetsky (2006) are able to obtain closed-form solutions for European-style plain-vanilla options, survival probabilities, credit default swap spreads, and corporate bonds in the JDCEV model by exploring the powerful link between CEV and Bessel processes. By adopting the hybrid credit-equity JDCEV architecture modeling framework, Dias et al. (2015) are restricted to the volatility and default intensity specifications that are implicit in the JDCEV model. By contrast, since we do not need to be restricted to such specific modeling assumptions we are able to quickly and accurately price DBKO options for a larger class of models. We illustrate our numerical method on an *extended jump to default constant elasticity of variance* (hereafter, EJD-CEV) model, which nests the JDCEV model as a special case.

[2.2]We recall that Davydov and Linetsky (2003) considered also interest rate knock-out options in the Cox et al. (1985) term structure model, while Carr and Crosby (2010) studied foreign exchange double-no-touch options. Even though our focus is on equity derivatives, our approach is also suitable for pricing interest rate knock-out options and double-no-touch options, even in the absence of a closed-form solution for the transition density.

In summary, our method can be considered as an alternative powerful computational tool for pricing DBKO options. Since we are able to quickly construct the whole value function and not just the price, we can easily observe the behavior of the option price through time and different initial values. Moreover, the NSBF representation also presents an easy way to calculate the derivatives of the value function and consequently the 'Greeks' of the option, and thus it can be used for the design of hedging strategies. Given its accuracy, efficiency, and easy implementation, the novel valuation method can be used also for analyzing the empirical performance of models for barrier option valuation under alternative underlying asset pricing dynamics, e.g. Jessen and Poulsen (2013).

The remainder of the paper is structured as follows. Section 2.2 sets the general financial framework and defines the boundary value problem. Section 2.3 provides the main result of the paper (in Proposition 2.1): the representation of the solution to the boundary value problem and the price for a DBKO option. Section 2.4 illustrates the calculation of the so-called 'Greeks'. Next sections are dedicated to the algorithm implementation and numerical examples. First, we present, in section 2.5, some recurrence formulas which are more robust and efficient for computation of the coefficients that appear in the direct representations of the value function and its derivatives presented in previous sections. Then, section 2.6 offers the conceptual algorithm for the computation of the price of DBKO options. Section 2.7 presents numerical experiments for the EJDCEV framework. For illustrative purposes, the analysis is separated into two different horizons: medium (six months) and short (one day). The final section presents the concluding remarks and the possible directions for further research.

2.2 Modelling framework

This section presents the general financial model for our pricing method and describes the boundary value problem associated to an option contract containing two barrier (knock-out) provisions. We recall that the holder of such a DBKO option has the right to receive, at the expiration date T, a payoff $f(y) = (y - K)^+$ in the case of a call option, or $f(y) = (K - y)^+$ for the case of a put option, if the underlying asset price (Y) remains in the range (L, U). The real constants $U > L > 0$ are designated by the upper and lower bounds (i.e., the knock-out trigger barrier levels), whereas $K \in \mathbb{R} : L < K < U$ is the strike price.[2.3]

2.2.1 The general financial model setup

Hereafter, and during the trading interval $[0, T]$, for some fixed time T (> 0), uncertainty is generated by a probability space $(\Omega, \mathcal{G}, \mathbb{Q})$, where the equivalent martingale measure $\mathbb{Q}$ associated to the numéraire "money market account" is taken as given. The price dynamics of the underlying asset is assumed to be governed, under the risk-neutral measure $\mathbb{Q}$, by the time-homogeneous (or time invariant) diffusion

$$dY_t = \mu(Y_t) Y_t dt + \sigma(Y_t) Y_t dB_t, \tag{2.1}$$

with initial value $Y_0 = y_0$, and where the functions $\mu(y)$ and $\sigma(y)$ are, respectively, the (state dependent) instantaneous drift and instantaneous volatility (whose regularity properties will be formally defined later in Assumption 2.1), whereas $(B_t)_{t \geq 0} \in \mathbb{R}$ is a standard Wiener process defined under measure $\mathbb{Q}$.

[2.3] To simplify the notation, it is assumed that the valuation date of each contract is today (i.e., the current time $t = 0$). Moreover, in the case of a knock-out event it is assumed that there is no rebate. Nevertheless, the valuation of rebates can be straightforwardly accomplished using the insights presented in Remark 2.3

To explain the development of our pricing methodology we consider a European-style DBKO option contract whose payoff at the expiry date T is a function of the single state variable Y. Given the contractual clauses of such derivative security, the process is considered on the interval $[L, U]$, where L and U are, respectively, the lower and upper bounds of the DBKO option contract. The end-points L and U are set to be knock-out boundaries, because if at any time between the initial date of the contract and its expiration either the upper barrier or the lower barrier is hit, then the option contract is canceled (i.e. it is knocked out). We are considering the case with no rebate for simplicity. However, it is possible to incorporate a rebate value, as shown in Remark 2.3.

As in Davydov and Linetsky (2003), if any of these end-points is a regular boundary, we adjoin a killing boundary condition at that end-point, sending the process to a cemetery state $\{\Delta\}$ at the first hitting time of the end-point. Consequently, the hitting time for our problem (with two knock-out provisions) is defined by

$$\tau_{\{L,U\}} = \inf \{s \geq t : Y_s \notin (L, U)\}.$$

We also consider the possibility that the process may be killed by a sudden jump to $\{\Delta\}$, i.e. the spot price is allowed to jump to zero from the interior of the interval. This implies that the default event forces the option knock-out. There is no recovery value (in the case of a DBKO put) upon default.

This is accomplished by imposing a killing time defined as

$$\tau_h = \inf \left\{ s \geq 0 : \int_0^s h(Y_u)\, du \geq \mathcal{E} \right\},$$

where $h(y) \geq 0$ is the default intensity or the hazard rate, whereas $\mathcal{E}$ is an exponential random variable with unit mean, independent of Y and time. Therefore, the combined stopping time of the process is denoted by

$$\tau = \min\left\{\tau_{\{L,U\}}, \tau_h\right\}. \tag{2.2}$$

Remark 2.1 *The abuse of notation is in place; to simplify notation, the stopped process set on the domain $[L,U] \cup \{\Delta\}$ is denoted by the same letter Y as the original process. This avoids bloating the paper with many technical details that are standard in the literature—see, for instance, Rogers and Williams (1994, Section III.3.18), Borodin and Salminen (2002, Section II.4), Øksendal (2003, Section 8.2) and Mendoza-Arriaga et al. (2010). We notice that the defaultable asset price process is adapted not to the filtration $\mathbb{F} = \{\mathcal{F}_t, t \geq 0\}$ generated by the predefault process, but rather to the enlarged filtration $\mathbb{G} = \{\mathcal{G}_t : t \geq 0\}$, obtained as $\mathcal{G}_t = \mathcal{F}_t \vee \mathcal{D}_t$, where $\{\mathcal{D}_t, t \geq 0\}$ is a default indicator process, with $\mathcal{D}_t = \mathbf{1}_{\{t>\tau_h\}}$.*

As usual, to ensure that the constructed (killed) process remains a martingale it is necessary to set the drift of equation (2.1) as

$$\mu(y) = \bar{r}(y) - \bar{q}(y) + h(y), \tag{2.3}$$

where $\bar{r}(y)$ and $\bar{q}(y)$ are the (time-homogeneous) continuously compounded interest rate and dividend yield.

In summary, the main purpose of this paper is to develop an efficient and flexible pricing methodology for computing risk-neutral expectations of the form

$$v(y,t) = E_y\left[e^{-\int_t^T [\bar{r}(Y_s)+h(Y_s)]ds} f(Y_T)\, \mathbf{1}_{\left\{\tau_{\{L,U\}}>T\right\}}\right]. \tag{2.4}$$

This will be accomplished by applying the NSBF expansion to the associated Sturm-Liouville problem.

2.2.2 The boundary value problem

Let us introduce the differential operator

$$\mathcal{A} = \frac{1}{2}\sigma^2(y)\, y^2 \partial_{yy} + \mu(y)\, y \partial_y - (\bar{r}(y) + h(y)). \tag{2.5}$$

Then, the value function (2.4) is the solution of the following boundary value problem

$$\begin{cases} \mathcal{A}v(y,t) = -v_t, & (y,t) \in (L,U) \times [0,T), \\ v(y,T) = f(y), & y \in (L,U), \\ v(L,t) = v(U,t) = 0, & t \in [0,T]. \end{cases} \tag{2.6}$$

The pricing of the DBKO option will be performed by solving problem (2.6). For convenience, we rewrite the operator $\mathcal{A}$ in the following form

$$\mathcal{A} = \frac{1}{w(y)}\left(\frac{d}{dy}\left(p(y)\frac{d}{dy}\right) - q(y)\right),$$

where

$$p(y) = \exp\left(\int^y \frac{2\mu(s)}{s\sigma^2(s)} ds\right), \quad w(y) = \frac{2p(y)}{\sigma^2(y)y^2}, \quad \text{and} \quad q(y) = [\bar{r}(y) + h(y)]\, w(y). \tag{2.7}$$

At this point, we can set the needed conditions for the coefficients of the process Y_t through the problem (2.6). In this illustration paper we are looking only at the regular case, so we will need the following assumptions:

Assumption 2.1 *The functions p, p', q, w and w' are real valued and continuous on $[L, U]$. Additionally, it is assumed that p' and w' are absolutely continuous and that $p > 0$, $\sigma > 0$ and $w > 0$.*

Assumption 2.2 *The payoff function f is square integrable.*

Application of Fourier' separation of variables method to the partial differential equation in (2.6)—see, for example, Mikhailov (1978) and Pinchover and Rubinstein (2005) for a general exposition of the method and Davydov and Linetsky (2003) for financial applications—, leads to the eigenfunction expansion of the value function (2.4) as

$$v(y,t) = \sum_{n=1}^{\infty} f_n \varphi_n(y) e^{-\lambda_n (T-t)}, \tag{2.8}$$

where the pairs (λ_n, φ_n) are solutions of the Sturm-Liouville problem

$$\begin{cases} (p(y)\varphi_n'(y))' - q(y)\varphi_n(y) = -\lambda_n w(y)\varphi_n(y) \qquad y \in (L,U) \\ \varphi_n(U) = \varphi_n(L) = 0 \end{cases}. \tag{2.9}$$

The functions φ_n form a complete orthogonal basis for the space $L_w^2([L,U])$. The coefficients f_n are the Fourier coefficients of the function f relative to the basis $\{\varphi_n\}_{n\in\mathbb{N}}$ with scalar product

$$\langle g_1, g_2 \rangle = \int_L^U g_1(s) g_2(s) w(s)\, ds. \tag{2.10}$$

The Hilbert space $L_w^2([L,U])$ with the above defined scalar product is denoted by H_w. The function f can be explicitly decomposed as

$$f(y) = \sum_{n=1}^{\infty} f_n \varphi_n(y), \tag{2.11}$$

where f_n are the Fourier coefficients of the payoff function f defined as

$$f_n = \frac{\langle f, \varphi_n \rangle}{\langle \varphi_n, \varphi_n \rangle}.$$

We recall that Assumption 2.2 guarantees that the series converges to the function f in L^2_w norm. We note also that Assumption 2.1 ensures that problem (2.9) is a regular Sturm-Liouville problem. The eigenvalues are real, positive and can be listed as $\lambda_1 < \lambda_2 < .. < \lambda_n < ...$, with $\lim_{n\to\infty} \lambda_n = +\infty$.[2.4]

Remark 2.2 *We further notice that for the put and call barrier options under consideration, problem* (2.6) *possesses non-consistent (discontinuous) boundary conditions. For the barrier call option the value function is discontinuous at the point* (U, T)*, i.e.* $v(U, T) = 0 \neq \lim_{y\to U} v(y, T) = f(U) = U - K$*. A similar observation can be made for the point* (L, T) *in the barrier put case. Nevertheless, in both cases the value function is still in the space* H_w *and can be represented by its Fourier series* (2.11)*.*

Remark 2.3 *Consider the case of the call option with rebate* $R > 0$*. The upper boundary condition for the problem* (2.6) *changes to*

$$v(U, t) = R.$$

The boundary conditions (2.6) *become non-homogeneous. For the direct application of the presented method we have to first transform our value function. Let us define the new function*

$$\tilde{v}(y, t) = v(y, t) - \frac{y - L}{U - L} R,$$

[2.4] Decomposition (2.8) and other related topics, such as properties of the eigenfunctions, can be consulted in Birkhoff and Rota (1989, Chapter 10) and Stakgold and Holst (2011, Chapter 7). The analysis of the spectral decomposition directly applied to finance problems may be found in Linetsky (2004).

which satisfies the following boundary problem

$$\begin{cases} (i) & \mathcal{A}\tilde{v} + \mathcal{A}\left(\frac{y-L}{U-L}R\right) = -\tilde{v}_t, & y \times t \in (L,U) \times (0,T) \\ (ii) & \tilde{v}(L,t) = \tilde{v}(U,t) = 0, & t \in [0,T] \\ (iii) & \tilde{v}(y,T) = d(y), & y \in (L,U) \end{cases}, \tag{2.12}$$

with homogeneous boundary conditions. The details can be consulted in Pinchover and Rubinstein (2005, Ch. 6.6). The interesting observation is that from a mathematical point of view the solution $v(y,t)$ *becomes smoother if* $R = U - K$*, i.e. the boundary conditions become consistent.*

2.3 An analytical representation through NSBF of the value function

This section presents the pricing formula for the DBKO option using the NSBF representation for the Sturm-Liouville problem (2.9) recently proposed by Kravchenko et al. (2017b) for the one-dimensional Schrödinger equation—i.e. the case with $w(y) = 1$—and then extended to a more general function $w(y)$ in Kravchenko and Torba (2018). In a nutshell, this powerful technique consists in the representation of the solutions of the Sturm-Liouville problem (2.9) and their derivatives in terms of NSBF with explicit formulas for the coefficients.

To extend this approach to our option pricing problem, let us first introduce the space $H_w^{1,0}$. This is the subspace of the functions $u \in L_w^2([L,U] \times [0,T])$, that possesses the first derivative $\partial_x u$ in the sense of distributions and $\partial_x u, u \in L_w^2([L,U] \times [0,T])$—see, for example, Mikhailov (1978, Chapter III.2) for further details. Next proposition provides our main theoretical result.

Proposition 2.1 *Under Assumptions 2.1 and 2.2, the value function* (2.4) *is the solution to problem* (2.6) *and can be represented as*

$$v(y,t) = \sum_{n=1}^{\infty} f_n \left[\frac{\sin(\omega_n l(y))}{\rho(y)} + 2\sum_{m=0}^{\infty} (-1)^m \alpha_{2m+1}(y)\, j_{2m+1}(\omega_n l(y)) \right] e^{-\omega_n^2 (T-t)}. \quad (2.13)$$

The series converges in the norm of the space $H_w^{1,0}$*.*[2.5] *Moreover the series converges uniformly with respect to* $y \in [L,U]$ *and* $t \in [0,T_0] \subset [0,T)$*.*

Before providing a formal proof of Proposition 2.1 and for the sake of completeness, let us first highlight some important details aiming to offer a better exposition. Consider the following identities:

- The eigenfunctions, solutions to the Sturm-Liouville problem (2.9) are[2.6]

$$\varphi_n(y) = \frac{\sin(\omega_n l(y))}{\rho(y)} + 2\sum_{m=0}^{\infty} (-1)^m \alpha_{2m+1}(y)\, j_{2m+1}(\omega_n l(y)). \quad (2.14)$$

- The spherical Bessel functions of the first kind, $j_\nu(y)$, are given by

$$j_\nu(y) = \sqrt{\frac{\pi}{2y}} J_{\nu+\frac{1}{2}}(y),$$

  where $J_\mu(y)$ are the Bessel functions of the first kind shown in Gradshteyn and Ryzhik (2007, 8.461.1).

- The function $l(y)$ is defined by[2.7]

$$l(y) := \int_L^y \sqrt{\frac{w(s)}{p(s)}} ds = \sqrt{2} \int_L^y \frac{1}{s\sigma(s)} ds, \quad y \in [L,U].$$

[2.5] The price of the DBKO option is given by $v(y_0,0)$ and the corresponding series converges in the norm $L_w^2([L,U])$.

[2.6] Note that these functions are not normalized.

[2.7] A detailed analysis of the role of this transformation in this decomposition and in the transmutation operators theory can be found in Kravchenko et al. (2016).

- The function $\rho(y)$ is defined by

$$\rho(y) = [p(y) w(y)]^{1/4} = \sqrt{2}\left(\frac{p(y)}{\sigma(y) y}\right)^{1/2}, \quad y \in [L, U].$$

- The roots of the eigenvalues λ_n, denoted as ω_n, are solutions of the equation

$$\frac{\sin(\omega l(U))}{\rho(U)} + 2\sum_{m=0}^{\infty} (-1)^m \alpha_{2m+1}(U) j_{2m+1}(\omega l(U)) = 0, \quad \omega \in \mathbb{R}. \tag{2.15}$$

- The functions $\alpha_n(y)$, $n \geq 0$ are defined as

$$\alpha_n(y) = \frac{2n+1}{2}\left(\sum_{k=0}^{n} \frac{l_{k,n}\Phi_k(y)}{(l(y))^k} - \frac{1}{\rho(y)}\right), \quad y \in (L, U]. \tag{2.16}$$

  The efficient recursive method for computing α_n will be presented in Section 2.5.

- $l_{k,n}$ is the coefficient of x^k in the Legendre polynomial of order n—see, for instance, Abramowitz and Stegun (1972, Chapter 8).

- $\Phi_k(y)$ are the formal powers that will be defined in Definition 2.1.

The formal powers $\Phi_k(y)$ are constructed on the basis of one non-vanishing solution g of the equation[2.8]

$$(p(y) g'(y))' - q(y) g(y) = 0, \quad y \in [L, U], \tag{2.17}$$

with an initial condition set as

$$g(L) = \frac{1}{\rho(L)}. \tag{2.18}$$

Definition 2.1 *Let p, q, w satisfy Assumption 2.1 and let g be a non-vanishing solution of equation* (2.17) *that satisfies condition* (2.18). *Then, the associated formal powers*

[2.8] For p, p' and q continuous on $[L, U]$ such solution exists, see Kravchenko and Porter (2010, Remark 5).

are defined, for $k = 0, 1, 2, ...$, as

$$\Phi_k(y) = \begin{cases} g(y)\, Y^{(k)}(y), & k \text{ odd} \\ g(y)\, \tilde{Y}^{(k)}(y), & k \text{ even} \end{cases},$$

where two families of the auxiliary functions are defined as

$$Y^{(0)}(y) \equiv \tilde{Y}^{(0)}(y) \equiv 1,$$
$$Y^{(k)}(y) = \begin{cases} k \int_L^y Y^{(k-1)}(s) \frac{1}{g^2(s)p(s)} ds, & k \text{ odd} \\ k \int_L^y Y^{(k-1)}(s)\, g^2(s)\, p(s)\, ds, & k \text{ even} \end{cases},$$
$$\tilde{Y}^{(k)}(y) = \begin{cases} k \int_L^y \tilde{Y}^{(k-1)}(s)\, g^2(s)\, p(s)\, ds, & k \text{ odd} \\ k \int_L^y \tilde{Y}^{(k-1)}(s) \frac{1}{g^2(s)p(s)} ds, & k \text{ even} \end{cases}.$$

Remark 2.4 *We note that these formal powers arise in the Spectral Parameter Power Series (SPPS) representation for the solution of the Sturm-Liouville problem* (2.9)*. The SPPS method was introduced in Kravchenko (2008)—see also Kravchenko and Porter (2010) and Khmelnytskaya et al. (2015).*

Next we provide the formal proof of Proposition 2.1.

Proof. 2.1 (Proof of Proposition 2.1) *The application of the Fourier separation of the variables method to problem* (2.6) *leads to representation* (2.8)*. It is a weak solution of problem* (2.6)*—see, for example, Mikhailov (1978, Chapter VI.2, Theorem 3) and Evans (1998, Chapter 7.1, Theorems 3 and 4). Application of Kravchenko and Torba (2018, Theorem 3.1) gives representation* (2.13) *and guarantees the approximation of the eigenfunctions uniformly in ω. Let us denote by $f_N(y) = \sum_{n=1}^{N} f_n \varphi_n(y)$ the approximation of the function f of the order N. For any $\varepsilon > 0$, there is a N such that*

$\|f - f_N\|_{L^2_w} \leq \varepsilon_N$*, where* $\varepsilon_N \to 0$ *when* $N \to \infty$*. Applying Mikhailov (1978, Chapter VI.2, Theorem 3), we have the following estimate*

$$\|v - v_N\|_{H^{1,0}_w} \leq C \|f - f_N\|_{L^2_w[L,U]} \leq C\varepsilon_N.$$

The uniform convergence of the series is due to majorization by decreasing sequence $e^{-\lambda_n T_0}$*.*

In summary, Proposition 2.1 provides a powerful computational technique with the potential to be applied in a wide range of finance applications due to the fact that the NSBF representation can be used as a simple and efficient numerical method. Furthermore, the proposed novel representation is applicable to a large class of option pricing models and it represents not only the price but also the entire value function. This feature allows us to view the behavior of the option price under different initial values for the asset (i.e., to construct the value surface as will be shown in Figure 2.1).

