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Efficient Space-Time Spectral Methods for Second-Order Problems on Unbounded Domains

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Abstract In this paper, we propose efficient space-time spectral methods for problems on unbounded domains. For this purpose, we first introduce two series of new basis functions on the half/whole line by matrix decomposition techniques. The new basis functions are mutually orthogonal in both L^2 and H^1 inner products, and lead to diagonal systems for second order problems with constant coefficients. Then we construct efficient space-time spectral methods based on Laguerre/Hermite-Galerkin methods in space and dual-Petrov-Galerkin formulations in time for problems defined on unbounded domains. Using these suggested methods, higher accuracy can be obtained. We also demonstrate that the use of simultaneously orthogonal basis functions in space may greatly simplify the implementation of the space-time spectral methods.

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1 Introduction

The spectral method possesses high accuracy, and so plays an important role in numerical solutions of differential and integral equations, see [2–4,6,8,9,15,22] and the references therein. As we know, the Fourier system $\{e^{ikx}\}$ is the most desirable basis owing to the facts: (i) the availability of Fast Fourier transform (FFT); and (ii) the diagonal mass and stiff matrices under any linear differential operator with constant coefficients. However, it is well-known that the Fourier method is only suitable for periodic problems due to the Gibbs phenomena. For non-periodic problems, one has to select other kinds of orthogonal polynomials, e.g. Jacobi, Laguerre or Hermite polynomials as basis functions, which are the eigenfunctions of certain singular Sturm–Liouville problems.

During the past decades, more and more attentions were paid to various problems defined on unbounded domains. The Laguerre and Hermite spectral methods have been widely used for solving differential equations on unbounded (or even exterior) domains, see [12,13,18,19,21,24,29,30] and the references therein.

Laguerre/Hermite spectral-Galerkin methods with compact combinations of orthogonal systems (cf. [21]) lead to optimal algorithms in terms of both conditioning and finite banded structures of the linear systems. For example, the integrated Laguerre polynomial basis [21] leads to a diagonal stiffness matrix and penta-diagonal mass matrix for the differential operator $\mathcal{L}_\lambda[u] = u'' - \lambda^2 u$ (with constant λ and homogeneous Dirichlet boundary conditions). However, in many situations, it is more advantageous to use Fourier-like basis functions. In [23], a polynomial basis, which stems from Legendre polynomials and is mutually orthogonal in both L^2 and H^1 inner products, was constructed by solving discrete eigen-value problems on finite domains. Such an eigen-basis leads to efficient spectral-element approaches on structured meshes in [31]. The first objective of this paper is to find new kinds of Laguerre/Hermite basis functions which are simultaneously orthogonal in both L^2 and H^1 inner products and lead to diagonal systems for second order problems with constant coefficients on unbounded domains.

For the time-dependent PDEs, high-order spectral methods in space coupled with a low-order finite difference scheme in time always create a mismatch in accuracy. The accuracy in time usually results in a severe time step restriction which may be prohibitive for higher-order differential equations. Thus, for certain type of time-dependent PDEs, we should use spectral methods for both space and time. Space-time spectral methods were initially proposed in [26] for solving first order hyperbolic equation. They were further developed and analyzed for parabolic equations [7,23,25,27] and advection-diffusion problems [1]. More recently, space-time spectral methods were studied in detail for fractional equations. And we also note that space-time spectral methods were extended to spectral or *hp* finite element cases [20,32] for more flexibility. For more information, see [16,17,28] and the references therein. The main objective of this paper is to propose efficient space-time spectral methods for problems on unbounded domains. For this purpose, we construct simultaneously orthogonal Laguerre/Hermite basis functions on the half/whole line by matrix decomposition techniques, and then present efficient space-time spectral methods based on simultaneously orthogonal Laguerre/Hermite-Galerkin methods in space and a dual-Petrov-Galerkin formulation in time for problems defined on unbounded domains. Using the suggested methods, higher accuracy can be obtained. We also demonstrate that the use of simultaneously orthogonal Laguerre/Hermite basis functions in space may greatly simplify the implementation of the space-time spectral methods.