2.4 The analytical representation of 'Greeks'

Since Proposition 2.1 presents an analytical representation of the value function, we are then able to offer a similar representation for its derivatives, commonly known as 'Greeks' in the option pricing literature. This should be a useful computational tool for both academics and practitioners, since numerical differentiation is known to be problematic in this kind of problems.

2.4.1 Delta

Let $y_0 \in (L, U)$. The Delta can be represented as

$$\Delta = \frac{\partial v}{\partial y}(y_0, 0) = \sum_{n=1}^{\infty} f_n \varphi_n'(y_0) e^{-\omega_n^2 T}, \tag{2.19}$$

where

$$\begin{aligned}\varphi_n'(y) = \sqrt{\frac{w(y)}{p(y)}} \Bigg(\frac{1}{\rho(y)} \left[G_2(y)\sin(\omega_n l(y)) + \omega_n \cos(\omega_n l(y))\right] + \\ + 2\sum_{m=0}^{\infty} (-1)^m \beta_{2m+1}(y) j_{2m+1}(\omega_n l(y)) \Bigg) - \\ - \frac{\rho'(y)}{\rho(y)} \left(\frac{\sin(\omega_n l(y))}{\rho(y)} + 2\sum_{m=0}^{\infty} (-1)^m \alpha_{2m+1}(y) j_{2m+1}(\omega_n l(y)) \right),\end{aligned}$$

the functions $G_2(y)$ and $\beta_m(y)$ are presented in the next section. The expressions for the φ_n' are adapted from Kravchenko and Torba (2018, Section 5). The representation (2.19) is valid if the function $\frac{\partial v}{\partial y}$ is continuous at $(y_0, 0)$. The conditions for this can be consulted at Ladyzhenskaya et al. (1988, Theorem 12.1).

2.4.2 Vega

For the calculation of the Vega, we assume that the instantaneous volatility σ is differentiable and $\sigma'(y_0) \neq 0$. Then by the application of the chain rule and the derivative of the inverse function theorem, we have

$$\nu = \frac{\partial v}{\partial \sigma}(\sigma(y_0), 0) = \frac{\partial v}{\partial y}(y_0, 0) \frac{1}{\sigma'(y_0)} = \frac{\Delta}{\sigma'(y_0)}. \tag{2.20}$$

For the constant σ we cannot apply this formula.[2.9]

[2.9] In particular, see Shaw (1998, Section 12.2) for the GBM model.

2.4.3 Theta

The direct differentiation with respect to t of (2.13) provides us with a formula for the Theta

$$\theta = \frac{\partial v}{\partial t}(y_0, 0) = \sum_{n=1}^{\infty} f_n \lambda_n \varphi_n(y_0) e^{-\lambda_n T}. \tag{2.21}$$

As in the case of the Delta, it is necessary to assume the continuity of $\frac{\partial v}{\partial t}$ at $(y_0, 0)$.

2.5 Recurrence formulas for the coefficients $\alpha_n(y)$ and $\beta_n(y)$

For the (efficient and robust) computation of the coefficient functions $\alpha_n(y)$ and $\beta_n(y)$ it is convenient to use recurrence formulas borrowed from Kravchenko and Torba (2018). These formulas increase the robustness of the calculations by solving the numerical issue in (2.16) related to the fast growth of the Legendre coefficients.

We first introduce

$$A_n(y) = l^n(y)\,\alpha_n(y) \quad \text{and} \quad B_n(y) = l^n(y)\,\beta_n(y). \tag{2.22}$$

The following formulas hold for $n = 2, 3, \ldots$

$$A_n(y) = \frac{2n+1}{2n-3}\left(l^2(y)\,A_{n-2}(y) + (2n-1)\,g(y)\,\tilde{\theta}_n(y)\right)$$

and

$$\begin{aligned} B_n(y) &= \frac{2n+1}{2n-3}\Bigg\{ l^2(y)B_{n-2}(y) + 2(2n-1)\Bigg(\sqrt{\frac{p(y)}{w(y)}}\left(g'(y)\rho(y) + g(y)\rho'(y)\right)\frac{\tilde{\theta}_n(y)}{\rho(y)} \\ &\quad + \frac{\tilde{\eta}_n(y)}{\rho^2(y)g(y)}\Bigg) - (2n-1)l(y)A_{n-2}(y)\Bigg\}, \end{aligned}$$

where

$$\tilde{\theta}_n(y) = \int_A^y \left(\frac{\tilde{\eta}_n(x)}{\rho^2(x)\, g^2(x)} - \frac{l(x)\, A_{n-2}(x)}{g(x)} \right) \sqrt{\frac{w(x)}{p(x)}} dx$$

and

$$\tilde{\eta}_n(y) = \int_A^y \left(l(x)(g'(x)\rho(x) + g(x)\rho'(x)) + (n-1)\rho(x)g(x)\sqrt{\frac{w(x)}{p(x)}} \right) \rho(x) A_{n-2}(x) dx.$$

The initial values A_0, A_1, B_0 and B_1 can be calculated from

$$\alpha_0(y) = \frac{1}{2}\left(g(y) - \frac{1}{\rho(y)} \right) \quad \text{or} \quad A_0(y) = \alpha_0(y),$$
$$\alpha_1(y) = \frac{3}{2}\left(\frac{\Phi_1(y)}{l(y)} - \frac{1}{\rho(y)} \right) \quad \text{or} \quad A_1(y) = \frac{3}{2}\left(\Phi_1(y) - \frac{1}{\rho(y)\, l(y)} \right),$$

and

$$\beta_0(y) = \sqrt{\frac{p(y)}{w(y)}} \left(\alpha_0'(y) + \frac{\rho'(y)}{\rho(y)} \alpha_0(y) \right) - \frac{G_1(y)}{2\rho(y)},$$
$$\beta_1(y) = \frac{\alpha_1(y)}{l(y)} + \sqrt{\frac{p(y)}{w(y)}} \left(\alpha_1'(y) + \frac{\rho'(y)}{\rho(y)} \alpha_1(y) \right) - \frac{3G_2(y)}{2\rho(y)},$$

with

$$\alpha_0'(y) = \frac{1}{2}\left(g'(y) + \frac{\rho'(y)}{\rho^2(y)} \right),$$
$$\alpha_1'(y) = \frac{3}{2}\left(\frac{\left(g'(y)\, Y^{(1)}(y) + \frac{1}{g(y)p(y)} \right) l(y) - g(y)\, Y^{(1)}(y) \sqrt{\frac{w(y)}{p(y)}}}{l^2(y)} + \frac{\rho'(y)}{\rho^2(y)} \right),$$

and

$$G_1(y) = \tilde{h} + G_2(y), \tag{2.23}$$

$$G_2\left((y)\right)=\frac{1}{2}\int_L^y\frac{1}{(pw)^{1/4}}\left(\frac{q}{(pw)^{1/4}}-\left[p\left\{(pw)^{-1/4}\right\}'\right]'\right)(s)\,ds$$
$$=\left.\frac{\rho\rho'}{2w}\right|_L^y+\frac{1}{2}\int_L^y\left[\frac{q}{\rho^2}+\frac{(\rho')^2}{w}\right](s)\,ds, \tag{2.24}$$

where

$$\tilde{h}=\sqrt{\frac{\rho(L)}{w(L)}}\left(\frac{g'(L)}{g(L)}+\frac{\rho'(L)}{\rho(L)}\right). \tag{2.25}$$

There is a useful practical test for the verification of the coefficients α_n and β_n—its details may be consulted in Kravchenko and Torba (2018, Equations 7.1-7.3)—, that is

$$\sum_{m=0}^{\infty}\alpha_m(y)=\frac{\left(G_1(y)+G_2(y)\right)l(y)}{2\rho(y)} \tag{2.26}$$

$$\sum_{m=0}^{\infty}(-1)^m\alpha_m(y)=\frac{\tilde{h}l(y)}{2\rho(y)} \tag{2.27}$$

and

$$\sum_{m=0}^{\infty}\beta_m(y)=l(y)\left[\frac{q(y)}{4\rho(y)w(y)}-\frac{1}{4w(y)}\left[p(y)\left(\frac{1}{\rho(y)}\right)'\right]'+\frac{\tilde{h}G_2(y)+G_2^2(y)}{2\rho(y)}\right], \tag{2.28}$$

$$\sum_{m=0}^{\infty}(-1)^m\beta_m(y)=l(y)\left[\frac{1}{4\rho(y)}\left(\frac{q(L)}{w(L)}-\frac{\rho(L)}{w(L)}\left[p(y)\left(\frac{1}{\rho(y)}\right)'\right]'\Bigg|_{y=L}\right)+\frac{\tilde{h}G_2(y)}{2\rho(y)}\right]. \tag{2.29}$$

The relations (2.26) - (2.29) can also be used as an indicator for the optimal choice of the number K of coefficients in the truncated series (2.13) and (2.14) to include in computations, monitoring the differences between the right sides of equations (2.26) - (2.29) and the partial sums of these.

Remark 2.5 *When computing the coefficients $\alpha_n(y)$ and $\beta_n(y)$ it is important to prop-*

erly perform the division by $l(y)^n$. Here we present a simple scheme that proved to be useful—the detail and the proofs can be consulted in Kravchenko and Torba (2018, Section 7). Let us first note that the functions α_n are increasing functions in the neighborhood of L. Then, let $\{y_i\}_{1\leq i\leq N_\epsilon}$ be the ordered set of N_ϵ points of some neighborhood of L, $[L, L+\epsilon]$, with $y_1 = L < y_2 < ... < y_{N_\epsilon} = L+\epsilon$. For each coefficient function α_n consider[2.10]

$$\tilde{y} = \underset{y\in\{y_i\}}{argmin}\ \alpha(y).$$

Let also k_0 be the index of $\tilde{y}$ (i.e. $y_{k_0} = \tilde{y}$). Hence, we can set $\alpha_n(y) = 0$ for all $n < k_0$. They are larger only due to the numerical error. A similar construction can be performed for the coefficients $\beta_n(y)$.

2.6 Implementation of the pricing algorithm

For the sake of completeness and to better describe important details of our pricing methodology, let us now provide the conceptual steps for implementing our algorithm:

1. Compute the coefficients p, q and w of the associated Sturm-Liouville problem using (2.7).

2. Create or choose an indefinite integration scheme. In this paper, we have used the Newton-Cotes six point integration rule—see Kravchenko et al. (2017b) for discussions on the use of other possible methods.

3. Construct or find any non-vanishing solution g to equation (2.17) that satisfies (2.18). In our implementation, we have used the SPPS method presented in

[2.10] For a function $f : X \to Y$, the $argmin$ over a subset S of X is defined as $\underset{x\in S\subseteq X}{argmin}\, f(x) := \{x : x\in S \wedge \forall y\in S : f(y)\geq f(x)\}$.

Kravchenko and Porter (2010). For example, if $q(y) \equiv 0$ (as in the case of the standard CEV model), we can choose $g(y) = \frac{1}{\rho(L)}$ as a particular solution.

4. Construct the formal power $\Phi^{(1)}$ using Definition 2.1, compute the constant $\tilde{h}$ and the functions $G_1(y)$ and $G_2(y)$ using formulas (2.25), (2.23) and (2.24), respectively.

5. Compute recursively the coefficients $A_m(y)$ and $B_m(y)$ using the representation highlighted in Section 2.5.

6. Compute coefficients $\alpha_m(y)$ and $\beta_m(y)$ using equations (2.22) and verify them using relations (2.26) - (2.29) and Remark 2.5. We notice that this procedure can incorporate a test for estimating an optimal M (truncation parameter for the series (2.14) and for the second sum in the series (2.13)) to be used.

7. Find the eigenvalues $\lambda_n = \omega_n^2$ from equation (2.15). Note that the values of the spherical Bessel functions j_{2m+1} for varying indices $m = 0, 1, \ldots, M$ at the same point x can be computed efficiently using backward-recursive formula, see Abramowitz and Stegun (1972, Equation 10.1.19)

$$j_m(x) = \frac{2(m+1)}{x} j_{m+1}(x) - j_{m+2}(x).$$

8. Construct the eigenfunctions of the problem (2.9) given by (2.14).

9. Decompose function f into the Fourier series (2.11) using the eigenfunctions φ_n.

10. Construct the function v through a truncated expression (2.8). By N we denote the number of terms in the truncated series.

11. Calculate the Greeks via expressions (2.19)-(2.21).

Remark 2.6 *Notice that the proposed algorithm can be significantly simplified if we are interested only in the price of the option $v(y_0, 0)$. If this is the case, then in steps 4, 5 and 6 we only need terms relative to A_n and $\alpha_n(y)$. Moreover, after calculating f_n we do not need to keep the eigenfunctions, but only values at the point y_0. Further, at step 10, we construct only $v(y_0, t)$ and step 11 is not necessary.*

2.7 Computational experiments and particular examples

In this section we apply the algorithm described in the previous section to the EJD-CEV model, whose details will be described next. For illustrative purposes, we have separated the examples in two different time horizons, the medium (six months) and the short (one day). This particular choice will highlight the eigendata needed for the accurate computations and the sensibility of the model to the chosen parameters.

We note that for the regular Sturm-Liouville problems that we are considering in this paper, the asymptotics for the eigenvalue growth is of the order of n^2, e.g. Polianin and Zaitsev (1970, Section 2.13). In the case of the long horizon the exponential term $e^{-\lambda_n(T-t)}$, with $T-t$ of order $\frac{1}{2}$, decays rapidly and the representation (2.13) converges quickly. Hence, few eigenvalues and eigenfunctions are needed to secure a good approximation. For the short horizon case, with $T-t$ of order $\frac{1}{360}$, that is analyzed in the second set of numerical experiments, we need more eigenvalues to have an accurate approximation for the option value. We further note that the NSBF method calculates the required eigendata with the same accuracy. This NSBF's important property, of not loosing accuracy for the highest order eigenvalues, makes it an exciting tool for applications to problems requiring large sets of eigenvalues.

Another computational advantage of our method is that there is no need in any two-dimensional grid for computation. The formulas for the steps 1-9 are one-dimensional. In order to make the integration errors negligible and to concentrate mainly on the numerical performance we have used an overwhelming number of mesh points (10000) on the interval $[L, U]$ to represent all the functions involved, moreover, even 3000 mesh points produced close results. Once all the coefficients are obtained, the computation of the value function and Delta may be performed only for the arguments $(y,t) \in [L,U] \times [0,T]$ required by application. E.g., option price can be obtained as the value of v at one point $(y_0, 0)$; the value surface requires calculation of the function v on a mesh of about 101×101 points, etc. Even though the main purpose here is to present the ability of the algorithm to be used in a wide variety of modeling contexts and not the optimization speed, the very small computational burden that is required is remarkable.

All the calculations where done in Matlab R2015a.

2.7.1 The EJDCEV model

The volatility specification under the time-homogeneous version of the JDCEV model is given by

$$\sigma(y) = \delta y^{\beta}, \tag{2.30}$$

with $\delta > 0$ and $\beta \in \mathbb{R}$. The drift is given by expression (2.3), with $\bar{r} > 0$, $\bar{q} \geq 0$ and hazard rate

$$h(y) := h_1(y) = b + c\sigma^2(y),$$

with $b > 0$ and $c > 0$. The properties of the constructed diffusion with different parameterizations can be consulted in Carr and Linetsky (2006) and Mendoza-Arriaga et al. (2010). The nice feature of the JDCEV model is its analytical tractability, due to the special form of the assumed hazard rate $h_1(y)$. The advantage of the NSBF representation is that it allows us to consider different default intensity specifications without any additional effort. Following Campbell and Taksler (2003), we have also considered a default intensity specification guaranteeing a positive relationship between the default probability and volatility. Hence, in our variant of the JDCEV model, that we name as the EJDCEV, the default intensity is assumed to be dependent of the constant parameter $\gamma \geq 0$ as

$$h(y) := h_1^{alt}(y) = b + c\sigma^{\gamma}(y). \tag{2.31}$$

It is important to point out that we are not restricted to functions of the form h_1^{alt}; we can choose any positive continuously differentiable function. This feature allows the possibility of obtaining a wide alternative of default rates when calibrating the model to market prices.

Medium horizon (6 months)

For this set-up, we adopt the parameter configuration considered in Dias et al. (2015, Table 2, Panel C), that is $y_0 = 100$, $L = 90$, $U = 120$, $T = 0.5$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, and $\sigma_0 = 0.25$. As usual, the scale parameter δ is calculated, for each β value[2.11], through the relation

$$\sigma_0 = \delta y_0^{\beta}, \tag{2.32}$$

while keeping the initial instantaneous volatility $\sigma_0 = 0.25$.

Table 2.1 shows the prices of European-style DBKO call and put options and the corresponding Greeks under the EJDCEV model for different moneyness levels with $K \in \{95, 100, 105\}$, $\beta \in \{0.5, 0.0, -1.0, -2.0\}$ and $\gamma \in \{0, 1, 2\}$. We further note that the six cases with $\gamma = 2$ and $\beta \in \{-1.0, -2.0\}$ originate the values of DBKO put op-

[2.11] Notice that our β is equivalent to the $\overline{\beta}$ considered in Dias et al. (2015).

tions shown in Dias et al. (2015, Table 2, Panel C). A direct comparison reveals that the results are exactly the same (rounded to four decimal places of accuracy), which gives further evidence on the robustness of our algorithm. More importantly, this also allows us to test our methodology under a larger set of volatility and default intensity specifications that until now were not possible to be tackled in the literature.

Table 2.1: Prices and 'Greeks' of European-style DBKO options.

Parameters			Call Option: $f(y)=(y-K)^{+}$				Put Option: $f(y)=(K-y)^{+}$			
			Price	Greeks			Price	Greeks		
K	β	γ	$v(100,0)$	Δ	ν	θ	$v(100,0)$	Δ	ν	θ
95	0.5	0	0.7314	-0.0332	-26.5669	4.9860	0.0029	-0.0001	-0.1101	0.0201
95	0.5	1	1.5057	0.0179	14.3442	6.5544	0.0168	0.0002	0.1364	0.0744
95	0.5	2	1.5572	0.0417	33.3312	6.3003	0.0222	0.0006	0.4438	0.0912
95	0.0	0	0.7163	-0.0319		5.0712	0.0023	-0.0001		0.0166
95	0.0	1	1.6417	0.0251		7.0686	0.0148	0.0002		0.0652
95	0.0	2	1.7117	0.0518		6.7849	0.0198	0.0006		0.0802
95	-1.0	0	0.6905	-0.0300	12.0097	5.2996	0.0014	-0.0001	0.0263	0.0111
95	-1.0	1	1.9733	0.0432	-17.2851	8.2401	0.0114	0.0002	-0.0865	0.0496
95	-1.0	2	2.0860	0.0771	-30.8585	7.8538	0.0157	0.0005	-0.2135	0.0615
95	-2.0	0	0.6421	-0.0280	5.5973	5.3842	0.0008	0.0000	0.0078	0.0071
95	-2.0	1	2.3959	0.0675	-13.5059	9.5993	0.0087	0.0002	-0.0419	0.0375
95	-2.0	2	2.5570	0.1107	-22.1395	9.0265	0.0123	0.0005	-0.0964	0.0469
100	0.5	0	0.4568	-0.0207	-16.5434	3.1114	0.0270	-0.0013	-1.0175	0.1860
100	0.5	1	0.8695	0.0105	8.4109	3.7784	0.1307	0.0014	1.0802	0.5772
100	0.5	2	0.8778	0.0237	18.9282	3.5444	0.1655	0.0042	3.3387	0.6801
100	0.0	0	0.4561	-0.0202		3.2256	0.0218	-0.0010		0.1563
100	0.0	1	0.9700	0.0150		4.1676	0.1181	0.0016		0.5189
100	0.0	2	0.9881	0.0301		3.9064	0.1517	0.0043		0.6143
100	-1.0	0	0.4571	-0.0198	7.9187	3.5041	0.0137	-0.0006	0.2535	0.1071
100	-1.0	1	1.2159	0.0269	-10.7784	5.0594	0.0962	0.0018	-0.7382	0.4167
100	-1.0	2	1.2574	0.0469	-18.7457	4.7137	0.1272	0.0044	-1.7458	0.4979
100	-2.0	0	0.4385	-0.0190	3.8045	3.6716	0.0082	-0.0004	0.0781	0.0709
100	-2.0	1	1.5313	0.0437	-8.7342	6.1011	0.0779	0.0019	-0.3774	0.3328
100	-2.0	2	1.6006	0.0699	-13.9770	5.6109	0.1059	0.0042	-0.8350	0.4012
105	0.5	0	0.2314	-0.0104	-8.3529	1.5750	0.1004	-0.0047	-3.7580	0.6899
105	0.5	1	0.4019	0.0049	3.9499	1.7435	0.4133	0.0044	3.4963	1.8212
105	0.5	2	0.3948	0.0107	8.5777	1.5909	0.5054	0.0129	10.2860	2.0713
105	0.0	0	0.2373	-0.0105		1.6764	0.0828	-0.0038		0.5924
105	0.0	1	0.4611	0.0073		1.9763	0.3842	0.0053		1.6823
105	0.0	2	0.4570	0.0140		1.8016	0.4762	0.0137		1.9220
105	-1.0	0	0.2522	-0.0109	4.3457	1.9300	0.0544	-0.0025	0.9987	0.4244
105	-1.0	1	0.6092	0.0137	-5.4756	2.5241	0.3317	0.0065	-2.5939	1.4293
105	-1.0	2	0.6129	0.0230	-9.2182	2.2859	0.4227	0.0147	-5.8633	1.6465
105	-2.0	0	0.2536	-0.0109	2.1851	2.1184	0.0342	-0.0016	0.3217	0.2940
105	-2.0	1	0.8049	0.0233	-4.6594	3.1840	0.2853	0.0070	-1.4099	1.2092
105	-2.0	2	0.8184	0.0361	-7.2223	2.8436	0.3736	0.0149	-2.9815	1.4039

This table shows the prices of European-style DBKO call and put options and the corresponding Greeks under the EJDCEV model, with $y_0=100$, $K\in\{95,100,105\}$, $L=90$, $U=120$, $T=0.5$, $\bar{r}=0.1$, $\bar{q}=0$, $b=0.02$, $c=0.5$, $\gamma\in\{0,1,2\}$, $\beta\in\{0.5,0.0,-1.0,-2.0\}$, and $\sigma_0=0.25$.

We notice that the determination of the spectral parameters in step 7 was performed by interpolation with a grid of equally distributed 100 points on the interval $(0, 15)$ for the practical purposes and the grid of 1000 points on the interval $(0, 50)$ for the construction of the illustration of Table 2.2 and the following graphs. The practical reasoning is to cut out the eigenvalues $\lambda_n > 15^2$ due to the term $e^{\lambda_n(T-t)}$ in our formulas, this indirectly sets the parameter N somewhere around 6, as can be observed in Table 2.2. Figure 2.1 illustrates the value function under the JDCEV model using the aforementioned parameters coupled with $K = 100$, $\beta = -1$ and $\gamma = 2$. Using the same set of parameters, Figure 2.2 shows the detail of the approximation of the function $f(y) = (y - K)^+$ at the boundary for $t = T$. It is possible to observe a sharp decline at the boundary U, this is the illustration of the Remark 2.2.

Table 2.2: Eigenvalues.

	Parameters			
n	$\beta = 1, \gamma = 1$	$\beta = 1, \gamma = 2$	$\beta = -2, \gamma = 1$	$\beta = -2, \gamma = 2$
1	4.4047	4.1314	4.0997	3.6155
6	144.3068	144.0338	112.8959	112.4098
11	484.0679	483.7949	377.105	376.6189
16	1023.6885	1023.4155	796.731	796.2449
21	1763.1687	1762.8956	1371.7741	1371.288
26	2702.5083	2702.2352	2102.2343	2101.7481
31	3841.7073	3841.4343	2988.1115	2987.6253
36	5180.7659	5180.4929	4029.4057	4028.9196
41	6719.684	6719.411	5226.117	5225.6309

This table shows the eigenvalues for different γ and β parameters, with $y_0 = 100$, $K = 100$, $L = 90$, $U = 120$, $T = 0.5$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, and $\sigma_0 = 0.25$.

Figure 2.3 shows prices of European-style DBKO call options for different initial asset values S_0. The left-hand side plot sets $\gamma = 1$ for different β values. The right-hand side plot sets $\beta = -1$ for different γ values. We note that with the chosen parametrization for this model, the term $e^{\lambda_n T}$ decays very rapidly and thus we only need to compute few eigenvalues to obtain accurate prices.

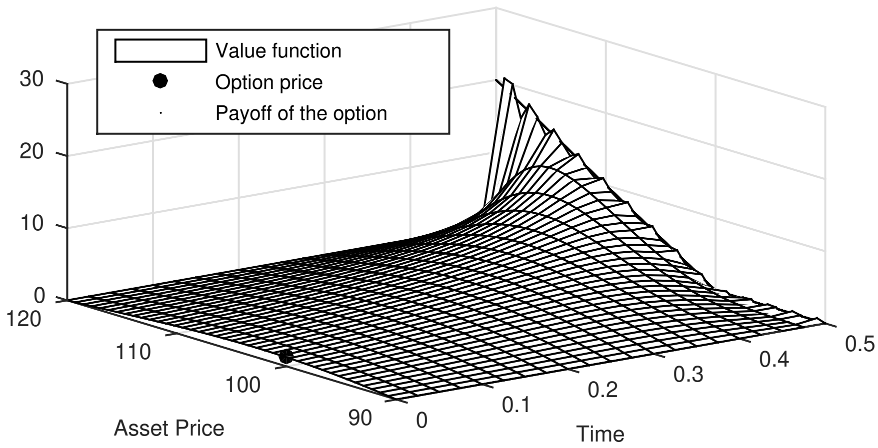

Figure 2.1: This figure illustrates the value function, the payoff and the price of a European-style DBKO call option, with $y_0 = 100$, $K = 100$, $L = 90$, $U = 120$, $T = 0.5$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, $\gamma = 2$, $\beta = -1$, and $\sigma_0 = 0.25$.

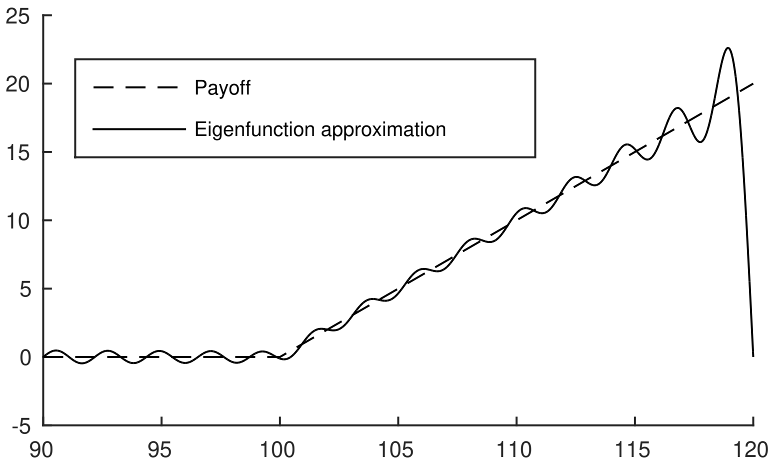

Figure 2.2: This figure illustrates the payoff function approximation by an eigenfunction expansion for a European-style DBKO call option, with $N = 27$ eigenfunctions and $y_0 = 100$, $K = 100$, $L = 90$, $U = 120$, $T = 0.5$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, $\gamma = 2$, $\beta = -1$, and $\sigma_0 = 0.25$.

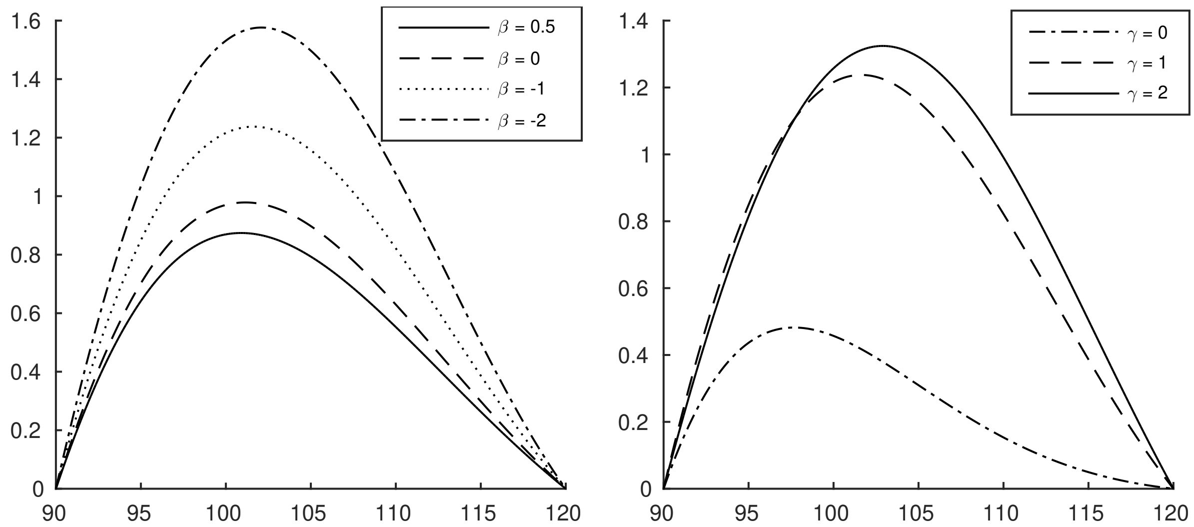

Figure 2.3: This figure prices European-style DBKO call options for different initial asset values y_0. The left-hand side plot sets $\gamma = 1$ for different β values. The right-hand side plot sets $\beta = -1$ for different γ values. The remaining parameters are: $K = 100$, $L = 90$, $U = 120$, $T = 0.5$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, and $\sigma_0 = 0.25$.

Short horizon (1 day)

In the case of the short horizon, the time is of the order $\frac{1}{360}$ and, hence, the term $e^{-\lambda_n(T-t)}$ decays much slower as n grows. For this case, in step 7, we have used 1000 points for the interval $(0, 100)$. Some values are presented in Table 2.2. In order to illustrate the convergence and the necessity of calculating accurately a significant number of eigenvalues, we introduce the contribution of the partial sum from equation (2.8), defined as

$$Contrib\,(n_1, n_2) = \sum_{n=n_1}^{n_2} f_n \varphi_n e^{-\lambda_n(T-t)}. \tag{2.33}$$

We observe, in Table 2.3, that the value of the parameter β under the short horizon does not have much influence on the price. However, the γ parameter associated with default intensity is relevant. It is important to note that although the prices of the options for different β values differ slightly, the corresponding Sturm-Liouville problems are very different. This can be observed in Tables 2.2 and 2.4. The observation of the Table 2.4 induces the choice of N around 45.

Table 2.3: Prices for one-day to maturity European-style DBKO calls.

	$\gamma = 3$	$\gamma = 2$	$\gamma = 1$	$\gamma = 0$
$\beta = -2$	0.54297	0.54622	0.55950	0.61518
$\beta = 1$	0.54300	0.54634	0.55976	0.61516

This table shows prices for one-day to maturity European-style DBKO call options for different γ and β parameters, with $y_0 = 100$, $K = 100$, $L = 90$, $U = 120$, $T = 1/360$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, and $\sigma_0 = 0.25$.

Table 2.4: Contribution values for one-day to maturity European-style DBKO calls.

n	$\beta = -2, \gamma = 2$	$\beta = -2, \gamma = 1$	$\beta = 1, \gamma = 2$	$\beta = 1, \gamma = 1$
1-5	-0.94494	-1.60020	1.54180	1.77004
6-10	1.81670	2.60534	-1.15441	-1.41771
10-15	-0.23014	-0.31208	0.19023	0.24668
16-20	-0.10622	-0.14909	-0.03420	-0.04298
21-25	0.00934	0.01343	0.00311	0.00400
26-30	0.00157	0.00224	-0.00021	-0.00026
31-35	-0.00010	-0.00014	0.00001	0.00001
36-40	-0.00001	-0.00001	0.00000	0.00000
41-45	0.00000	0.00000	0.00000	0.00000
$>$45	0.00000	0.00000	0.00000	0.00000
Price	0.54622	0.55950	0.54634	0.55976

This table shows the value of the contribution defined in equation (2.33) for one-day to maturity European-style DBKO call options for different γ and β parameters, with $y_0 = 100$, $K = 100$, $L = 90$, $U = 120$, $T = 1/360$, $\bar{r} = 0.1$, $\bar{q} = 0$, $b = 0.02$, $c = 0.5$, and $\sigma_0 = 0.25$.

2.8 Concluding remarks and future research

This paper provides a new methodology for pricing (and hedging) European-style DBKO options via the application of the NSBF decomposition of the Sturm-Liouville equation associated to the corresponding boundary value problem. The illustration of the method was done through the EJDCEV model. The modeling techniques applied in this paper open several avenues for future research. For instance, it should be possible to apply the NSBF decomposition and similar constructions to other singular problems that naturally appear in many financial applications, e.g. plain-vanilla options (unbounded domains), default cases (singularities in the coefficients) and others. It would also be interesting to apply the method to calibrate a parametric curve of parameters to real market data. Finally, it has also the potential to be applied to stopping time problems and related subjects.

3. Solution of parabolic free boundary problems using transmuted heat polynomials

Abstract: A numerical method for free boundary problems for the equation

$$u_{xx} - q(x)u = u_t \tag{3.1}$$

is proposed. The method is based on recent results from transmutation operators theory allowing one to construct efficiently a complete system of solutions for equation (3.1) generalizing the system of heat polynomials. The corresponding implementation algorithm is presented.

3.1 Introduction

Free boundary problems (FBPs) for parabolic equations are of considerable interest in physics (e.g., the Stefan problem) and in financial mathematics (e.g., the problem of pricing of an American option). One of the relatively simple and practical methods proposed for solving FBPs involving the heat equation is the heat polynomials method (see Colton (1976), Reemtsen and Lozano (1982), Colton and Reemtsen (1984), Reemtsen and Kirsch (1984), Sarsengeldin et al. (2014), Kharin et al. (2016)) based on the fact that the system of the heat polynomials represents a complete family of solutions of the heat equation. In the book Colton (1976) D. Colton proposed to extend this method onto parabolic equations with variable coefficients by constructing an appropriate transmutation operator and obtaining with its aid the corresponding transmuted heat polynomials. However, the construction of the transmutation operator is a difficult problem itself. In the present work we show that the transmuted heat polynomials required for Colton's approach can be constructed without knowledge of the transmutation operator by a simple and robust recursive integration procedure. To this aim a recent result from Campos et al. (2012) concerning a mapping property of the transmutation operators is used.

This makes possible to extend the heat polynomials method onto equations of the form

$$u_{xx} - q(x)u = u_t. \tag{3.2}$$

We mention that linear parabolic equations of a more general form with coefficients depending on one variable reduce to (3.2) (see, e.g., (Colton, 1976, Chap. 2) or Miyazawa (1989)).

Thus, we propose a numerical method for approximate solution of a class of FBPs involving (3.2). This method of transmuted heat polynomials will be designated by THP. The main aim of this paper is to explain it in detail and to propose a simple to implement algorithm for its application.

The subject of FBPs appears in many different fields and applications, as such, presents a large variety of formulations and still open questions. We will not be focusing on the existence and uniqueness of the solution in this paper assuming that it exists in the classical sense.

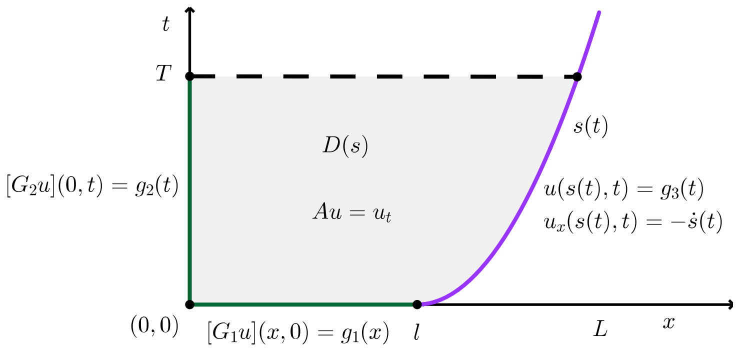

Figure 3.1: Illustration of Problem 3.1 statement

The paper is structured as follows. In Section 3.2 we state the FBP. In Section 3.3 we define transmutation operators and present some of their properties motivating the development of the THP method. In Section 3.4 we construct the conceptual algorithm for the implementation of the THP method for solving FBPs. In Section 3.5 we consider an example with an exact solution, with its aid we illustrate the performance of the method. In Section 3.6 we discuss the possibilities of generalization of our construction and its application to more general FBPs.

3.2 Statement of the problem

Consider the differential expression

$$\mathbf{A} = \frac{\partial^2}{\partial x^2} - q(x)$$

with $q \in C[0, L]$, $q : [0, L] \to \mathbb{C}$.

Every $s \in C^1[0, T]$, such that $0 < s(x) \leq L$ for all $x \in [0, T)$ and $s(0) = l$, defines a domain

$$D(s) = \left\{(x, t) \in \mathbb{R}^2 : 0 < x < s(t), 0 < t < T\right\}, \tag{3.3}$$

see Figure 3.1. Consider the first order linear differential operators $\mathbf{G}_1 = \gamma_{11}(x) + \gamma_{12}(x)\frac{\partial}{\partial x}$ and $\mathbf{G}_2 = \gamma_{21}(t) + \gamma_{22}(t)\frac{\partial}{\partial x}$, where γ_{ij} are some given continuous functions.

Problem 3.1 *Find functions* (u, s) *such that*

(i) $s \in C^1[0, T]$ *and such that* $0 < s(x) \leq L$ *for all* $x \in [0, T)$ *and* $s(0) = l$*,*

(ii) $u \in C^{2,1}\big(D(s)\big)$*,*

(iii) *the following equation is satisfied on* $D(s)$

$$\mathbf{A}u(x,t) = u_t(x,t), \qquad (x,t) \in D(s), \tag{3.4}$$

(iv) *and the following boundary conditions are satisfied*

$$\left[\mathbf{G}_1 u\right](x,0) = g_1(x), \qquad x \in (0,l), \qquad l \leq L, \tag{3.5}$$

$$\left[\mathbf{G}_2 u\right](0,t) = g_2(t), \qquad t \in (0,T), \tag{3.6}$$

$$u\big(s(t),t\big) = g_3(t), \qquad t \in (0,T), \tag{3.7}$$

$$u_x\big(s(t),t\big) = -\dot{s}(t), \qquad t \in (0,T), \tag{3.8}$$

here the dot over the function s *means the derivative with respect to the variable* t*. The last condition is usually known as the equation of heat balance or as the Stefan condition.*

This problem is broadly studied in literature (see, e.g., Friedman (1964), Rubinshtein (1971), Crank (1984), Meirmanov (1992), Fasano and Primicerio (1979) and Tarzia (2000) for additional bibliography). In particular, the classical one dimensional one phase Stefan problem is a special case of Problem 3.1. Since the subject of this paper is the approximate numerical method for solution of Problem 3.1, we make the following assumption.

Assumption 3.3 *There exists a unique solution to Problem 3.1.*

A relevant example of an existence and uniqueness result is given in (Fasano and Primicerio, 1979, Theorem 1), see Remark 3.7 below.

3.3 Transmuted heat polynomials

3.3.1 Heat polynomials

The heat polynomials are defined for $n \in \mathbb{N}_0$ as (see, e.g., Rosenbloom and Widder (1959) and Widder (1962))

$$h_n(x,t) = \sum_{k=0}^{[n/2]} c_k^n x^{n-2k} t^k, \qquad \text{where } c_k^n = \frac{n!}{(n-2k)!k!}$$

and $[\cdot]$ denotes the entire part of the number. The first five heat polynomials are

$$h_0(x,t) = 1, \qquad h_1(x,t) = x, \qquad h_2(x,t) = x^2 + 2t,$$
$$h_3(x,t) = x^3 + 6xt, \qquad h_4(x,t) = x^4 + 12x^2t + 12t^2.$$

The set of the heat polynomials $\{h_n\}_{n\in\mathbb{N}_0}$ represents a complete system of solutions for the heat equation

$$u_{xx} = u_t \tag{3.9}$$

on any domain $D(s)$ defined by (3.3) (see Colton and Watzlawek (1977)).

3.3.2 Formal powers and the transmutation operator

Let f be a nonvanishing (in general, complex valued) solution of the equation

$$\left(\frac{d^2}{dx^2} - q(x)\right) f(x) = 0, \qquad x \in (0, L), \tag{3.10}$$

such that

$$f(0) = 1. \tag{3.11}$$

The existence of such solution[3.1] for any complex valued $q \in C[0, L]$ was proved in Kravchenko and Porter (2010) (see also Camporesi and Di Scala (2011)).

Consider two sequences of recursive integrals (see Kravchenko (2009), Kravchenko et al. (2016), Kravchenko and Porter (2010))

$$X^{(0)}(x) \equiv 1, \qquad X^{(n)}(x) = n \int_0^x X^{(n-1)}(s) \left(f^2(s)\right)^{(-1)^n} \mathrm{d}s, \qquad n = 1, 2, \ldots$$

and

$$\widetilde{X}^{(0)} \equiv 1, \qquad \widetilde{X}^{(n)}(x) = n \int_0^x \widetilde{X}^{(n-1)}(s) \left(f^2(s)\right)^{(-1)^{n-1}} \mathrm{d}s, \qquad n = 1, 2, \ldots.$$

Definition 3.2 *The family of functions $\{\varphi_n\}_{n=0}^{\infty}$ constructed according to the rule*

$$\varphi_n(x) = \begin{cases} f(x) X^{(n)}(x), & n \textit{ odd}, \\ f(x) \tilde{X}^{(n)}(x), & n \textit{ even}, \end{cases} \tag{3.12}$$

*is called the system of **formal powers** associated with f.*

[3.1] In fact the only reason for the requirement of the absence of zeros of the function f is to make sure that the auxiliary functions (3.12) be well defined. As was shown in Kravchenko and Torba (2014) this can be done even without such requirement, but corresponding formulas are somewhat more complicated.

The formal powers arise in the spectral parameter power series (SPPS) representation for solutions of the Sturm-Liouville equation, see Kravchenko (2008), Kravchenko and Porter (2010), Khmelnytskaya et al. (2015), Kravchenko et al. (2016).

The following result from Marchenko (1952) (see also Kravchenko et al. (2017b) and Kravchenko and Torba (2015) for additional details) and from Campos et al. (2012) guarantees the existence of a transmutation operator associated with f and shows its connection with the system of formal powers.