The rest of this paper is organized as follows. In the next section, we construct a new series of simultaneously orthogonal Laguerre functions on the half line, present the space-time spectral method for a time-dependent problem and derive an optimal error estimate. We also present some numerical results demonstrating the effectiveness of the proposed approach. In Sect. 3, a new series of simultaneously orthogonal Hermite functions on the whole line is given. As an example, we propose a new space-time spectral method for the Black–Scholes-type equation and present some numerical results showing the high accuracy of this new approach. The final section is for concluding remarks.

2 Simultaneously Orthogonal Basis Functions on the Half Line and Its Applications

Let $\Lambda = (0, +\infty)$ and $\chi(x)$ be certain a weight function. For integer $r \geq 0$, we define the weighted Sobolev space $H^r_\chi(\Lambda)$ in the usual way, with the inner product $(\cdot,\cdot)_{r,\chi,\Lambda}$, the semi-norm $|\cdot|_{r,\chi,\Lambda}$ and the norm $||\cdot||_{r,\chi,\Lambda}$. In particular, the inner product and the norm of $L^2_\chi(\Lambda)$ are denoted by $(\cdot,\cdot)_{\chi,\Lambda}$ and $\|\cdot\|_{\chi,\Lambda}$, respectively. For simplicity, we denote $\dfrac{d^k v}{dx^k}$ by $\partial_x^k v$. For integer $r \geq 1$,

$$ {}_0H^r_\chi(\Lambda) = \{v \in H^r_\chi(\Lambda) \mid \partial_x^k v(0) = 0,\ 0 \leq k \leq r-1\}. $$

We omit the subscript χ in notations whenever $\chi(x) \equiv 1$.

2.1 The Generalized Laguerre Functions

The generalized Laguerre polynomial of degree $l \geq 0$ is defined by (cf. [13])

$$ L_l^{(\alpha,\beta)}(x) = \frac{1}{l!} x^{-\alpha} e^{\beta x} \partial_x^l \left(x^{l+\alpha} e^{-\beta x} \right), \qquad \alpha > -1, \quad \beta > 0, \tag{2.1} $$

which is the l-th eigenfunction of the following Sturm–Liouville problem,

$$ \partial_x (x^{\alpha+1} e^{-\beta x} \partial_x v(x)) + \lambda_l x^\alpha e^{-\beta x} v(x) = 0 \tag{2.2} $$

with the eigenvalue $\lambda_l = \beta l$.

They satisfy the following relations,

$$ L_l^{(\alpha,\beta)}(x) = L_l^{(\alpha+1,\beta)}(x) - L_{l-1}^{(\alpha+1,\beta)}(x), \qquad l \geq 1, \tag{2.3} $$

$$ \partial_x L_l^{(\alpha,\beta)}(x) = -\beta L_{l-1}^{(\alpha+1,\beta)}(x), \qquad l \geq 1, \tag{2.4} $$

$$ -x\partial_x L_l^{(\alpha,\beta)}(x) = (l+\alpha) L_{l-1}^{(\alpha,\beta)}(x) - l L_l^{(\alpha,\beta)}(x), \qquad l \geq 1. \tag{2.5} $$

Let $\omega_{\alpha,\beta}(x) = x^\alpha e^{-\beta x}$. We have

$$ \int_\Lambda L_l^{(\alpha,\beta)}(x) L_{l'}^{(\alpha,\beta)}(x) \omega_{\alpha,\beta}(x) dx = \gamma_l^{(\alpha,\beta)} \delta_{l,l'}, \tag{2.6} $$

where $\delta_{l,l'}$ is the Kronecker function and

$$\gamma_l^{(\alpha,\beta)} = \frac{\Gamma(l+\alpha+1)}{\beta^{\alpha+1} l!}. \tag{2.7}$$

We next recall the generalized Laguerre functions. For any real number $\alpha > -1$ and $\beta > 0$, the generalized Laguerre functions are defined by (cf. [14])

$$\hat{L}_l^{(\alpha,\beta)}(x) = e^{-\frac{\beta}{2}x} L_l^{(\alpha,\beta)}(x), \qquad l \geq 0. \tag{2.8}$$

In particular, if $\alpha = 0$, we denote $\hat{L}_l^{\beta}(x) = \hat{L}_l^{(0,\beta)}(x)$.