Theorem 3.1 *Let $q \in C[0, L]$. Then there exists a unique complex valued function $K(x, y) \in C^1\big([0, L] \times [-L, L]\big)$ such that the Volterra integral operator*

$$\mathbf{T}u(x) = u(x) + \int_{-x}^{x} K(x, y)u(y)\,dy$$

defined on $C[0, L]$ satisfies the equality

$$\mathbf{A}\mathbf{T}[u] = \mathbf{T}\left[\frac{d^2u}{dx^2}\right]$$

for any $u \in C^2[0, L]$ and

$$\mathbf{T}\,[1] = f.$$

Note that if $v = \mathbf{T}u$ then $v(0) = u(0)$ and $v'(0) = u'(0) + f'(0)u(0)$.

Theorem 3.2 (Campos et al. (2012))

$$\mathbf{T}\,[x^n] = \varphi_n(x) \qquad \textit{for any } n \in \mathbb{N}_0.$$

3.3.3 Construction of the transmuted heat polynomials

Denote $H_n = \mathbf{T}[h_n]$. Thus, $H_n(x,t) = h_n(x,t) + \int_{-x}^{x} K(x,y)h_n(y,t)\,dy$. The functions H_n are called the **transmuted heat polynomials** Kravchenko et al. (2017c).

We have $\left(\mathbf{A} - \frac{\partial}{\partial t}\right) H_n = \mathbf{A}\mathbf{T}h_n - \frac{\partial}{\partial t}\mathbf{T}h_n = \mathbf{T}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}\right) h_n = 0$ and hence every H_n is a solution of the equation

$$\mathbf{A}u = u_t. \tag{3.13}$$

The set $\{H_n\}_{n\in\mathbb{N}_0}$ is a complete system of solutions of (3.13) in the following sense.

Proposition 3.2 *Let u be a classical solution of (3.13) in $D(s)$, continuous in the closure $\bar{D}(s)$. Then for any compact set $D_c \subset D(s)$ and any given $\varepsilon > 0$ there exist N and constants $a_0, \dots, a_N$ such that*

$$\max_{(x,t)\in D_c} \left| u(x,t) - \sum_{n=0}^{N} a_n H_n(x,t) \right| < \varepsilon.$$

Moreover, if $s(t)$ can be extended to a function analytic in the disk $\{t \in \mathbb{C} : |t| \le T\}$, the uniform approximation property is valid on the whole set $\bar{D}$.

Proof. 3.2 *Suppose first that $q \in C^1[0,L]$. Note that any compact set D_c can be covered by a subset $D_a \subset \bar{D}(s)$ of the form $D_a = \{(x,t) \in \mathbb{R}^2 : 0 \le x \le x_1(t) \le s(t),\ 0 \le t \le T\}$ with analytic function $x_1(t)$. For the set D_a the proof is completely similar to that of (Colton, 1976, Theorem 2.3.3) with the only change that the transmutation operator $\mathbf{T}$ and its inverse are used. For the general case $q \in C[0,L]$ one approximates q by a C^1 function.*

Theorem 3.3 *The transmuted heat polynomials admit the following form*

$$H_n(x,t) = \sum_{k=0}^{[n/2]} c_k^n \varphi_{n-2k}(x) t^k.$$

Proof. 3.3 *This equality is an immediate corollary of Theorem 3.2. Indeed, we have* $H_n(x,t) = \mathbf{T} h_n(x,t) = \sum_{k=0}^{[n/2]} c_k^n \mathbf{T}\left[x^{n-2k}\right] t^k$*, where Theorem 3.2 is used.*

The explicit form of the functions H_n presented in this theorem makes possible the construction of the approximate solution to Problem 3.1 by the THP method.

3.4 Description of the method

We proceed to the step by step construction of the THP method, summarizing the algorithm at the end of the section.

Assume that we have already calculated the formal powers φ_k and the functions H_n. Further, let N be the highest index of the formal power considered, or equivalently the highest degree in x of the considered heat polynomials. We denote by

$$u_N(x,t) = \sum_{n=0}^{N} a_n H_n(x,t) \tag{3.14}$$

the approximation of the solution $u(x,t)$, and by $\bar{a} = (a_0, ..., a_N)^T$ the column-vector of the unknown coefficients. Note that by construction functions u_N satisfy equation (3.4), all we need is to find suitable coefficients $\bar{a}$.

Denote by $\{t_i\}$ an ordered set of $N_t + 1$ points of the interval $[0,T]$, with $t_0 = 0 < t_1 < ... < t_{N_t} = T$, $\bar{t} = (t_0, ..., t_{N_t})^T$, and by $\{x_i\}$ an ordered set of $N_x + 1$ points of the initial boundary, with $x_0 = 0 < x_1 < ... < x_{N_x} = l$, $\bar{x} = (x_0, ..., x_{N_x})^T$.

Consider a set of $K+1$ linearly independent differentiable functions, $\beta_k : [0,T] \to \mathbb{R}$. We are looking for the free boundary in the form

$$s_K(t) = \sum_{k=0}^{K} b_k \beta_k(t).$$

Denote the vector of the unknown coefficients[3.2] by $\bar{b} = (b_0, ..., b_K)^T$. For any function v defined on the set of points $\{y_i\}_{i=0,1,...,N_y}$ the following notation is introduced

$$v(\bar{y}) = \left(v(y_0), ..., v\left(y_{N_y}\right)\right)^T.$$

A numerical approximation problem consists in finding a set of the coefficients $\left(\bar{a}, \bar{b}\right)$ that best fits the conditions of Problem 3.1 with the following norm chosen

$$\|v(\bar{y})\|^2 = \sum_{i=0}^{N_y} |v(y_i)|^2.$$

The following magnitudes are to be minimized,

$$\begin{aligned}
I_1\left(\bar{a}, \bar{b}\right) &= \left\| [\mathbf{G}_1 u_N](\bar{x}, 0) - g_1(\bar{x}) \right\|, \\
I_2\left(\bar{a}, \bar{b}\right) &= \left\| [\mathbf{G}_2 u_N](0, \bar{t}) - g_2(\bar{t}) \right\|, \\
I_3\left(\bar{a}, \bar{b}\right) &= \left\| u_N\left(s_K(\bar{t}), \bar{t}\right) - g_3(\bar{t}) \right\|, \\
I_4\left(\bar{a}, \bar{b}\right) &= \left\| (u_N)_x \left(s_K(\bar{t}), \bar{t}\right) + \dot{s}_K(\bar{t}) \right\|.
\end{aligned}$$

Each of them is related to a boundary condition from (3.5)–(3.8). With introduction of the value function

$$F\left(\bar{a}, \bar{b}\right) = \sum_{i=1}^{4} I_i^2\left(\bar{a}, \bar{b}\right), \tag{3.15}$$

the minimization problem can be stated as follows.

[3.2] It is possible to search for the free boundary in a more general form, see Section 3.6.3.

Problem 3.2 *Find*[3.3]

$$\arg\min_{(\bar{a},\bar{b})} F\left(\bar{a},\bar{b}\right),$$

subject to

$$0 < s_K(t) \leq L, \qquad t \in [0,T]. \tag{3.16}$$

Note that instead of the uniform norm chosen in Reemtsen and Lozano (1982) for the heat polynomials method, we used the L_2 norm in the value function (3.15). The main reason for such choice was to take advantage of the presence of the so-called separable linear parameters (see (Ross, 1990, Chap. 6.2), see also Herrera-Gomez and Porter (2017)) and to reduce the number of parameters in the value function. Indeed, for each fixed $\bar{b}$, the constrained minimization Problem 3.2 reduces to an unconstrained linear least squares problem for parameters $\bar{a}$ and can be easily solved exactly (see Subsection 3.4.1). That is, for each $\bar{b}$ we can define

$$\bar{a}(\bar{b}) := \arg\min_{\bar{a}} F\left(\bar{a},\bar{b}\right). \tag{3.17}$$

So instead of minimizing the value function F over an $N+K+2$ dimensional space of parameters $(\bar{a},\bar{b})$, the problem can be reduced to minimization of the function

$$\tilde{F}(\bar{b}) := F\big(\bar{a}(\bar{b}),\bar{b}\big)$$

over a $K+1$ dimensional space. Such reformulation of the original optimization problem leads to a more robust convergence of numerical optimization algorithms, c.f., Herrera-Gomez and Porter (2017). We state this new minimization problem as follows.

[3.3] For a function $f : X \to Y$, the $\arg\min$ over a subset S of X is defined as

$$\arg\min_{x\in S\subseteq X} f(x) := \{x : x \in S \wedge \forall y \in S : f(y) \geq f(x)\}.$$

Problem 3.3 *Find*

$$\arg\min_{\bar{b}} \tilde{F}\left(\bar{b}\right)$$

subject to

$$0 < s_K(t) \leq L, \qquad t \in [0,T]. \tag{3.18}$$

3.4.1 Linear minimization problem

Let a vector $\tilde{b}$ be fixed. We have to solve the linear least squares problem (3.17). Let us denote the corresponding approximate boundary by $\tilde{s}$,

$$\tilde{s}(t) = \sum_{i=0}^{N_\beta} \tilde{b}_i \beta_i(t).$$

Note that problem (3.17) is equivalent to solving the overdetermined system of linear equations (resulting from the boundary conditions (3.5)–(3.8))

$$[\mathbf{G}_1 u_N]\left(\bar{x},0\right) = \sum_{n=0}^{N} a_n B_n\left(\bar{x}\right), \qquad u_N\left(\tilde{s}\left(\bar{t}\right),\bar{t}\right) = \sum_{n=0}^{N} a_n D_n\left(\bar{t}\right),$$

$$[\mathbf{G}_2 u_N]\left(0,\bar{t}\right) = \sum_{n=0}^{N} a_n C_n\left(\bar{t}\right), \qquad \left(u_N\right)_x\left(\tilde{s}\left(\bar{t}\right),\bar{t}\right) = \sum_{n=0}^{N} a_n E_n\left(\bar{t}\right),$$

where

$$B_n\left(\bar{x}\right) = \begin{cases} c_0^n \gamma_{11}(\bar{x})\varphi_n(\bar{x}) + c_{\frac{n-1}{2}}^n \gamma_{12}(\bar{x})\varphi_1'(\bar{x}), & n \text{ odd}, \\ c_0^n \gamma_{11}(\bar{x})\varphi_n(\bar{x}), & n \text{ even}, \end{cases} \tag{3.19}$$

$$C_n\left(\bar{t}\right) = \begin{cases} c_{\frac{n-1}{2}}^n \gamma_{22}(\bar{t})\bar{t}^{\frac{n-1}{2}}, & n \text{ odd}, \\ c_{\frac{n}{2}}^n \gamma_{21}(\bar{t})\bar{t}^{\frac{n}{2}}, & n \text{ even}, \end{cases} \tag{3.20}$$

$$D_n(\bar{t}) = \sum_{k=0}^{[n/2]} c_k^n \varphi_{n-2k}(\tilde{s}(\bar{t})\bar{t}^k, \qquad E_n(\bar{t}) = \sum_{k=0}^{[n/2]} c_k^n \varphi_{n-2k}'(\tilde{s}(\bar{t}))\bar{t}^k, \tag{3.21}$$

or in the matrix form

$$\mathbf{B}\bar{a} \simeq \mathbf{g}, \tag{3.22}$$

where

$$\mathbf{B} = \begin{pmatrix} B_0(\bar{x}) & \dots & B_N(\bar{x}) \\ C_0(\bar{t}) & \dots & C_N(\bar{t}) \\ D_0(\bar{t}) & \dots & D_N(\bar{t}) \\ E_0(\bar{t}) & \dots & E_N(\bar{t}) \end{pmatrix} \quad \text{and} \quad \mathbf{g} = \begin{pmatrix} g_1(\bar{x}) \\ g_2(\bar{t}) \\ g_3(\bar{t}) \\ \dot{\tilde{s}}(\bar{t}) \end{pmatrix}.$$

Note that the derivatives φ' in (3.21) do not require numerical differentiation and can be obtained in a closed form from (3.12).

The solution of this overdetermined system coincides (Madsen and Nielsen, 2010, Thm. 5.14) with the unique solution of the following fully determined system of linear equations

$$\mathbf{C}\bar{a} = \mathbf{h}, \qquad \text{where } \mathbf{C} = \mathbf{B}^T\mathbf{B} \text{ and } \mathbf{h} = \mathbf{B}^T\mathbf{g}. \tag{3.23}$$

See also Lawson and Hanson (1995) or Nocedal and Wright (2006) for various methods of efficient solution of equation (3.22) or (3.23). In particular, we used the Moore-Penrose pseudo-inverse method.

3.4.2 Implementation

Here we present the algorithm of the implementation of the THP method for Problem 3.1.

1. Find a particular solution of equation (3.10) satisfying (3.11). For example, the SPPS method presented in Kravchenko and Porter (2010) can be used.

2. Construct the formal powers on an interval from 0 to some $L > l$. In this paper we represented all the functions involved by their values on a uniform mesh and used the Newton-Cotes six point integration rule. Since we may need the values of the formal powers at arbitrary points $\tilde{s}(\bar{t}) \subset [0, L]$, we approximated the formal powers by splines passing through their values on the selected mesh. Spline integration can be used as well for the construction of the formal powers, c.f., Khmelnytskaya et al. (2013). See also Kravchenko et al. (2017b) for the discussion of other possible methods.

3. Compute the coefficients B_n and C_n given by (3.19) and (3.20) and the respective functions g_1 and g_2. Since these conditions are independent of the free boundary (i.e. of the choice of $\tilde{b}$), they need to be computed only once.

4. Construct a function that solves problem (3.17) for each given set of coefficients $\tilde{b}$.

5. Construct the value function $\tilde{F}(b)$ using (3.15).

6. Solve the constrained minimization Problem 3.3 using any suitable algorithm, see, e.g., Nocedal and Wright (2006). For the numerical illustration we used the Matlab function `fmincon`. Note that for faster convergence we may initially solve the minimization Problem 3.3 for some small value $K' < K$ and use the coefficients b_k^0, $k = 0, \ldots, K'$ obtained as an initial value for the optimization algorithm for larger value K.

3.5 Numerical illustration

3.5.1 Example with an exact solution and a tractable free boundary

For the numerical experiment we constructed an example of an FBP admitting an exact solution.

For every $s \in C^1[0,1]$, with $s(0) = 1$ consider the domain

$$D(s) = \left\{(x,t) \in \mathbb{R}^2 : 0 < x < s(t),\, 0 < t < 1\right\}.$$

Problem 3.4 *Find the pair* (s,u) *such that* $s \in C^1[0,1]$, $u \in C^{2,1}\left(D(s)\right)$ *and*

$$u_{xx} - x^2 u = u_t, \qquad (x,t) \in D(s),$$

with the following boundary conditions

$$u(x,0) = e^{-\frac{x^2}{2}}, \qquad x \in [0,1], \tag{3.24}$$

$$u_x(0,t) = 0, \qquad t \in (0,1), \tag{3.25}$$

$$u(s(t),t) = e^{-\operatorname{Ei}^{-1}\left(2C - 2e^{-t}\right) - t}, \qquad t \in (0,1), \tag{3.26}$$

$$u_x(s(t),t) = -\dot{s}(t), \qquad t \in (0,1), \tag{3.27}$$

where

$$C = \frac{1}{2}\operatorname{Ei}\left(\frac{1}{2}\right) + 1 \approx 1.2271,$$

and Ei^{-1} *stands for the inverse function of the exponential integral* Ei,

$$\operatorname{Ei}(x) = -\,\mathrm{v.\,p.}\int_{-x}^{\infty} \frac{e^{-t}}{t}\,dt.$$

Problem 3.4 possesses an exact solution u given by

$$u(x,t) = e^{-\frac{x^2}{2}-t}, \qquad (x,t) \in D(s), \tag{3.28}$$

and the free boundary

$$s\left(t\right) = \sqrt{2\,\mathrm{Ei}^{-1}\left(2C - 2e^{-t}\right)}, \qquad t \in \left[0,1\right]. \tag{3.29}$$

Remark 3.7 *The existence and the uniqueness of the solution for $t \in [0,1]$ is guaranteed by (Fasano and Primicerio, 1979, Theorem 1). For the application of the theorem it is necessary to use the transformation $v(x,t) = u(x,t) + \gamma(t)$, where $\gamma(t) = \exp\left(-\mathrm{Ei}^{-1}\left(2C - 2e^{-t}\right) - t\right)$.*

3.5.2 Numerical illustration

We proceed by presenting numerical results delivered by the algorithm described in Section 3.4. All the calculations were carried out in Matlab R2012a.

A particular solution to equation (3.10) and the formal powers (3.12) were represented by their values on a 2000-points uniform mesh. The Newton-Cotes integration rule was used for their computation. The number of formal powers considered was set at $N = 12$. Finally the function `spapi` was used to create splines approximating the formal powers. For computing the Ei^{-1} we have used a polynomial interpolation on a fine grid for the function Ei. The values for the function Ei were constructed by the series expansions presented in (Gradshteyn and Ryzhik, 2007, (8.214)), see also Pecina (1986).

The sets of points $\{t_i\}$ and $\{x_i\}$ considered are both equidistant grids of 101 points. The free boundary s is sought in terms of polynomials. The condition $s(0) = 1$ inspires the following form

$$s_K(\bar{t}) = 1 + \sum_{j=1}^{K} b_j \bar{t}^j.$$

In our calculations we have considered $K = 6$.

The linear problem (3.17) was solved by using the Matlab function `pinv`. We have found the solution to Problem 3.3 using the Matlab routine `fmincon`.

The proposed algorithm converged rapidly for various initial free boundaries tested. On Figure 3.2 we present one of the initial boundaries, the exact free boundary $s(t)$ calculated from equation (3.29) and the difference between the exact free boundary $s(t)$ and the obtained approximation $s_K(t)$. The obtained approximate boundary was

$$\begin{aligned} s_K(t) = 1 + 0.60657885t - 0.30458770t^2 + 0.03631846t^3 + \\ + 0.06761711t^4 - 0.05111378t^5 + 0.01270860t^6, \end{aligned} \tag{3.30}$$

here and after the coefficients are presented up to the eighth decimal place. The coefficients of the vector $\bar{a}$ that corresponds to the solution of the linear problem (3.17) with $\bar{b}$ consisting of the coefficients from (3.30) are

$$\begin{aligned} &a_0 = 1.00000201, && a_1 = -3.88882172 \cdot 10^{-6}, && a_2 = -5.00020660 \cdot 10^{-1}, \\ &a_3 = 2.67326664 \cdot 10^{-5}, && a_4 = 4.16822991 \cdot 10^{-2}, && a_5 = -2.03778980 \cdot 10^{-5}, \\ &a_6 = -1.38990292 \cdot 10^{-3}, && a_7 = 4.02691726 \cdot 10^{-6}, && a_8 = 2.43785480 \cdot 10^{-5}, \\ &a_9 = -2.56424452 \cdot 10^{-7}, && a_{10} = -2.28538929 \cdot 10^{-7}, && a_{11} = 4.70925279 \cdot 10^{-9}, \\ &a_{12} = 7.12497038 \cdot 10^{-10}. \end{aligned}$$

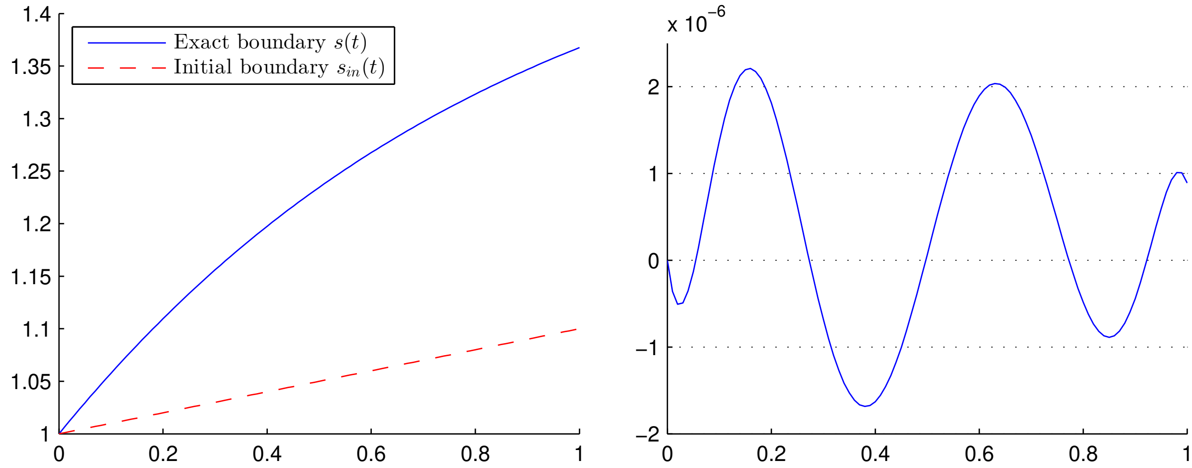

Figure 3.2: Left: the initial boundary $s_{in}(t) = 1 + 0.1t$ and the exact boundary $s(t)$ for the Problem 3.4. Right: the difference between the exact boundary $s(t)$ and the approximate boundary $s_K(t)$.

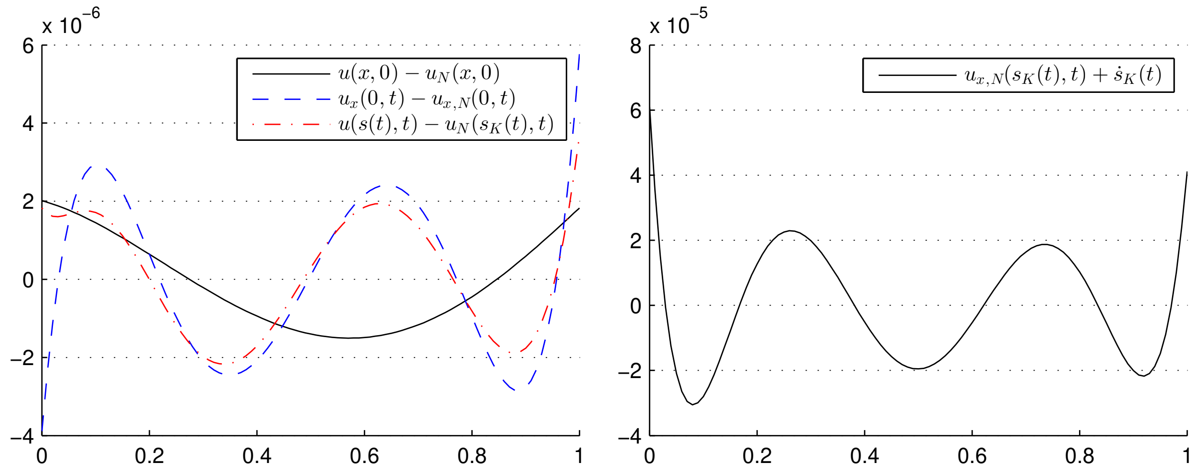

Figure 3.3: Accuracy of fulfillment of the boundary conditions (3.24)–(3.27) for the approximate solution u_N and approximate free boundary s_K obtained by the algorithm. On the left: conditions (3.24)–(3.26), on the right: condition (3.27).

Figure 3.3 illustrates the accuracy of fulfillment of the boundary conditions (3.24)–(3.27). The absolute value of the difference between the exact solution (3.28) and the obtained approximate solution in the domain $D(s)$ is presented on Figure 3.4.

Note that for the problem considered one may look for an approximate solution in the

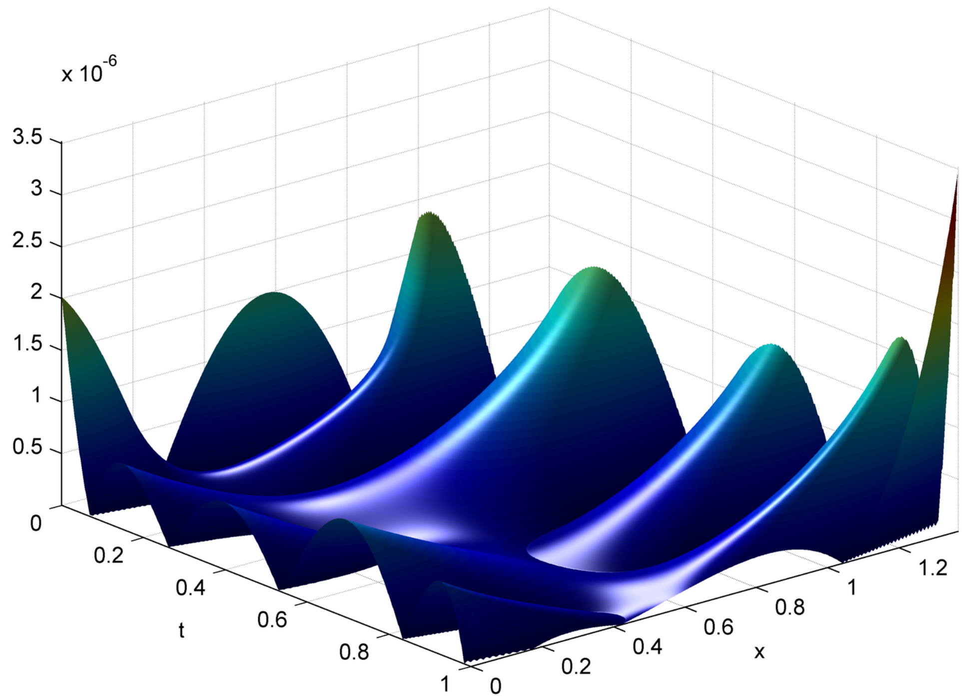

Figure 3.4: The absolute difference $|u(x,t) - u_N(x,t)|$ between the exact and the approximate solutions for the Problem 3.4 in the domain $D(s)$.

form

$$u_N(x,t) = \sum_{n=0}^{N/2} a_{2n} H_{2n}(x,t),$$

i.e., having only even coefficients a_{2n}. In such way the boundary condition (3.25) is satisfied automatically. The proposed algorithm can be applied with minimal modifications for such simplified form of an approximate solution, however we did not observe any gain in the obtained result, the original formulation of the algorithm performed equally well.

3.6 Possible extensions of the method to more general FBPs and final remarks

3.6.1 Generalization of the operator A

The presented method can be extended onto operators of the form

$$\mathbf{C} = \alpha_1(x)\frac{\partial^2}{\partial x^2} + \alpha_2(x)\frac{\partial}{\partial x} + \alpha_3(x)$$

with sufficiently regular coefficients $\alpha_i(x)$. For the construction of the formal powers in this case see Kravchenko and Torba (2018). The FBPs with this type of operators are very common in financial applications.

3.6.2 Generalizations of the conditions on a free boundary

Linear generalization

The conditions (3.7) and (3.8) are sometimes referred to as Stefan's conditions. Our algorithm can be applied to more general conditions of the type

$$\mathbf{G}_3 u(s(t), t) = g_3\big(t, s(t), \dot{s}(t)\big),$$
$$\mathbf{G}_4 u(s(t), t) = g_4\big(t, s(t), \dot{s}(t)\big),$$

for some first order linear differential operators $\mathbf{G}_3$ and $\mathbf{G}_4$, and where g_3 and g_4 are given functions of three variables.

Nonlinear generalization

For some FBPs we can only express the conditions (3.7) and (3.8) as

$$g_3\big(t, s(t), \dot{s}(t), u(s(t), t), u_x(s(t), t)\big) = 0,$$
$$g_4\big(t, s(t), \dot{s}(t), u(s(t), t), u_x(s(t), t)\big) = 0,$$

where g_3 and g_4 are given functions of five variables. In this case the elegant decomposition into a linear and nonlinear problems will be lost, however the hierarchic structure of the minimization problem remains, i.e., the minimization Problem 3.2 can be reduced to the Problem 3.3 with the only difference that the auxiliary problem (3.17) may be nonlinear.

3.6.3 Nonlinear form of the boundary

Often in applications some additional information is available about the free boundary structure. With this additional knowledge (or for other reasons) the linear decomposition of the boundary might not be appropriate. It is easy to see that we can still apply the algorithm assuming that

$$s_K = \xi\left(b_0, ..., b_K\right),$$

for the known function ξ. This nonlinear structure can slow down the algorithm for the search of the minimum in Problems 3.2 or 3.3, due to the constraints (3.16) and (3.18) respectively. In our particular Matlab implementation, we have used `fmincon` function that performs better with a linear constraint on the boundary than a nonlinear one.

3.6.4 Concluding remarks

A method for approximate solution of a large variety of FBPs is proposed. It is based on a possibility to construct a complete system of solutions of a parabolic equation called transmuted heat polynomials. The numerical implementation is relatively simple and direct. The time required for computations is within seconds. The method admits extensions onto a much larger class of FBPs then that discussed in the paper.

4. Generalized exponential basis for efficient solving of homogeneous diffusion free boundary problems: Russian option pricing

Abstract: This paper develops a method for solving free boundary problems for time-homogeneous diffusions. We combine the complete exponential system of solutions for the heat equation, transmutation operators and recently discovered Neumann series of Bessel functions representation for solutions of Sturm-Liouville equations to construct a complete system of solutions for the considered partial differential equations. The conceptual algorithm for the application of the method is presented. The valuation of Russian options with finite horizon is used as a numerical illustration. The solution under different horizons is computed and compared to the results that appear in the literature.

JEL Classification: G13, C60.

4.1 Introduction

One of the approaches for solving boundary value problems for partial differential equations (PDE's) is based on complete systems of solutions (CSS). In particular, several CSS have been used in different models such as: fundamental solutions (the well known method of fundamental solutions or discrete sources) Kupradze (1967), Alexidze (1991), Fairweather and Karageorghis (1998) and Doicu et al. (2000); heat polynomials Colton (1976), Reemtsen and Lozano (1982), Colton and Reemtsen (1984), Sarsengeldin et al. (2014) and Kravchenko et al. (2017c); wave polynomials in Khmelnytskaya et al. (2013) among many others. For the present paper the following family $\{e_n^{\pm}\}_{n\in\mathbb{N}}$ of exponential solutions of the heat equation

$$h_{xx} = h_t, \tag{4.1}$$

defined as

$$e_n^{\pm}(x,t) = \exp(\pm i\omega_n x - \omega_n^2 t), \tag{4.2}$$

are of particular interest. Here the constants ω_n are chosen such that the limit

$$d := \lim_{n\to\infty} \frac{n}{\omega_n^2} > 0 \tag{4.3}$$

exists. In Colton (1980), the completeness of this system of solutions was proved for bounded domains satisfying certain smoothness properties.

As a rule, the approach based on CSS cannot be directly applied to equations with variable coefficients, because CSS are not available in a closed form. In Colton (1976), there was developed the idea to extend the approach of CSS to equations with variable coefficients with the aid of transmutation operators whenever they are known or can be constructed efficiently. However, the construction of the transmutation operators is itself a complicated task.

In the present paper, we propose the construction of the CSS generalizing exponential solutions (4.2) for the equation

$$\mathbf{C}u(y,t) := \frac{1}{w\left(y\right)}\left(\frac{\partial}{\partial y}\left(p\left(y\right)\frac{\partial}{\partial y}\right) - q\left(y\right)\right)u(y,t) = u_t(y,t). \tag{4.4}$$

These generalized exponential solutions represent a CSS for equation (4.4) and are the images of the exponential solutions (4.2) under the action of the transmutation operator. Moreover, they can be computed by a simple robust recursive integration procedure which does not require the knowledge of the transmutation operator itself. This makes possible to extend the numerical methods (minimization problems) for free boundary problems (FBP's) for the heat equation to the time homogeneous parabolic equations, in particular, to the finite horizon Russian option (FHRO) valuation problem that we analyze in detail in this paper.

In Kravchenko et al. (2017a), a numerical method was developed for the classical one dimensional Stefan like problem for the time-homogeneous parabolic operator using the CSS of the transmuted heat polynomials, that was referred to as THP method. It is well known that the CSS based on polynomials result in badly conditioned matrices, making the application of THP complicated for the practical computations. This is the case for the FHRO. Fortunately, there are alternative CSS for the heat equation (4.1), for which we also know their transmuted images.

In practice, the FBP's are often challenging for numerical methods. For example, the boundary conditions arising in relation to the FHRO problem are non consistent (the solution or its derivative can not be continuous along the boundary). This leads to all

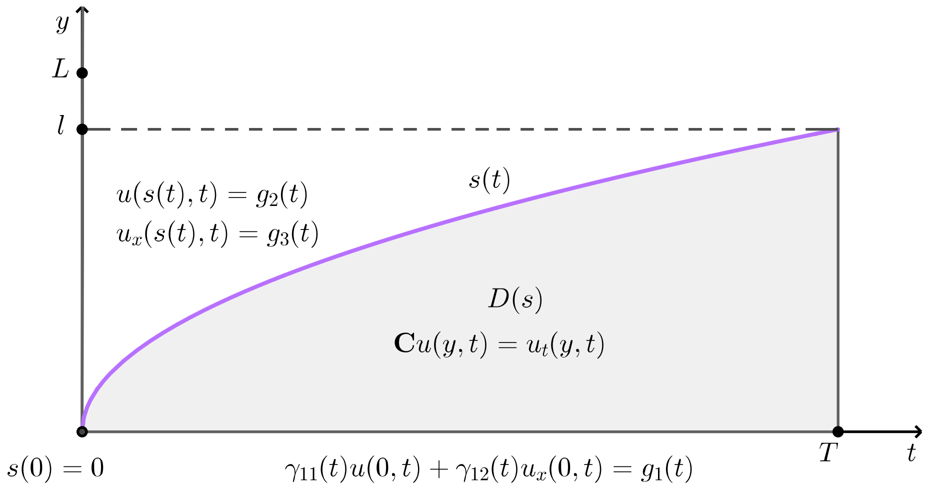

Figure 4.1: Free boundary problem.

sort of different computational issues. We present a step by step algorithm and discuss the numerical issues that we have encountered. The method that we propose takes into account known properties of the solution (such as monotone increase of the free boundary) and of the functions from the CSS (possibility to automatically satisfy one of the boundary conditions) making the computations easier and more predictable.

Even though there are several quantitative studies on the FHRO, e.g. Duistermaat et al. (2005), Kimura (2008) and Jeon et al. (2016), it seems that there is no agreement on the exact value for the option. We contribute to this discussion confirming the values from Jeon et al. (2016) and providing possible explanation of the discrepancy with Kimura (2008).

The parabolic FBP's arise in many fields, and hence the method proposed has a lot of potential for further applications and developments. In particular, for the financial engineering applications presenting path-dependence and early exercise features such as lookback options, American options, etc. In this paper, for the FHRO, we are restricted to the Black and Scholes (1973) and Merton (1973) (BSM) model (and respective infinitesimal generator) since it is not clear how to generalize the problem to different diffusions and keep the resulting FBP two dimensional (see also Kamenov (2008) for Bachelier model). However, for other financial (and non-financial) applications, where the FBP can be formulated using a general operator (4.4), our method can be applied as well. This is, for example, the case of American option where the underlying asset follows time-homogeneous diffusion process.

The paper is structured as follows. In Section 4.2, we state the FBP. In Section 4.3, we introduce the transmutation operators and highlight some of the relevant theoretical results. In Section 4.4, we introduce the notion of the CSS and see how it can be used to approximate the solutions of the PDE (4.4). We also show how to explicitly construct the transmuted CSS for the case of the generalized trigonometric series. In Section 4.5, we state the minimization problem and summarize an algorithm for the solution. In Section 4.6, we introduce the FHRO and set-up the corresponding FBP. The quantitative results for the FHRO, the discussion of the numerical issues and the comparison with existing in the literature results are presented in Section 4.7. Section 4.8 presents some concluding remarks.

4.2 The free boundary problem

Consider the differential expression $\mathbf{C}$ from (4.4) where the functions p, q and w satisfy the following assumption.

Assumption 1 *The functions p, p', q, w and w' are real valued and continuous on $[0, L]$. Additionally, it is assumed that p' and w' are absolutely continuous and that $p > 0$ and $w > 0$.*

Every non-negative function $s \in C^1[0, T]$, such that $s(0) = 0$ and $0 < s(t) \leq L$, $t \in$

$(0,T]$, defines a domain

$$D(s) = \{(y,t) \in \mathbb{R}^2 : 0 < y < s(t), 0 < t < T\}, \tag{4.5}$$

as shown on Figure 4.1.

Problem 4.5 *Find functions $u(y,t)$ and $s(t)$ such that*

$$\mathbf{C}u(y,t) = u_t(y,t), \qquad (y,t) \in D(s), \tag{4.6}$$

$$\gamma_{11}(t)u\left(0,t\right) + \gamma_{12}(t)u_y(0,t) = g_1\left(t\right), \qquad t \in \left(0,T\right), \tag{4.7}$$

$$u\left(s\left(t\right),t\right) = g_2\left(t\right), \qquad t \in \left(0,T\right), \tag{4.8}$$

$$u_y\left(s\left(t\right),t\right) = g_3\left(t\right), \qquad t \in \left(0,T\right), \tag{4.9}$$

where γ_{1j} for $j \in \{1,2\}$ and g_k for $k \in \{1,2,3\}$ are analytic functions.

The aim of this paper is to illustrate the application of the numerical method based on the transmutation operators theory to Problem 4.5. To avoid the questions of the existence and uniqueness of solution specific to each problem, we will make the following assumption.

Assumption 2 *There exists a unique solution to Problem 4.5.*

The basic idea of a numerical method based on a CSS is that any linear combination of the functions from the CSS is already a solution to (4.6). Hence one may construct the linear combination that will satisfy (approximately) the boundary conditions of Problem 4.5. As was mentioned in the introduction, for many practical problems the boundary conditions are inconsistent resulting that the uniform norm is not a choice for measuring the quality of an approximate solution, and some kind of L_2 norm is more convenient. For this reason we will make the following assumption guaranteeing the proposed numerical method to work.

Assumption 3 *The solution to Problem 4.5 continuously depends on the boundary data in a suitable L_2 norm.*

Remark 4.8 *This problem includes as a special case the classical degenerate one dimensional Stefan problem. For these types of problems the dependence of the functions g_2 and g_3 on the function s and its derivatives can be specified—see Rose (1960) for example. For our method this does not represent additional difficulty. The definition of Problem 4.5 may also include additional conditions that can be necessary to guarantee the existence and the uniqueness of solution. We will see this in the example for the FHRO constructed further.*

4.3 Transmutation operators

In this section we present our main operational tool: the transmutation operator.

Definition 4.3 *Let E_1 and F_1 be linear subspaces of the linear topological spaces E and F, respectively. Consider the pair of operators $\mathbf{A} : E_1 \to E$ and $\mathbf{B} : F_1 \to F$. A linear invertible operator $\mathbf{T} : F \to E$ defined on the whole F is called a* ***transmutation operator*** *for the pair of operators $\mathbf{A}$ and $\mathbf{B}$ if the following conditions are met:*

1. *The operator $\mathbf{T}$ is continuous in F, its inverse $\mathbf{T}^{-1}$ is continuous in E;*

2. *$T(F_1) \subset E_1$;*

3. *The following operator equality is valid*

$$\mathbf{AT} = \mathbf{TB},$$

or which is the same

$$\mathbf{A} = \mathbf{TBT}^{-1}.$$

We are particularly interested in the case of $\mathbf{A}$ being the differential operator $\mathbf{C}$ defined in (4.4) and $\mathbf{B}$ being the second derivative. The idea is to transmute the solutions of the heat equation (4.1) into the solutions of the parabolic equation (4.6).[4.1] Throughout this section we consider equation (4.4) to be defined for $y \in [A, B]$, and Assumption 1 to hold on the segment $[A, B]$.

In the work of Kravchenko et al. (2016) and Kravchenko and Torba (2018) using the Liouville transformation

$$x = l(y) := \int_{A_0}^{y} (w(s)/p(s))^{1/2} ds, \qquad y \in [A, B],$$

where the point A_0 is chosen such that

$$\int_{A}^{A_0} (w(s)/p(s))^{1/2} ds = \int_{A_0}^{B} (w(s)/p(s))^{1/2} ds =: b,$$

the transmutation operator for the operators $\mathbf{C}$ and ∂_{xx} was studied, for the spaces $E_1 = C^2[A, B]$, $E = C[A, B]$, $F_1 = C^2[-b, b]$ and $F = C[-b, b]$.

Remark 4.9 *Equation* (4.6) *is a separable PDE, which implies that we only have to construct a one-dimensional transmutation operator for the operator* $\mathbf{C}$*.*

[4.1] As an illustration, let $h(x, t)$ be a solution of (4.1), then if the operator $\mathbf{T}$ exists, $u = \mathbf{T}h$ will be the solution to equation (4.6), indeed $\mathbf{C}u - u_t = \mathbf{CT}h - \partial_t \mathbf{T}h = \mathbf{T}(\partial_{yy} h - \partial_t h) = 0$.

The transmutation operator $\mathbf{T}$ is known in the closed form only for few equations (4.6). However as we will show for the construction of the CSS the knowledge of the operator $\mathbf{T}$ itself is not indispensable. This construction is based on the fundamental result Theorem 4.4 that connects the images of the transmutation operator to the family of the recursive integrals, that are called **formal powers**, see Definition 4.4 below.