From (2.2), the function $\hat{L}_l^{(\alpha,\beta)}(x)$ is the l-th eigenfunction of the following Sturm–Liouville problem,

$$\partial_x(x^{\alpha+1}e^{-\beta x}\partial_x(e^{\frac{\beta}{2}x}v(x))) + \lambda_l x^{\alpha} e^{-\frac{\beta}{2}x} v(x) = 0, \qquad l \geq 0. \tag{2.9}$$

Let $\omega_\alpha(x) = x^\alpha$. By virtue of (2.6), the set of $\hat{L}_l^{(\alpha,\beta)}(x)$ forms a complete $L^2_{\omega_\alpha}(\Lambda)$-orthogonal system, i.e.

$$\int_\Lambda \hat{L}_l^{(\alpha,\beta)}(x)\hat{L}_{l'}^{(\alpha,\beta)}(x)\omega_\alpha(x)dx = \gamma_l^{(\alpha,\beta)}\delta_{l,l'}. \tag{2.10}$$

Thus, for any $v \in L^2_{\omega_\alpha}(\Lambda)$, we have

$$v(x) = \sum_{l=0}^{\infty} \hat{v}_l^{(\alpha,\beta)} \hat{L}_l^{(\alpha,\beta)}(x) \tag{2.11}$$

with

$$\hat{v}_l^{(\alpha,\beta)} = \frac{1}{\gamma_l^{(\alpha,\beta)}} \int_\Lambda v(x)\hat{L}_l^{(\alpha,\beta)}(x)\omega_\alpha(x)dx. \tag{2.12}$$

Consider the following problem with homogeneous boundary conditions,

$$\begin{cases} -\partial_x^2 u(x) + u(x) = f(x), \quad x \in \Lambda, \\ u(0) = 0, \quad \lim\limits_{x\to+\infty} u(x) = 0. \end{cases} \tag{2.13}$$

We usually use compact combinations of generalized Laguerre functions, which lead to optimal algorithms in terms of both conditioning and finite banded structures of the linear systems. Let

$$\phi_k(x) = \hat{L}_k^{\beta}(x) - \hat{L}_{k+1}^{\beta}(x), \quad k \geq 0. \tag{2.14}$$

It is obvious that $\phi_k(0) = 0$. Let

$$V_M = \text{span}\{\phi_0, \phi_1, \ldots, \phi_{M-1}\},$$

where M is a positive integer.

The Laguerre spectral-Galerkin approximation to (2.13) is to find $u_M \in V_M$ such that

$$(\partial_x u_M, \partial_x \psi)_\Lambda + (u_M, \psi)_\Lambda = (f, \psi)_\Lambda, \quad \forall \psi \in V_M. \tag{2.15}$$

We denote

$$a_{jk} = (\phi_k, \phi_j)_\Lambda, \quad b_{jk} = (\partial_x\phi_k, \partial_x\phi_j)_\Lambda,$$

and introduce the matrices

$$\boldsymbol{A} = (a_{jk})_{0 \le k, j \le M-1}, \quad \boldsymbol{B} = (b_{jk})_{0 \le k, j \le M-1}.$$

By using the properties (2.3) and (2.4), we can deduce that $\boldsymbol{A}$ is a symmetric tridiagonal matrix, and $\boldsymbol{B} = \beta \boldsymbol{I}_M - \frac{\beta^2}{4}\boldsymbol{A}$ with $\boldsymbol{I}_M$ being the identity matrix of order M. Thus, the corresponding matrix of the scheme (2.15) is tridiagonal, but not an identity (or diagonal) matrix. In this section, our main aim is to construct new basis functions which lead to a diagonal matrix.