Let us define an auxiliary function

$$\rho(y) = [p(y)\, w(y)]^{1/4}.$$

Let f be a non-vanishing (in general, complex-valued) solution of the equation

$$(p(y)\, f'(y))' - q(y)\, f(y) = 0, \qquad y \in [A, B], \tag{4.10}$$

with an initial condition set as

$$f(A_0) = \frac{1}{\rho(A_0)}. \tag{4.11}$$

Since p and q satisfy Assumption 1, equation (4.10) has two linearly independent regular solutions f_1 and f_2 whose zeros alternate. We may construct a non-vanishing solution as $f = f_1 + if_2$ —Kravchenko and Porter (2010, Remark 5)

Definition 4.4 *Let p, q, w satisfy Assumption 1 and let f be a non-vanishing solution of equation (4.10) that satisfies condition (4.11). Then, the associated formal powers are defined, for $k = 0, 1, 2, ...$, as*

$$\Phi_k(y) = \begin{cases} f(y)\, Y^{(k)}(y), & k \text{ odd} \\ f(y)\, \tilde{Y}^{(k)}(y), & k \text{ even} \end{cases}, \qquad \Psi_k(y) = \begin{cases} \frac{1}{f(y)} Y^{(k)}(y), & k \text{ even} \\ \frac{1}{f(y)} \tilde{Y}^{(k)}(y), & k \text{ odd} \end{cases},$$

where two families of the auxiliary functions are defined as

$$Y^{(0)}(y) \equiv \tilde{Y}^{(0)}(y) \equiv 1,$$

$$Y^{(k)}(y) = \begin{cases} k\int_{A_0}^{y} Y^{(k-1)}(s)\frac{1}{f^2(s)p(s)}ds, & k \text{ odd} \\ k\int_{A_0}^{y} Y^{(k-1)}(s) f^2(s) p(s) ds, & k \text{ even} \end{cases},$$

$$\tilde{Y}^{(k)}(y) = \begin{cases} k\int_{A_0}^{y} \tilde{Y}^{(k-1)}(s) f^2(s) p(s) ds, & k \text{ odd} \\ k\int_{A_0}^{y} \tilde{Y}^{(k-1)}(s)\frac{1}{f^2(s)p(s)}ds, & k \text{ even} \end{cases}.$$

Theorem 4.4 (Kravchenko et al. (2016)) *Let p, q and w satisfy Assumption 1 for all $y \in [A, B]$ and let f be a non-vanishing solution of equation* (4.10) *that satisfies condition* (4.11)*, then there exists a unique complex valued function K and the transmutation operator $\mathbf{T}$ defined as*

$$\mathbf{T}h(y) = \frac{h(l(y))}{\rho(y)} + \int_{-l(y)}^{l(y)} K(y,t)h(t)dt,$$

for $h \in C[-b, b]$ and satisfying the equality

$$\mathbf{CT}h = \mathbf{T}\partial_{xx}h,$$

for any $h \in C^2[-b, b]$ such that

$$\mathbf{T}[1] = f(y).$$

Moreover, for any $n \in N \cup \{0\}$

$$\mathbf{T}[x^n] = \Phi_n(y) \tag{4.12}$$

and for $u = \mathbf{T}h$ the following boundary conditions are satisfied

$$u(A_0) = \frac{h(0)}{\rho(A_0)} \tag{4.13}$$

$$u'(A_0) = h(0)f'(A_0) + h'(0)\frac{1}{\rho(A_0)}\sqrt{\frac{w(A_0)}{p(A_0)}}. \tag{4.14}$$

The theorem provides tools for computation of the transmuted powers. It was used directly in Kravchenko et al. (2017a) for the application of the Transmuted heat polynomials (THP) method to the Stefan-like problem. In this paper, we will use a different CSS.

Remark 4.10 *This transmutation operator $\mathbf{T}$ has the following important property. Consider a function $u = \mathbf{T}v$. Then the values $u(y)$ for $y \in [A_0, B]$ are completely determined by the function v and the values of p, q, w on the segment $[A_0, B]$ and are independent of the values of p, q, w on $[A, A_0)$. For this reason we may consider the restriction of equation (4.6) onto $[A_0, B]$ and the operator $\mathbf{T}$ as the operator mapping functions from $C[-b, b]$ to functions from $C[A_0, B]$. Such operator is no longer invertible, however it is continuous and maps a solution of the heat equation into a solution of (4.6) and is sufficient to present the proposed numerical method. Moreover, it allows one to take into account the boundary conditions (4.13) and (4.14). For that reason from now on we assume that $A_0 = A$ in the Liouville transformation, and when we need the invertibility of $\mathbf{T}$, we continue the coefficients p, q, w to the left arbitrarily asking only that Assumption 1 be fulfilled. Moreover, in the rest of the present paper we consider $A_0 = 0$.*

4.4 Transmutation of the complete systems of solutions

Let $D = \{(y,t) : y_1(t) < y < y_2(t), t \in (0,T]\}$, where $0 \le y_i(t) \le L$, $i \in \{1,2\}$, are continuous functions, be a subset of $\mathbb{R}^2$.

Definition 4.5 *The set of solutions* $\{u_n\}_{n\in\mathbb{N}}$ *of equation* (4.6) *is said to be a* ***complete system of solutions in the closed region*** $\bar{D}$ *if for any* $u \in C(\bar{D}) \cap C^{2,1}(D)$*, a solution to* (4.6)*, and for any* $\varepsilon > 0$ *there exist an integer* $N = N(\varepsilon)$ *and constants* $a_0, ..., a_N$ *such that*

$$\max_{(y,t)\in\bar{D}} \left|u(y,t) - u^N(y,t)\right| < \varepsilon,$$

where

$$u^N(y,t) = \sum_{n=0}^{N} a_n u_n(y,t). \tag{4.15}$$

The completeness of a system of functions in the sense of Definition 4.5 may be difficult to establish, and the following weaker form of the definition may be sufficient for practical applications.

Definition 4.6 *The set of solutions* $\{u_n\}_{n\in\mathbb{N}}$ *of equation* (4.6) *is said to be a* ***complete system of solutions*** *if for any* $u \in C^{2,1}(D)$*, a solution to* (4.6)*, for any compact subset* $K \subset D$ *and for any* $\varepsilon > 0$ *there exist an integer* $N = N(\varepsilon, K)$ *and constants* $a_0, ..., a_N$ *such that*

$$\max_{(y,t)\in K} \left|u(y,t) - u^N(y,t)\right| < \varepsilon.$$

The following proposition allows us, on the basis of the CSS for the heat equation, to construct the CSS for equation (4.6). Let

$$b = \int_0^L (w(s)/p(s))^{1/2} ds.$$

Proposition 4.3 *Let $\{v_n\}_{n\in\mathbb{N}}$ be a CSS for the heat equation on a rectangle $[-b, b] \times [\delta, T]$ for all sufficiently small $\delta > 0$. Consider the system of the transmuted functions $\{u_n\}_{n\in\mathbb{N}}$, i.e.*

$$u_n = \mathbf{T}[v_n], \tag{4.16}$$

where $\mathbf{T}$ is defined in Theorem 4.4 (see Remark 4.10). Then the system $\{u_n\}_{n\in\mathbb{N}}$ is a CSS for equation (4.6) *in D.*

Proof. 4.4 *Consider a continuation of the coefficients p, q, w onto $[-L_1, L]$ such that the Liouville transformation satisfies $l(-L_1) = l(L) = b$ and Assumption 1 holds on $[-L_1, L]$.*

Let $u(y, t) \in C^{2,1}(D)$ be a real valued solution to (4.6)*, $K \subset D$ a compact subset and $\varepsilon > 0$. Consider the preimage $u_l = l^{-1}(u)$ of the solution u under the Liouville transformation. Let $K_l = l^{-1}(K)$. Then there exist a constant $\delta > 0$ and functions $s_1(t)$ and $s_2(t)$, analytic on a disk in the complex plane containing the segment $[\delta, T]$ such that the domain $D(s_1, s_2) = \{(x, t) : s_1(t) \leq x \leq s_2(t),\, t \in [\delta, T]\}$ satisfies*

$$K_l \subset D(s_1, s_2) \subset [0, b] \times [0, T].$$

The solution u_l is a classical solution of the Liouville transformed parabolic equation in $D(s_1, s_2)$, continuous in $\bar{D}(s_1, s_2)$. Similarly to the proofs of Theorem 2.3.2 and 2.3.3 from Colton (1976) u_l can be extended to the solution of the same equation on the rectangle $[-b, b] \times [\delta, T]$, and its Liouville transformation (which we denote by $\tilde{u}$) is then a solution of (4.6) *on $[-L_1, L] \times [\delta, T]$.*

Consider $v = \mathbf{T}^{-1}\tilde{u}$. Then v is a solution of the heat equation on $[-b, b] \times [\delta, T]$. Since the system $\{v_n\}_{n\in\mathbb{N}}$ is a CSS for the heat equation on the region $[-b, b] \times [\delta, T]$, there *exist a constant N and such constants $a_0, \dots, a_N$ that*

$$\max_{(x,t)\in[-b,b]\times[\delta,T]} \left| v(x,t) - \sum_{n=0}^{N} a_n v_n(x,t) \right| < \frac{\varepsilon}{\|\mathbf{T}\|}.$$

Hence

$$\max_{(y,t)\in[-L_1,L]\times[\delta,T]} \left| \tilde{u}(y,t) - \sum_{n=0}^{N} a_n u_n(y,t) \right| = \max_{(y,t)\in[-L_1,L]\times[\delta,T]} \left| \mathbf{T}v(y,t) - \sum_{n=0}^{N} a_n \mathbf{T}v_n(y,t) \right|$$
$$< \frac{\varepsilon}{\|\mathbf{T}\|} \cdot \|\mathbf{T}\| = \varepsilon.$$

Now the proof follows observing that $K \subset [-L_1, L] \times [\delta, T]$.

Remark 4.11 *Note that the transmuted CSS defined by (4.16) does not depend on a continuation of the coefficients p, q, w*

Remark 4.12 *The technique developed in Colton (1976) and used in the proof of Proposition 4.3 requires the boundaries $y_{1,2}$ of the region to be separated, i.e., $y_1(t) < y_2(t)$, $t \in [0, T]$ and thus allows us to work with an approximation to the original problem in which $y_1(0) = y_2(0)$.*

The idea to use the transmutation operator to transmute the CSS for the construction of the solutions was studied in the monographs Colton (1976, 1980). At the time, the representation (4.12) for the transmuted powers and the representations of the next section were unknown, which limited the practical application of Colton's theory.

4.4.1 Transmutation of the exponential CSS

In the work of Kravchenko et al. (2017b) a representation for the solutions to equation

$$\mathbf{C}u = \omega^2 u,$$

was obtained in terms of Neumann series of Bessel functions. This representation can be used to construct a CSS for equation (4.6). Consider the set of functions $\{e_n^{\pm}\}_{n\in\mathbb{N}}$ defined in (4.2) where ω_n are chosen such that the limit (4.3) exists. The next proposition guarantees that it is in fact the CSS.

Let $D = \{(x,t) : s_1(t) < x < s_2(t),\ 0 < t < t_0\}$, where s_1 and s_2 are analytic functions of t for $0 \le t \le t_0$ and $s_1(t) < s_2(t)$ for $0 \le t \le t_0$.

Proposition 4.4 (Colton (1980, Cor. 5.4)) *Let $h \in C^{2,1}(D) \cap C(\bar{D})$ be a solution to the heat the equation (4.1) in D. Then there exists an integer N and constants $a_0^{\pm}, ..., a_N^{\pm}$ such that*

$$\max_{\bar{D}} \left| h(x,t) - \sum_{n=0}^{N} a_n^{\pm} e_n^{\pm}(x,t) \right| < \varepsilon.$$

Since under the change of the variable $t \mapsto t + \delta$ each function $e_n^{\pm}$ remains the same up to a multiplicative constant, the system $\{e_n^{\pm}\}_{n\in\mathbb{N}}$ is the CSS in the sense required for Proposition 4.3.

Each of the basis functions e_n is a solution to the heat equation (4.1). We define the transmuted basis functions as follows

$$E_n^{\pm}(y,t) = \mathbf{T}[e_n^{\pm}(x,t)] = e^{\omega_n^2 t}\mathbf{T}[e^{\pm i\omega_n x}].$$

Application of Theorem 4.4 guarantees us that they are solutions to equation (4.6), i.e.

$(\mathbf{C}-\partial_t)E_n^{\pm} = (\mathbf{C}\mathbf{T}e_n^{\pm} - \partial_t \mathbf{T}e_n^{\pm}) = \mathbf{T}(\partial_{xx}-\partial_t)e_n^{\pm} = 0$ and the application of Proposition 4.3 guarantees that they form a CSS for equation (4.6) on any compact contained in $[0, L] \times (0, T]$.

For the construction of functions $E_n^{\pm}$ we can use the explicit form of the transmuted solutions $\mathbf{T}[\cos(\omega x)]$ and $\mathbf{T}[\sin(\omega x)]$, since

$$\mathbf{T}[e^{\pm i\omega_n x}] = \mathbf{T}[\cos(\omega_n x)] \pm i\mathbf{T}[\sin(\omega_n x)],$$

presented in Kravchenko and Torba (2018).

4.4.2 Representation of the transmuted Sine and Cosine

Two linearly independent solutions of equation

$$\mathbf{C}u = \omega^2 u \tag{4.17}$$

can be obtained as images of $\cos \omega x$ and $\sin \omega x$, linearly independent solutions of the equation $z'' = \omega^2 z$, under the action of the transmutation operator $\mathbf{T}$, and will be denoted by

$$c(\omega, y) = \mathbf{T}[\cos(\omega x)], \qquad \text{with} \quad c(\omega, 0) = 1/\rho(0) \quad \text{and} \quad c'(\omega, 0) = \tilde{h}, \tag{4.18}$$

and

$$s(\omega, y) = \mathbf{T}[\sin(\omega x)], \qquad \text{with} \quad s(\omega, 0) = 0 \quad \text{and} \quad s'(\omega, 0) = \frac{\omega}{\rho(0)}\sqrt{\frac{w(0)}{p(0)}}, \tag{4.19}$$

where

$$\tilde{h} = \sqrt{\frac{\rho(0)}{w(0)}} \left(\frac{f'(0)}{f(0)} + \frac{\rho'(0)}{\rho(0)} \right)$$

and f is a solution of (4.10) that satisfies (4.11) and appears in Theorem 4.4.

Theorem 4.5 (Kravchenko and Torba (2018, Theorem 4.1)) *Let the functions p, q and w satisfy the conditions from the Assumption 1 and f be the solution of (4.10) satisfying (4.11) and such that $f \neq 0$ for all $y \in [0, L]$. Then two linearly independent solutions c and s of equation (4.17) for $\omega \neq 0$ can be written in the form*

$$c(\omega, y) = \frac{\cos(\omega l(y))}{\rho(y)} + 2 \sum_{m=0}^{\infty} (-1)^m \alpha_{2m}(y) j_{2m}(\omega l(y)) \tag{4.20}$$

and

$$s(\omega, y) = \frac{\sin(\omega l(y))}{\rho(y)} + 2 \sum_{m=0}^{\infty} (-1)^m \alpha_{2m+1}(y) j_{2m+1}(\omega l(y)), \tag{4.21}$$

where j_k stands for the spherical Bessel function of order k,

$$l(y) := \int_0^y (w(s)/p(s))^{1/2} \, ds,$$

with the coefficients defined by

$$\alpha_m(y) = \frac{2n+1}{2} \left(\sum_{k=0}^{m} \frac{l_{k,m} \Phi_k(y)}{l^k(y)} - \frac{1}{\rho(y)} \right), \tag{4.22}$$

where Φ_k are taken from Definition 4.4, and $l_{k,m}$ is the coefficient of x^k in the Legendre polynomial of order m. The solutions c and s satisfy the initial conditions (4.18) and (4.19). The series in (4.20) and (4.21) converge uniformly with respect to y on $[0, L]$ and converge uniformly with respect to ω on any compact subset of the complex plane of *the variable ω. Moreover, for the functions*

$$c^M(\omega,y)=\frac{\cos(\omega l(y))}{\rho(y)}+2\sum_{m=0}^{[M/2]}(-1)^m\alpha_{2m}(y)j_{2m}(\omega l(y))$$

and

$$s^M(\omega,y)=\frac{\sin(\omega l(y))}{\rho(y)}+2\sum_{m=0}^{[(M-1)/2]}(-1)^m\alpha_{2m+1}(y)j_{2m+1}(\omega l(y))$$

the following estimates hold

$$\begin{aligned}\left|c(\omega,y)-c^M(\omega,y)\right| &\leq \sqrt{2l(y)}\varepsilon_M(l(y))\max_{y\in[0,L]}\frac{1}{|\rho(y)|},\\ \left|s(\omega,y)-s^M(\omega,y)\right| &\leq \sqrt{2l(y)}\varepsilon_M(l(y))\max_{y\in[0,L]}\frac{1}{|\rho(y)|}\end{aligned}$$

for any $\omega\in\mathbb{R}$, $\omega\neq 0$, and

$$\begin{aligned}\left|c(\omega,y)-c^M(\omega,y)\right| &\leq \varepsilon_M(l(y))\sqrt{\frac{\sinh(2Cl(y))}{C}}\max_{y\in[0,L]}\frac{1}{|\rho(y)|},\\ \left|s(\omega,y)-s^M(\omega,y)\right| &\leq \varepsilon_M(l(y))\sqrt{\frac{\sinh(2Cl(y))}{C}}\max_{y\in[0,L]}\frac{1}{|\rho(y)|}\end{aligned}$$

for any $\omega\in\mathbb{C}$, $\omega\neq 0$ belonging to the strip $|\operatorname{Im}\omega|\leq C$, $C\geq 0$, where ε_M is a function satisfying $\varepsilon_M\to 0$, as $M\to\infty$.

Remark 4.13 *For $\omega=0$ the two linearly independent solutions can be represented as*

$$\begin{aligned}&c(0,y)=\mathbf{T}[1]=f(y),\\ &\tilde{s}(0,y)=\lim_{\omega\to 0}\mathbf{T}\left[\frac{\sin(\omega x)}{\omega}\right]=\mathbf{T}[x]=\Phi_1(y).\end{aligned}$$

We also have the representation for the derivatives of the solutions in (Kravchenko and

Torba, 2018, Section 5),

$$c'(\omega,y)=\sqrt{\frac{w(y)}{p(y)}}\left[\frac{1}{\rho(y)}(G_1(y)\cos(\omega l(y))-\omega\sin(\omega l(y)))+2\sum_{m=0}^{\infty}(-1)^m\mu_{2m}(y)j_{2m}(\omega l(y))\right]$$
$$-\frac{\rho'(y)}{\rho(y)}c(\omega,y)$$

and

$$s'(\omega,y)=\sqrt{\frac{w(y)}{p(y)}}\left[\frac{1}{\rho(y)}(G_2(y)\sin(\omega l(y))+\omega\cos(\omega l(y)))+2\sum_{m=0}^{\infty}(-1)^m\mu_{2m+1}(y)j_{2m+1}(\omega l(y))\right]$$
$$-\frac{\rho'(y)}{\rho(y)}s(\omega,y),$$

where

$$G_1\left(y\right)=G_2\left(y\right)+\tilde{h},\qquad G_2\left(y\right)=\left.\frac{\rho\rho'}{2w}\right|_0^y+\frac{1}{2}\int_0^y\left[\frac{q}{\rho^2}+\frac{\left(\rho'\right)^2}{w}\right](s)\,ds,$$

and

$$\begin{aligned}\mu_m(y):=\frac{2m+1}{2\rho(y)}\Bigg[\sum_{k=0}^{m}\frac{l_{k,m}}{l^k(y)}\left(k\frac{\Psi_{k-1}(y)}{\rho(y)}+\rho(y)\sqrt{\frac{p(y)}{w(y)}}\left(\frac{f'(y)}{f(y)}+\frac{\rho'(y)}{\rho(y)}\right)\Phi_k(y)\right)\\-\frac{m(m+1)}{2l(y)}-G_2(y)-\frac{\tilde{h}}{2}(1+(-1)^n)\Bigg].\end{aligned}\tag{4.23}$$

We can use Theorem 4.5 to represent the transmuted base functions and their derivatives as follows

$$E_n^{\pm}(y,t)=\left(c\left(\omega_n,y\right)\pm is(\omega_n,y)\right)e^{-\omega_n^2t},\tag{4.24}$$

$$\partial_y\left(E_n^{\pm}(y,t)\right)=\left(c'\left(\omega_n,y\right)\pm is'(\omega_n,y)\right)e^{-\omega_n^2t},\tag{4.25}$$

$$\partial_t\left(E_n^{\pm}(y,t)\right)=-\omega_n^2\left(c\left(\omega_n,y\right)\pm is(\omega_n,y)\right)e^{-\omega_n^2t}.\tag{4.26}$$

4.4.3 Recurrence formulas

The representations (4.22) and (4.23) are not practical for efficient computation of a large number of the coefficients due to the fast growth of the Legendre coefficients $l_{k,m}$ when $m \to \infty$. An alternative, robust for the computations recurrence formulas, were developed in Kravchenko and Torba (2018). We introduce

$$A_n(y) = l^n(y)\,\alpha_n(y) \qquad \text{and} \qquad B_n(y) = l^n(y)\,\mu_n(y), \tag{4.27}$$

and then the following formulas hold for $n = 2, 3, ...$

$$A_n(y) = \frac{2n+1}{2n-3}\left(l^2(y)\,A_{n-2}(y) + (2n-1)\,f(y)\,\tilde{\theta}_n(y)\right) \tag{4.28}$$

and

$$\begin{aligned} B_n(y) = \frac{2n+1}{2n-3}\Bigg[& l^2(y)B_{n-2}(y) + 2(2n-1)\left(\sqrt{\frac{p(y)}{w(y)}}\,(f'(y)\rho(y) + f(y)\rho'(y))\,\frac{\tilde{\theta}_n(y)}{\rho(y)}\right. \\ & \left. + \frac{\tilde{\eta}_n(y)}{\rho^2(y)f(y)}\right) - (2n-1)l(y)A_{n-2}(y)\Bigg], \end{aligned} \tag{4.29}$$

where

$$\tilde{\theta}_n(y) = \int_0^y \left(\frac{\tilde{\eta}_n(x)}{\rho^2(x)\,f^2(x)} - \frac{l(x)\,A_{n-2}(x)}{f(x)}\right)\sqrt{\frac{w(x)}{p(x)}}dx$$

and

$$\tilde{\eta}_n(y) = \int_0^y \left(l(x)(f'(x)\rho(x) + f(x)\rho'(x)) + (n-1)\rho(x)f(x)\sqrt{\frac{w(x)}{p(x)}}\right)\rho(x)A_{n-2}(x)dx.$$

The initial values A_0, A_1, B_0 and B_1 can be calculated from

$$A_0(y) = \frac{1}{2}\left(f(y) - \frac{1}{\rho(y)}\right), \qquad A_1(y) = \frac{3}{2}\left(\Phi_1(y) - \frac{l(y)}{\rho(y)}\right),$$

and

$$B_0(y) = \sqrt{\frac{p(y)}{w(y)}}\left(f'(y) + \frac{f(y)\rho'(y)}{\rho(y)}\right) - \frac{G_1(y)}{2\rho(y)},$$

$$B_1(y) = \frac{3}{2}\left[\frac{1}{f(y)\rho^2(y)} + \sqrt{\frac{p(y)}{w(y)}}\left(\frac{\rho'(y)}{\rho(y)} + \frac{f'(y)}{f(y)}\right)\Phi_1(y) - \frac{G_2(y)l(y)+1}{\rho(y)}\right].$$

For the discussion on the computational details see Kravchenko and Torba (2018) and Kravchenko et al. (2017b).