2.2 Simultaneously Orthogonal Laguerre Functions on the Half Line

Since the matrix $\boldsymbol{A}$ (associated with the basis $\{\phi_j\}$) is a symmetric tridiagonal matrix, we can easily compute its eigenpairs, which are all real and positive. Let $\boldsymbol{Q} = (q_{kj})_{k,j=0,\ldots,M-1}$ be the matrix formed by the orthogonal eigenvectors of $\boldsymbol{A}$ and $\boldsymbol{\Gamma} = diag(\{\gamma_i\}_{i=0}^{M-1})$ be the diagonal matrix with main diagonal being the corresponding eigenvalues, i.e.

$$\boldsymbol{A}\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{\Gamma}, \qquad \boldsymbol{Q}^t\boldsymbol{Q} = \boldsymbol{I}_M.$$

Since the matrix $\boldsymbol{Q}$ is nonsingular, the linear combination

$$\varphi_k(x) = \sum_{j=0}^{M-1} q_{jk}\phi_j(x), \qquad 0 \le k \le M-1 \tag{2.16}$$

forms a new basis of V_M satisfying the following properties,

$$(\varphi_l, \varphi_i)_\Lambda = \sum_{k,j=0}^{M-1} q_{kl}q_{ji}(\phi_k, \phi_j)_\Lambda = \sum_{k,j=0}^{M-1} q_{ji}a_{jk}q_{kl} = (\boldsymbol{Q}^t\boldsymbol{A}\boldsymbol{Q})_{il} = \gamma_i\delta_{il}, \tag{2.17}$$

$$\begin{aligned}(\partial_x\varphi_l, \partial_x\varphi_i)_\Lambda &= \sum_{k,j=0}^{M-1} q_{kl}q_{ji}(\partial_x\phi_k, \partial_x\phi_j)_\Lambda = \sum_{k,j=0}^{M-1} q_{ji}b_{jk}q_{kl} \\ &= \sum_{k,j=0}^{M-1} q_{ji}\left(\beta\delta_{jk} - \frac{\beta^2}{4}a_{jk}\right)q_{kl} = \left(\beta - \frac{\beta^2}{4}\gamma_i\right)\delta_{il}.\end{aligned} \tag{2.18}$$

From (2.17) and (2.18), we find that the new basis functions $\{\varphi_k\}_{k=0}^{M-1}$ is mutually orthogonal in both L^2 and H^1 inner products. In other words, the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ under this new basis $\{\varphi_k\}_{k=0}^{M-1}$ are both diagonal. An immediate consequence of (2.17)–(2.18) is that

$$(\partial_x\varphi_l, \partial_x\varphi_i)_\Lambda = \gamma_l^{-1}\left(\beta - \frac{\beta^2}{4}\gamma_l\right)(\varphi_l, \varphi_i)_\Lambda,$$

which implies

$$(\partial_x\varphi_l, \partial_x v)_\Lambda = \gamma_l^{-1}\left(\beta - \frac{\beta^2}{4}\gamma_l\right)(\varphi_l, v)_\Lambda, \quad \forall v \in V_M. \tag{2.19}$$

2.3 Applications for Two Dimensional Problems

As an illustrative example, we consider the following problem:

$$\begin{cases} -\Delta u + \alpha u = f, \qquad (x, y) \in \Sigma = \Lambda \times \Lambda, \\ u(0, y) = u(x, 0) = 0, \\ \lim\limits_{x \to +\infty} u(x, y) = \lim\limits_{y \to +\infty} u(x, y) = 0, \end{cases} \tag{2.20}$$

where the data α and f are given such that the above problem is well-posed.

Let $\{\varphi_k, \gamma_k\}$ be the same as before. Define the approximation space

$$\mathcal{V}_M = \mathrm{span}\{\varphi_k(x)\varphi_j(y) : 0 \le k, j \le M - 1\}. \tag{2.21}$$