4.5 Minimization problem

In this section we describe the scheme of the numerical method proposed. In the previous section, we saw that any solution to the PDE (4.6) can be approximated by a linear combination of functions from the CSS of transmuted exponential functions. We denote by u^N this approximation and by a_n, $n \in \{0, \ldots, N\}$ the respective coefficients—see equation (4.15). Note that we reordered the set of the functions $E_n^{\pm}(y,t)$ into the sequence $\{u_n(y,t)\}_{n=0}^{\infty}$ by setting, e.g., $u_{2n} = E_n^+$ and $u_{2n+1} = E_n^-$. We also denote by $\bar{t} = (t_0, ..., t_{N_t})$ an ordered numerical set of $N_t + 1$ points on the interval $[0, T]$, with $t_0 = 0 < t_1 < ... < t_{N_t} = T$. Similarly, we construct the vector $\bar{y} = (y_0, ..., y_{N_y})$, on an interval $[y_0, y_{N_y}]$, the bounds will be specified further. We look for the free boundary in the form

$$s_K(t) = \sum_{k=0}^{K} b_k \beta_k(t), \tag{4.30}$$

where $\beta_k : [0,T] \to \mathbb{R}$, $k = 0, 1..., K$ is a set of $K + 1$ linearly independent functions.[4.2]

Recall that any expression of the form (4.15) is a solution to (4.6). Hence, our problem now reduces to finding the coefficients $\bar{a} = (a_0, ..., a_N)$ for the approximate solution and

[4.2] We can choose a more general representation for the boundary if needed. See Kravchenko et al. (2017a) for the discussion.

$\bar{b} = (b_0, ..., b_K)$ for the free boundary in such a way that the approximate solution is close to the exact solution of Problem 4.5. For this purpose, according to Assumption 3, it is sufficient to minimize the discrepancy for the boundary conditions (4.7)–(4.9) in a suitable L_2 norm. We consider the following one for each boundary condition

$$\|v(\bar{t})\|^2 = \|(v(t_0), ..., v(t_{N_t}))\|^2 = \sum_{i=0}^{N_t}{}'' |v(t_i)|^2 , \tag{4.31}$$

where the double prime indicates that the first and the last terms of the sum are to be halved. This formula is the discrete approximation for the L_2 norm on the segment $[0, T]$, and for different choices of the points t_k reduces either to trapezoidal rule (for uniformly distributed points t_k) or to the highly accurate Lobatto–Tchebyshev integration rule of the first kind (for t_k being Tchebyshev nodes), see (Davis and Rabinowitz, 1984, (2.7.1.14)). With this representation, the minimization problem that we have to solve takes the following form.

Problem 4.6 *Find* [4.3]

$$\arg\min_{(\bar{a},\bar{b})} F\left(\bar{a}, \bar{b}\right) ,$$

subject to

$$s_K(0) = 0, \qquad 0 < s_K(t) \leq L, \qquad t \in (0, T], \tag{4.32}$$

where

$$F\left(\bar{a}, \bar{b}\right) = \sum_{i=1}^{3} I_i^2 \left(\bar{a}, \bar{b}\right) \tag{4.33}$$

[4.3] For a function $f : X \to Y$, the $\arg\min$ over a subset S of X is defined as

$$\arg\min_{x\in S\subseteq X} f(x) := \{x : x \in S \wedge \forall y \in S : f(y) \geq f(x)\} .$$

and

$$
\begin{aligned}
I_1\left(\bar{a}, \bar{b}\right) &= \left\| \left[\mathbf{G}_2 u^N\right](0, \bar{t}) - g_1(\bar{t}) \right\|, \\
I_2\left(\bar{a}, \bar{b}\right) &= \left\| u^N\left(s_K\left(\bar{t}\right), \bar{t}\right) - g_2(\bar{t}) \right\|, \\
I_3\left(\bar{a}, \bar{b}\right) &= \left\| \left(u^N\right)_x\left(s_K\left(\bar{t}\right), \bar{t}\right) - g_3(\bar{t}) \right\|.
\end{aligned}
$$

The value of the function F indicates the discrepancy with the exact solution.

Remark 4.14 *For fixed $\bar{b}$, the constrained Problem 4.6 reduces to the unconstrained least squares minimization problem for the coefficients $\bar{a}$ and can be solved exactly. That is, for each $\bar{b}$ we can define*

$$
\bar{a}(\bar{b}) := \arg\min_{\bar{a}} F\left(\bar{a}, \bar{b}\right). \tag{4.34}
$$

So instead of minimizing the value function F over an $N+K+2$ dimensional space of parameters $(\bar{a}, \bar{b})$, the problem can be reduced to minimization of the function

$$
\tilde{F}(\bar{b}) := F\left(\bar{a}(\bar{b}), \bar{b}\right) \tag{4.35}
$$

over a $K+1$ dimensional space. This reformulation of the problem leads to a more robust convergence of the numerical method— see Herrera-Gomez and Porter (2017). We will apply this technique to the FHRO in Section 4.7—see also Kravchenko et al. (2017a) for details in the THP case.

At this point, we can schematize the algorithm for constructing an approximate solution to Problem 4.5 starting from the exponential series (4.2) as a CSS for the heat equation and transmuting it to CSS for equation (4.6).

4.5.1 Conceptual algorithm

(i) Find a particular solution f for the equation (4.10) that satisfies (4.11). The SPPS method of Kravchenko and Porter (2010) can be used or any alternative analytical or numerical method.

(ii) Compute the coefficients α_n and μ_n using the recursive formulas (4.27), (4.28), (4.29).

(iii) Choose a sequence ω_n satisfying (4.3) and construct the functions $E_n^{\pm}(y,t)$, $n = 0, \ldots, N$ and their derivatives by formulas (4.24)–(4.26).

(iv) Choose the basis functions $\beta_0, \ldots, \beta_{N_k}$ for the approximation of the free boundary function in the form (4.30).

(v) Construct the minimization function $\tilde{F}$ from equation (4.35).

(vi) Run a minimization algorithm for the function $\tilde{F}$ under constraints (4.32).

The application of the above schematics on the valuation of FHRO will be presented in the next section.

4.6 The Russian option

The FHRO is a theoretical path-dependent financial contract, a special case of an American lookback option. It was first introduced and studied in Shepp and Shiryaev (1993, 1995). The owner of the Russian option has the right, but not the obligation, to exercise it any time and receive the supremum of stock archived during the period between the writing of an option ($t = 0$) and the exercise time. Originally, the Russian option was defined as a perpetual option (infinite horizon $T = \infty$) of the "reduced regret"—Shepp and Shiryaev (1993) and Duffie et al. (1993). The problem of pricing this option complicates if we want to treat finite horizon cases ($\infty > T > 0$).

The case where the underlying asset movement is given by the geometric Brownian motion, i.e. pricing under the BSM model, was widely studied. For the infinite horizon, there is a closed form solution, that for convenience of the reader is presented in the Appendix. For the finite horizon, the theoretical results can be consulted for instance in Ekström (2004), Peskir (2005) and Duistermaat et al. (2005). The Bachelier model was analyzed in Kamenov (2008, 2014). In the latest work some theoretical results for more general models are also presented.

One way of solving this pricing problem is to show that it satisfies a certain free boundary problem for the parabolic PDE. For the BSM model there are several quantitative studies, e.g. Duistermaat et al. (2005) by the method referred to as nth-order randomization, based on a method proposed by Carr (1998) for American options, Kimura (2008) applying the Laplace-Carlson transform and Jeon et al. (2016) defining an equivalent PDE problem with mixed boundary conditions and solving it using Mellin transform. These methods rely on the possibility of explicit solving the respective transformed problems and hence are restricted to the BSM model.

4.6.1 The set-up of the FBP for FHRO

The value of the FHRO depends on three variables: price of the underlying asset (s), the maximum of the underlying asset (m) and time (z). As we will see further, it can be reduced to the FBP with only two variables, due to the homogeneity property of the value function. The definition of the problem that we follow is from Ekström (2004, Theorem 1) and Kimura (2008). An equivalent derivation can be consulted in

Duistermaat et al. (2005, Theorem 3), Peskir (2005) and Peskir and Shiryaev (2006, Section 26.2.5).

Under the risk neutral measure the FHRO at the time $z \in [0, T]$, with $T > 0$ being the time horizon of the option price, is given by

$$V(s, m, z) = \operatorname*{ess\,sup}_{0 \le \theta_z \le T - z} E_{s,m}\left[e^{-r\theta_z} M_{\theta_z}\right],$$

where

$$M_z = m \vee \sup_{0 \le u \le z} S_u, \qquad z \ge 0,$$

is the supremum process,

$$S_z = s \exp\left\{\left(r - \delta - \frac{1}{2}\sigma_0^2\right) z + \sigma_0 B_z\right\}, \qquad z \ge 0,$$

is the price process for the underlying asset, with: $S_0 = s$ – the initial fixed value; $r > 0$ – the risk free rate of interest; $\delta \ge 0$ – the continuous dividend rate; $\sigma_0 > 0$ – the volatility coefficient of the asset price; B_z – the one-dimensional standard Brownian motion on a filtered probability space $\left(\Omega, \mathbb{F}, (\mathcal{F}_z)_{z \ge 0}, \mathbb{Q}\right)$; $(\mathcal{F}_z)_{z \ge 0}$ – the filtration generated by B_z; $\mathbb{Q}$ – the probability measure chosen so that the stock has a mean of return r; θ_z – the stopping time of the filtration $\mathbb{F}$; $E_{s,m}[\cdot] \equiv E[\cdot \mid \mathcal{F}_0] = E[\cdot \mid S_0 = s, M_0 = m]$ is calculated under the risk neutral measure $\mathbb{Q}$. Also, we define the early exercise boundary

$$S(m, z) = \inf\{s \in [0, m] : (s, m, z) \in \mathcal{C}\},$$

where $\mathcal{C} = \{(s, m, z) : V(s, m, z) > m\}$ is the so called continuation region. The function $S(m, z)$ is non-decreasing and continuous in z for $\delta > 0$, see (Ekström, 2004, Theorem 2) and Duistermaat et al. (2005)).

Theorem 4.6 (Ekström (2004, Theorem 1)) *The value of the FHRO is a solution* $V(s,m,z)$ *of the following free boundary problem:*

$$V_z + \frac{\sigma_0^2}{2} s^2 V_{ss} + (r-\delta) s V_s - rV = 0 \qquad \textit{for} \quad S(m,z) < s \le m$$

with boundary conditions:

$$\begin{gathered} V(s,m,z) = m \qquad \textit{if} \quad S(m,z) \ge s, \\ \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left(V(s, s+\varepsilon, z) - V(s,s,z) \right) = 0, \\ V(s,s,z) = 0 \qquad \textit{on} \quad S(m,z) = s, \\ V_s\left(s,m,z\right) \le V(1,1,z), \\ V(s,m,T) = m. \end{gathered}$$

The homogeneity of the function V, that is

$$V(ks, km, z) = kV(s,m,z), \qquad \text{for all } k \in \mathbb{R}^+,$$

suggests that the problem is two dimensional. Consider the following change of the dependent variable

$$V(s,m,z) = mV\left(\frac{s}{m}, 1, z\right) =: mu\left(1-y, t\right),$$

where

$$y = 1 - s/m \qquad \text{and} \qquad t = T - z \tag{4.36}$$

are the new independent variables. Moreover, we also introduce the following notation for the free boundary

$$b(t) := 1 - S(m, T-z)/m.$$

Then the FBP problem for the FHRO under the BSM model can be written as follows.

Problem 4.7 *Find functions $u(y,t)$ and $b(t)$, a monotone non-decreasing function, such that*

$$-u_t + \mathbf{M}u = 0, \qquad \textit{for } b\,(t) > y \geq 0, t \in [0,T], \tag{4.37}$$

where

$$\mathbf{M} = \frac{1}{2}\sigma_0^2\,(1-y)^2\,\partial_{yy} - (r-\delta)\,(1-y)\,\partial_y - r, \tag{4.38}$$

and the boundary conditions

$$u\,(b\,(t)\,,t) = 1, \tag{4.39}$$

$$u_y\,(b\,(t)\,,t) = 0, \tag{4.40}$$

$$u\,(0,t) + u_y\,(0,t) = 0, \tag{4.41}$$

$$u_y(y,t) + u(0,t) \geq 0, \tag{4.42}$$

$$b\,(0) = 0 \tag{4.43}$$

are satisfied.

Problem 4.7 compared to Problem 4.5 has an additional condition (4.42). This condition has to be taken into account in the proposed algorithm. Problem 4.5 has non-consistent boundary conditions, i.e., it is impossible to satisfy all the boundary conditions simultaneously at the point $(0,0)$. Indeed, conditions (4.39) and (4.40) imply $u(0,0) + u_y(0,0) = 1$, a contradiction to the condition (4.41). This observation already leads us to expect the computational difficulties near the origin.

Remark 4.15 *The classical transformation can be used to reduce the differential operator M from (4.38) to pqw form (4.6)—see e.g. Polyanin (2001, Sections 0.4.1-3).*

Remark 4.16 Theoretical results for the free boundary, asymptotics at the origin and the infinite horizon case. *In the case of the infinite horizon (i.e., perpetual option) the problem can be solved exactly—see Shepp and Shiryaev (1993, 1995). For the sake of completeness we have included the solution in the Appendix. The infinite horizon is an important bound that we can use in the minimization process, since we know that the value of the FHRO should be lower.*

The free boundary can not have a smooth behaviour at the origin. This was confirmed by the theoretical result established in Ekström (2004) and Peskir (2005). The asymptotics as $t \to 0$ *is given by*

$$b(t) \sim \sigma_0 \sqrt{t\,|\log(1/t)|}. \tag{4.44}$$

4.7 Numerical experiments

In this section, we analyze the application of the proposed algorithm as well as the arising numerical issues and their solutions. The results confirm the convergence of the method as well as some numerical values that appear in the bibliography for Problem 4.7.

4.7.1 First steps

For the implementation details of the first two steps of the proposed algorithm, i.e., construction of a particular solution f and of the coefficients α_n and μ_n we refer the reader to Kravchenko et al. (2017b), Kravchenko and Torba (2018), Kravchenko et al. (2017a) and only want to mention that since the maximum upper boundary b_∞ is known—see Appendix 4.10.1, we only need values of $E_n^{\pm}(y)$ on the interval $[0, b_\infty]$. In our computations we have used this knowledge and chose the interval $[0, L]$ to be a bit larger than

$[0, b_\infty]$. All the functions involved were represented by their values on 10000 points uniform mesh.

4.7.2 The choice of $\{\omega_n\}$

The optimal choice for the set $\{\omega_n\}$ is an open question. Since the condition (4.3) is for the convergence at infinity, we have total liberty for the choice of the first finite number of ω's. The only exception is that the pair of solutions for $\omega = 0$ is constructed as a part of the representation for $c(\omega, y)$ and $s(\omega, y)$ from Theorem 4.5, see Remark 4.13. For this reason we always include $\omega_0 = 0$ in the set $\{\omega_n\}$ and from now on we assume that $0 = \omega_0 < \omega_1 < \ldots < \omega_N < \ldots$.

In the experiments, we used a pseudo-random algorithm to generate $\{\omega_n\}$ that depend on the set up step $d > 0$ and density Δ and works as follows: it starts with $\omega_0 = 0$ and set $\omega_{n+1} = \omega_n + r_n + d$, where r_n is a random number between 0 and Δ. In our experience, too few leads to less accurate approximation, too many leads to functions linearly dependent up to machine error and hence the difficulty in solving the related linear problems. The upper bound for $\{\omega_n\}$ can be easily established: it is set where the value of $e^{-\omega_n T}$ becomes too small, (e.g., we have considered $|\omega_n T| < 20$). And we found that about $50 - 100$ values of ω_n allow us to obtain sufficiently accurate results, further increase in the number of ω_n does not lead to noticeable improvement.

This arbitrariness of the choice allows to test the algorithm under different choices of ω_n, though its convergence to almost the same values is another confirmation of its robustness.

4.7.3 Reduced system of solutions

The value function is approximated by a truncated series

$$u_N(y,t) = \sum_{n=0}^{N} \hat{a}_n^{\pm} E_n^{\pm}(y) e^{-\omega_n^2 t},$$

where

$$E_n^{\pm}(y) = \mathbf{T}[e^{\pm i\omega_n x}].$$

Since we know the value at $x = 0$ of the solutions forming the CSS $\{E_n^{\pm}\}_{n\in\mathbb{N}}$ and their derivatives, we can use this information to modify the CSS into one that a priori satisfies the condition (4.41), that will be denoted by $\{\tilde{E}_n\}$, and construct an approximate solution in the form

$$u_N(y,t) = \sum_{n=0}^{N} a_n \tilde{E}_n(y) e^{-\omega_n^2 t}. \tag{4.45}$$

It is worthwhile mentioning that we do not have a completeness result for this modified system of solutions, nevertheless we appeal to Assumption 3 and proceed as follows. If we can find coefficients for an approximate solution of the form (4.45) such that the remaining boundary conditions (4.39) and (4.40) are satisfied sufficiently well, we stay with these coefficients, if not, we use the complete system of functions $\{E_n^{\pm}\}_{n\in\mathbb{N}}$. Performed numerical experiments showed that there was no accuracy advantage in utilizing the complete system $\{E_n^{\pm}\}_{n\in\mathbb{N}}$.

Each of the functions $\tilde{E}_n$ can be written as a linear combination

$$\tilde{E}_n(y) = c(\omega_n, y) + \beta_n s(\omega_n, y),$$

where β_n are constants such that the condition $\tilde{E}_n(0) + (\tilde{E}_n)_y(0) = 0$ is fulfilled and hence (4.41) is valid for the truncated series, i.e.,

$$u_N(0,t) + (u_N)_y(0,t) = 0.$$

Consequently, for $n > 0$, using (4.18) and (4.19) we obtain

$$\beta_n = -\frac{\big(1 + f'(0)\big)p(0)}{\omega_n\sqrt{\frac{w(0)}{p(0)}}}.$$

For $n = 0$, i.e. $\omega_0 = 0$, according to Remark 4.13, the condition for β_0 takes the form $c(0,0) + c'(0,0) + \beta_0\tilde{s}'(0,0) = 0$ and hence

$$\beta_0 = -\big(1 + \rho(0)f'(0)\big)\sqrt{\frac{p(0)}{w(0)}}.$$

Thus, the first function for the transmuted basis is given by

$$\tilde{E}_0(y) = f(y) + \beta_0\Phi_1(y).$$

The computation of the value function (4.33) requires the possibility to compute values of $\tilde{E}_n(y)$ at arbitrary point $y \in [0, L]$. For that we have approximated these functions by splines using the routine `spapi` in Matlab.

4.7.4 Representation of the free boundary

The boundary asymptotics (4.44) presented in Remark 4.16 possesses factor $\sqrt{t}$ and unbounded derivative at $t = 0$ suggesting that the polynomial approximation is not the best choice for the free boundary and that the following form

$$s_K(t) = \sqrt{t}\left(\sum_{k=0}^{K} b_k t^{k/2}\right) \tag{4.46}$$

may be better. For faster convergence of the minimization we have orthonormalized the set of functions $\{t^{k/2}\}_{k=1,\ldots,K+1}$, using the $L^2(0,T)$ norm. We have for any polynomials P_n and P_m

$$\int_0^T \sqrt{t}P_n(\sqrt{t}) \cdot \sqrt{t}P_m(\sqrt{t})\,dt = 2\int_0^{\sqrt{T}} t^3 P_n(t)P_m(t)\,dt.$$

The orthogonal polynomials on the segment $[0, \sqrt{T}]$ with the weight t^3 coincide up to a multiplicative constant with the Jacoby polynomials $P_n^{(0,3)}\left(\frac{2t}{\sqrt{T}} - 1\right)$, see (Szegö, 1975, (4.1.2)). Hence using the formula (4.3.3) from Szegö (1975) we obtain that the orthonormalized set consists of the functions

$$\beta_k(t) = \sqrt{\frac{(k+2)t}{4T}}P_k^{(0,3)}\left(2\sqrt{\frac{t}{T}} - 1\right), \qquad k = 0, \ldots, K.$$

For the computations $K = 9$ was used.

The grid $\bar{t}$ was taken to contain 2000 points and was selected to be less dense near $t = 0$ (the problematic point) and more dense near $t = T$. For that we selected the points t_n as a half of the Tchebyshev points, by the formula $t_n = T\sin(n\pi/(2N_t))$. The point $t_0 = 0$ was excluded due to inconsistency of the boundary conditions at this point. We would like to mention that the norm (4.31) under such selection of the points t_n can be reduced to Lobatto-Tchebyshev integration rule of the first kind, see (Davis and Rabinowitz, 1984, (2.7.1.14)). We would also like to mention that the uniform distribution for the points t_n worked almost equally well.