Thus, the Laguerre-Galerkin spectral scheme for (2.20) is to find $u_M \in \mathcal{V}_M$ such that

$$(\nabla u_M, \nabla v)_\Sigma + \alpha(u_M, v)_\Sigma = (f, v)_\Sigma, \quad \forall v \in \mathcal{V}_M, \tag{2.22}$$

where the inner product on Σ is defined by

$$(u, v)_\Sigma = \int_\Sigma u(x, y)v(x, y)\mathrm{d}x\mathrm{d}y.$$

We expand the numerical solution as follows:

$$u_M(x, y) = \sum_{k,j=0}^{M-1} \tilde{u}_{kj}\varphi_k(x)\varphi_j(y).$$

Substituting the above equation into (2.22) and taking $v = \varphi_{k'}\varphi_{j'}$ with $k', j' = 0, 1, \ldots, M-1$, we get that

$$\begin{aligned} &\sum_{k,j=0}^{M-1} \tilde{u}_{kj}(\partial_x\varphi_k, \partial_x\varphi_{k'})_\Lambda(\varphi_j, \varphi_{j'})_\Lambda + \sum_{k,j=0}^{M-1} \tilde{u}_{kj}(\varphi_k, \varphi_{k'})_\Lambda(\partial_y\varphi_j, \partial_y\varphi_{j'})_\Lambda \\ &\quad + \alpha \sum_{k,j=0}^{M-1} \tilde{u}_{kj}(\varphi_k, \varphi_{k'})_\Lambda(\varphi_j, \varphi_{j'})_\Lambda = (f, \varphi_{k'}\varphi_{j'})_\Sigma, \qquad k', j' = 0, 1, \ldots, M-1. \end{aligned} \tag{2.23}$$

Denote

$$\begin{aligned} &a_{kk'} = (\varphi_k, \varphi_{k'})_\Lambda, && \boldsymbol{A} = (a_{kk'})_{0 \le k,k' \le M-1}, \\ &b_{kk'} = (\partial_x\varphi_k, \partial_x\varphi_{k'})_\Lambda, && \boldsymbol{B} = (b_{kk'})_{0 \le k,k' \le M-1}, \\ &f_{k'j'} = (f, \varphi_{k'}\varphi_{j'})_\Sigma, && \boldsymbol{F} = (f_{k'j'})_{0 \le k',j' \le M-1}, \\ &\boldsymbol{U} = (\tilde{u}_{kj})_{0 \le k,j \le M-1}. \end{aligned}$$

Then, the above system (2.23) can be rewritten in the following compact form,

$$(\alpha \boldsymbol{A}\boldsymbol{U}\boldsymbol{A}^t + \boldsymbol{B}\boldsymbol{U}\boldsymbol{A}^t + \boldsymbol{A}\boldsymbol{U}\boldsymbol{B}^t) = \boldsymbol{F}. \tag{2.24}$$

Rewrite (2.24) in the following form of tensor product,

$$(\alpha \boldsymbol{A} \otimes \boldsymbol{A}^t + \boldsymbol{B} \otimes \boldsymbol{A}^t + \boldsymbol{A} \otimes \boldsymbol{B}^t)\vec{u} = \vec{f}, \tag{2.25}$$

where

$$\begin{aligned}\vec{u} &= (\tilde{u}_{00}, \tilde{u}_{10}, \dots, \tilde{u}_{M-1,0};\\ &\quad \tilde{u}_{01}, \tilde{u}_{11}, \dots \tilde{u}_{M-1,1}; \dots; \tilde{u}_{0,M-1}, \tilde{u}_{1,M-1}, \dots, \tilde{u}_{M-1,M-1})^t,\\ \vec{f} &= (f_{00}, f_{10}, \dots, f_{M-1,0};\\ &\quad f_{01}, f_{11}, \dots, f_{M-1,1}; \dots; f_{0,M-1}, f_{1,M-1}, \dots, f_{M-1,M-1})^t.\end{aligned} \tag{2.26}$$

Remark 2.1 In the algebraic system, the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are both diagonal. Therefore, this algorithm is easily implemented.

2.4 An Efficient Space-Time Laguerre-Legendre Spectral Method

In this subsection, we propose an efficient space-time spectral method based on Laguerre-Legendre Galerkin method using simultaneously orthogonal functions (2.16) in space and a dual-Petrov-Legendre-Galerkin formulation in time.