4.7.5 Solution of the least squares minimization problem (4.34)

For the fixed $\bar{\tilde{b}}$, the minimization Problem 4.6 reduces to an unconstrained least squares minimization problem (4.34) that can be solved exactly. This solution will be denoted by $\tilde{a}$. It can be constructed as follows. Under the notation

$$\tilde{s}_K(t) = \sum_{k=0}^{K} \tilde{b}_k \beta_k(t),$$

for the free boundary with fixed coefficients $\bar{\tilde{b}}$, the boundary conditions (4.39) and (4.40) take the form

$$\bar{1} = u_N(\tilde{s}(\bar{t}), \bar{t}) = \sum_{n=0}^{N} \tilde{a}_n \tilde{E}_n(\tilde{s}(\bar{t})) e^{\omega_n \bar{t}},$$
$$\bar{0} = (u_N)_y(\tilde{s}(\bar{t}), \bar{t}) = \sum_{n=0}^{N} \tilde{a}_n \tilde{E}_n'(\tilde{s}(\bar{t})) e^{\omega_n \bar{t}}.$$

The relations for $\tilde{a}$ can be written in the matrix form as

$$\mathbf{D}\tilde{a} = \mathbf{g}, \tag{4.47}$$

where

$$\mathbf{D} = \begin{bmatrix} \tilde{E}_0(\tilde{s}(\bar{t})) e^{\omega_0 \bar{t}} & \dots & \tilde{E}_N(\tilde{s}(\bar{t})) e^{\omega_0 \bar{t}} \\ \tilde{E}_0'(\tilde{s}(\bar{t})) e^{\omega_0 \bar{t}} & \dots & \tilde{E}_N'(\tilde{s}(\bar{t})) e^{\omega_0 \bar{t}} \end{bmatrix} \quad \text{and} \quad \mathbf{g} = \begin{pmatrix} \bar{1} \\ \bar{0} \end{pmatrix}$$

The solution of this overdetermined system coincides with the unique solution of a fully determined one—see Madsen and Nielsen (2010, Theorem 5.14), Lawson and Hanson (1995) or Nocedal and Wright (2006) for various methods of solution. Note that the linear problem (4.47) is ill-conditioned, meanwhile is better than the one appearing in relation with the generalized head polynomials, see Kravchenko et al. (2017a). As a result, we were able to work with approximations (4.45) containing as many as 100 functions $\tilde{E}_n$. However direct solution of the system (4.47) results in large coefficients in the solution vector $\tilde{a}$ and hence in large round-off errors in the resulting approximate solution (4.45). This can be easily solved by applying Tikhonov regularization to find a solution vector $\tilde{a}$ having relatively small coefficients. We have used the Matlab package `Regularization Tools` by Christian Hansen (see, e.g., Hansen (1994)) to implement the regularization.

4.7.6 Minimization process

Minimization of the function $\tilde{F}$ from (4.35) was done with the help of `fmincon` function from Matlab. As the initial guess for the free boundary we took $s_K = c\beta_0$, where a constant c was such that $s_K(T) < b_\infty$.

Two additional implementation details were somewhat unexpected to us however resulted in more robust convergence and lower resulting minimum value for the function $\tilde{F}$.

Fist, instead of minimizing the function $\tilde{F}$, we run the minimization process for the function $\sqrt{\tilde{F}}$. As a result, if in an experiment for the function $\tilde{F}$ the lowest value found by `fmincon` was $1.3 \cdot 10^{-4}$, when applied to the function $\sqrt{\tilde{F}}$ the returned minimum value for the function $\tilde{F}$ was $5 \cdot 10^{-9}$.

Second, the robustness of the minimization process as well as the returned minimal value may improve by posing additional constrains for the problem, letting somehow the function `fmincon` to avoid local minimums. The problem formulation possesses constrain (4.32) and additionally (see formulation of Problem 4.7) asks the free boundary to be monotone non-decreasing function, which can be written for our approximate boundary as

$$s'_K(t) \geq 0, \qquad 0 < t \leq T. \tag{4.48}$$

Additionally to these two natural constrains we considered the following one: we asked the free boundary to be a concave function, such form of the boundary can be see in Kimura (2008), Jeon et al. (2016). That is, in terms for our approximate boundary we posed additionally

$$s''_K(t) \leq 0, \qquad 0 < t \leq T. \tag{4.49}$$

This additional constrain resulted to produce excellent results. For different choices of the exponents $\{\omega_k\}$ and different initial guesses for the free boundary, minimization process always converged to very close results. We have tried to improve the minimum by using returned vector $\bar{b}$ as an initial guess and running minimization process without additional constrain (4.49) however with no success. Other standard ideas like to run the minimization process for a small K and reuse the returned vector padded with zeros as an initial guess for larger K do not produce significant improvements.

4.7.7 Numerical results presentation

There are several quantitative studies in the literature on the FHRO for the BSM model. We will mainly compare our results with the Laplace–Carlson transform method (LCM) from Kimura (2008) for the long horizon and with the recursive integration method (RIM) from Jeon et al. (2016) for the short horizon.[4.4] For the short horizon we have other values for the comparison, produced by the binomial tree model (BTM) and also reported in Jeon et al. (2016). We will refer as TES (transmuted exponential system) for the results produced by the proposed method

We start by presenting in Figure 4.2 the solution u, value option surface. As expected, it

[4.4] We would like to thank Junkee Jeon for providing us additional values that where not presented in their paper.

increases with time (recall that in our notation $t = 0$ is the option expiry) and in the initial value of the coefficient s/m. The condition (4.42) is satisfied. The cuts for the value of the option in time T, i.e. $(y, u(y, T))$ and the free boundary $(t, s_K(t))$ are presented in Figure 4.3. We have chosen the following standard parameters for the model: $r = 0.05$, $\delta = 0.03$ and $\sigma_0 = 0.3$.

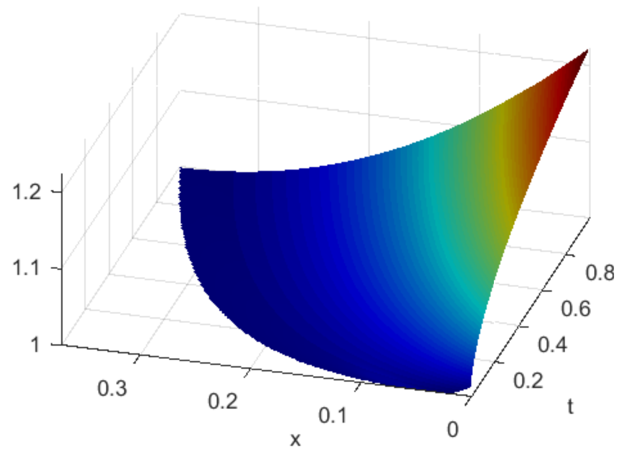

Figure 4.2: The value function for Problem 4.7, with parameters $r = 0.05$, $\delta = 0.03$, $\sigma_0 = 0.3$, $T = 1$.

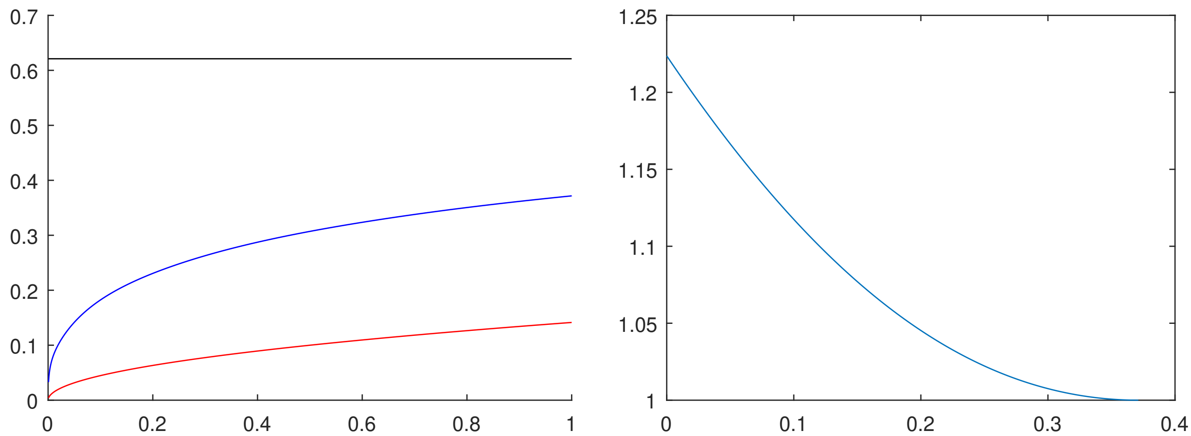

Figure 4.3: Left: the free boundary $s_K(t)$ (blue, upper), the initial boundary $s_{in} = 0.1\beta_0$ (red, lower) and the infinite horizon bound $b_\infty = 0.6211$ (top black line). Right: the value of the option, i.e. $u_N(y, T)$. Parameters (for both figures): $T = 1$, $\sigma = 0.3$, $\delta = 0.03$, $r = 0.05$, $N_t = 2001$, $K = 10$ and ω_n selected with a fixed step of $1/10$ and random step of $1/3$ (resulting in $N = 68$).

In Figure 4.4 the typical absolute errors that we obtain for the boundary conditions (4.39) and (4.40) are presented. Recall that condition (4.41) is satisfied by construction. In Figure 4.5 the typical absolute values of the coefficients $\bar{a}$ and $\bar{b}$ obtained by solving Problem 4.6 are presented. One can appreciate the smallness of the coefficients $\bar{a}$ due to the Tikhonov regularization and the rapid decrease in the coefficients $\bar{b}$ as the consequence of the applied orthonormalization.

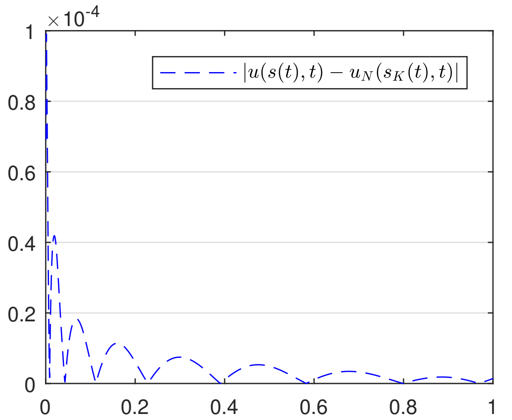

Figure 4.4: The typical approximation errors for the boundary conditions (4.39) and (4.40), with the same parameters as used to produce Figure 4.3.

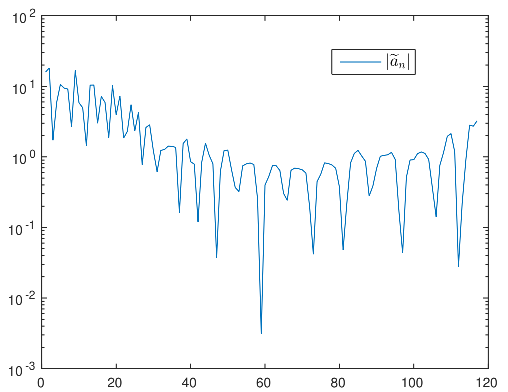

Figure 4.5: The typical absolute values of the coefficients $\tilde{a}$ and $\bar{b}$ for Problem 4.6, with the same parameters as used to produce Figure 4.3.

In Table 4.1 the values of the option for the different time horizons T are shown, bor-

	$u(0,T)$				$u(0.1,T)$				$u(0.2,T)$			
T	TES	LCM	BTM	RIM	TES	LCM	BTM	RIM	TES	LCM	BTM	RIM
1/3	1.1340		1.1324	1.1335	1.0462		1.0452	1.0454	1.0065		1.0062	1.0064
7/12	1.1744		1.1727	1.1742	1.0771		1.0761	1.0765	1.0208		1.0203	1.0203
1	1.2237	1.2188		1.2235	1.1175	1.1125			1.0453	1.0426		
2	1.3078				1.1891				1.0968			
5	1.4401	1.4228			1.3049	1.2890			1.1892	1.1741		
10	1.5508	1.5273			1.4029	1.3816			1.2712	1.2517		
40	1.6831				1.5208				1.3718			
100	1.6904				1.5273				1.3775			
∞	1.6904				1.5273				1.3769			

Table 4.1: Option value for Problem 4.7. The fixed parameters are $r = 0.05$, $\delta = 0.03$ and $\sigma_0 = 0.3$.

rowing the parameter configuration of Kimura (2008, Table 1) and Jeon et al. (2016, Table 1). One can appreciate an excellent agreement of the results produced by the proposed method with those delivered by the RIM and slightly worse agreement with the results produced by the BTM. The latter is due to the fact that even 10000 steps used is insufficient for the BTM to be precise to 4 figures. As for the results from Kimura (2008), there are two concerns. First, the method used in Kimura (2008) is based on the Laplace-Carlson transform and requires the option value to be defined for any $t \in (0, \infty)$ and to satisfy an equation similar to (4.37) for any $t > 0$. That is, a solution should have a continuation across the free boundary satisfying the same initial condition at $t = 0$. It is not clear why this rather strong assumption holds, and if not, how close is the obtained solution to the exact one. Second, the inversion of the Laplace-Carlson transform was computed by the Gaver-Stehfest method which is rather delicate to implement and can result in relative errors as high as several %, see Kuznetsov (2013) and references therein, no error analysis was presented. Nevertheless, our results are quite close to those of Kimura.

We can also observe from Table 4.1 that as T increases the algorithm converges to the infinite horizon value. For $T = 100$, we are already very close to the theoretical value of the perpetual option.

In Figure 4.6 the value of the option under different initial conditions is revealed. By the definition of y in (4.36) the option is more valuable if the initial supremum of the process is the same as the initial value of the underlying, i.e. $s/m = 1$. We present this curve under different financial parameters σ and r, that can be compared with Jeon et al. (2016, Figures 2 and 3).

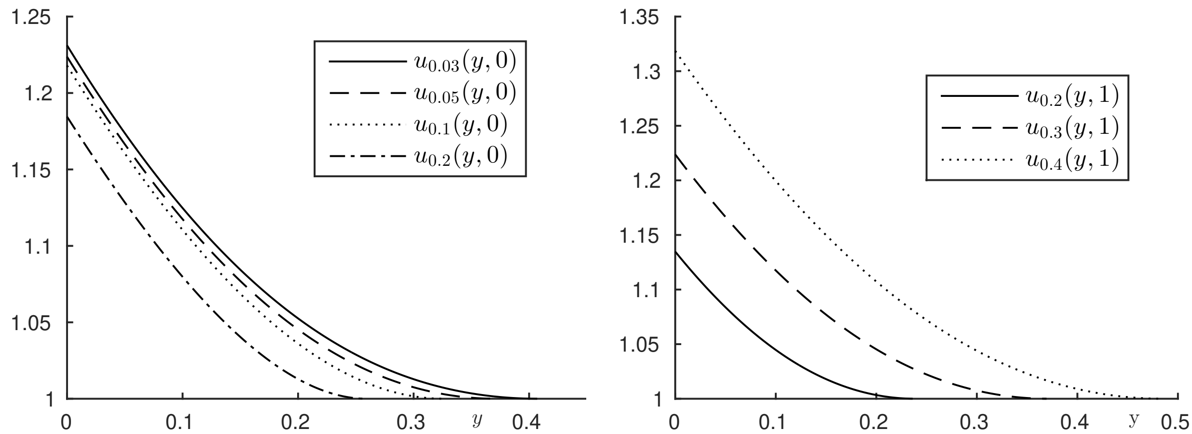

Figure 4.6: Option value under different initial conditions. The common parameters are $T = 1$, $\delta = 0.03$. Left: $r = 0.05$. Right: $\sigma_0 = 0.3$.

4.8 Final comments and future research

In summary, the proposed method has a lot of potential for further financial engineering applications possessing path-dependency and early exercise features such as look-back options, American options, etc. The method is not restricted to the BSM operator and can easily be applied to any other time-independent differential operator (4.4).

4.9 Acknowledgements

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4.10 Appendix

4.10.1 Russian option with infinite horizon under the BSM model

For the sake of completeness, we include the formula of Shepp and Shiryaev (1993) for the pricing of the perpetual Russian option. For $\delta > 0$, the upper boundary value is given by

$$b_\infty = 1 - \left(\frac{d_2(1-d_1)}{d_1(1-d_2)} \right)^{\frac{1}{d_1-d_2}},$$

where d_i, with $i \in 1, 2$, are the solutions to the quadratic equation

$$\frac{1}{2}\sigma^2 x^2 + (r - \delta - \frac{1}{2}\sigma^2)x - r = 0.$$

The value of the option is obtained from

$$u_\infty = \frac{1}{d_2 - d_1} \left\{ d_2 \left(\frac{s}{b_\infty} \right)^{d_1} - d_1 \left(\frac{s}{b_\infty} \right)^{d_2} \right\}.$$

The detailed analysis of this problem can be consulted in Peskir and Shiryaev (2006, Section VII, §26), Kimura (2008) and the references therein.

4.10.2 Transmuted heat polynomials

The heat polynomials are defined for $n \in \mathbb{N}$ as—see, e.g., Rosenbloom and Widder (1959) and Widder (1962),

$$h_n(x,t) = \sum_{k=0}^{[n/2]} c_k^n x^{n-2k} t^k,$$

where $[\cdot]$ denotes the entire part of the number and

$$c_k^n = \frac{n!}{(n-2k)!k!}.$$

The first five heat polynomials are

$$h_0(x,t) = 1, \quad h_1(x,t) = x, \quad h_2(x,t) = x^2 + 2t,$$
$$h_3(x,t) = x^3 + 6xt, \quad h_4(x,t) = x^4 + 12x^2 t + 12t^2.$$

The set of heat polynomials $\{h_n\}_{n \in \mathbb{N} \cup \{0\}}$ represents CSS for the heat equation

$$u_{xx} = u_t \tag{4.50}$$

on any domain $D(s)$ defined by (4.5)—see Colton and Watzlawek (1977).

Similarly to Kravchenko et al. (2017a), we will call the functions $H_n = \mathbf{T}[h_n]$ the **transmuted heat polynomials**[4.5]. As corollary of Theorem 4.4 we can show that H_n are solutions to equation (4.6), i.e., $(\mathbf{C} - \partial_t) H_n(y,t) = 0$. Moreover, the set $\{H_n\}_{n \in \mathbb{N}}$ is a CSS for (4.6) on any domain $D(s)$ defined by (4.5) due to Proposition 4.3 and the completeness of the system of heat polynomials Colton and Watzlawek (1977).

[4.5] In Kravchenko et al. (2017a) it is analyzed the case with $p \equiv 1$ and $r \equiv 1$.

Corollary 4.7 *The transmuted heat polynomials admit the following form*

$$H_n(y,t) = \sum_{k=0}^{[n/2]} c_k^n \Phi_{n-2k}(y)\, t^k. \tag{4.51}$$

Proof. 4.5 *This equality is an immediate corollary of Theorem 4.4. Indeed, we have* $H_n(x,t) = \mathbf{T}[h_n(x,t)] = \sum_{k=0}^{[n/2]} c_k^n \mathbf{T}[x^{n-2k}]t^k = \sum_{k=0}^{[n/2]} c_k^n \Phi_{n-2k}(y)\, t^k$*, where Theorem 4.4 is used.*

The explicit form (4.51) of the functions H_n allows the construction of the approximate solution to Problem 4.5 by the THP. The presented here is the extension of the results from Kravchenko et al. (2017a).

5. Final comments and future research

The thesis is composed by a set of three independent papers, and thus extended conclusions and contributions of each of them are referred in the text. In this section I concentrate on the importance of this study as whole.

The optimal stopping problems from mathematical finance can often be described as boundary problems for certain partial differential equation (PDE) or free boundary problems for PDE. Each of the chapters 2-4 presents a novel numerical method for the construction of an approximate solution using the transmutation operators in this type of problems. In chapter 2 it is considered a fixed boundary problem and in Chapters 3 and 4 are considered free boundary problems.

The methods have a strong theoretical background and the ability to numerically compute the corresponding solutions, which is often rare for this types of problems. They illustrate the potential of application of TO methods in the optimal stopping problems that appear in mathematical finance and other fields. For each analysed problem we were able to extend the pool of the applicable models and presented the numerical results that can be computed with at least state of the art precision.

For the DBKO, it was possible to extend the computational class of models to general time-homogeneous diffusion with an arbitrary default rate, opening the possibility to more realistic modelling of the market.

In the Stefan-like free boundary problem it was possible to step away from the classical case (heat equation) and compute the solution to the equation with potential. It is also worth mentioning that in this article was constructed an exact example that can be used by future researchers.

The ROFH paper shows that the method has the capacity to deal with problems that have non-consistent boundary conditions. For ROFH there was no agreement on the price of the option. The novel method for finding numerical solution under different horizon lengths was presented and has confirmed values that appeared in the literature for the short horizon and presenting the values for long horizons, setting this way a new benchmark for the problem.

The future research possibilities look promising. The constructed method for the ROFH can be applied to other path dependent options. It does not depend on any particular model, it should be possible to compute values for options under general time-independent diffusion models, such as American options, Asian options, etc. It is also very interesting to develop these constructions for singular models and have the opportunity to modulate the default scenarios. It might be possible to explore the knowledge of the form of the solution for estimating the implied model parameters from real data.

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