For simplicity, we consider the following time-dependent problem, and shift the time interval to $I = (-1, 1)$:

$$\begin{cases}\partial_t u(x,t) - \partial_x^2 u(x,t) + u(x,t) = f(x,t), \quad (x,t) \in \Omega_1 = \Lambda \times I,\\ u(0,t) = 0, \ \lim\limits_{x\to+\infty} u(x,t) = 0, \quad t \in (-1, 1],\\ u(x,-1) = u_0(x), \quad x \in \Lambda,\end{cases} \tag{2.27}$$

where $\Lambda = (0, +\infty)$ and f is a given function. Without loss of generality, we assume that $u_0 = 0$.

Let

$$\begin{aligned}S &= \{u \mid u \in C(I) \text{ and } u(-1) = 0\},\\ S^* &= \{u \mid u \in C(I) \text{ and } u(1) = 0\},\\ Q &= {}_0H^1(\Lambda) \otimes S, \quad \tilde{Q} = {}_0H^1(\Lambda) \otimes S^*.\end{aligned}$$

The weak formulation of the problem (2.27) is to find $u \in Q$ such that

$$(\partial_t u, v)_{\Omega_1} + (\partial_x u, \partial_x v)_{\Omega_1} + (u, v)_{\Omega_1} = (f, v)_{\Omega_1}, \quad \forall v \in \tilde{Q}. \tag{2.28}$$

Here, the space $L^2_\omega(\Omega_1)$ is defined as usual, with the inner product $(u, v)_{\omega,\Omega_1}$ and the norm $\|u\|_{\omega,\Omega_1}$.

We introduce the following finite-dimensional spaces

$$\begin{aligned}V_M &= {}_0H^1(\Lambda) \cap \tilde{\mathcal{P}}_M(\Lambda), \quad S_N = S \cap \mathcal{P}_N(I), \quad S_N^* = S^* \cap \mathcal{P}_N(I),\\ Q_{M,N} &= V_M \otimes S_N, \quad \tilde{Q}_{M,N} = V_M \otimes S_N^*,\end{aligned}$$

where $\mathcal{P}_N(I)$(resp. $\mathcal{P}_M(\Lambda)$) respect the space of polynomials of degree $\leq N$ on I (resp. of degree $\leq M$ on Λ), and $\tilde{\mathcal{P}}_M(\Lambda) = \{e^{-\frac{\beta}{2}x} v \mid v \in \mathcal{P}_M(\Lambda)\}$.

The spectral scheme of the problem (2.27) is to seek $u_{MN} \in Q_{M,N}$ such that

$$(\partial_t u_{MN}, \varphi)_{\Omega_1} + (\partial_x u_{MN}, \partial_x \varphi)_{\Omega_1} + (u_{MN}, \varphi)_{\Omega_1} = (f, \varphi)_{\Omega_1}, \quad \forall \varphi \in \tilde{Q}_{M,N}. \tag{2.29}$$

Since for any $\phi \in S_N$, we have $\dfrac{1-t}{1+t}\phi \in S_N^*$. Hence, the scheme (2.29) can be rewritten as the following weighted Galerkin formulation:

$$\begin{aligned}&(\partial_t u_{MN}, \phi)_{\chi^{1,-1},\Omega_1} + (\partial_x u_{MN}, \partial_x \phi)_{\chi^{1,-1},\Omega_1} + (u_{MN}, \phi)_{\chi^{1,-1},\Omega_1}\\ &\quad = (f, \phi)_{\chi^{1,-1},\Omega_1}, \quad \forall \phi \in Q_{M,N},\end{aligned} \tag{2.30}$$

where $\chi^{a,b}(t) = (1-t)^a(1+t)^b$ is the Jacobi weight function.

Remark 2.2 We shall find that the formulation (2.29) is most suitable for numerical implementation, and the weighted Galerkin formulation (2.30) is more convenient for error analysis.

2.5 Convergence Analysis

We first define the orthogonal projection in space ${}_0\pi^1_{M,\beta} : {}_0H^1(\Lambda) \to V_M$ as follows,

$$(\partial_x({}_0\pi^1_{M,\beta}v - v), \partial_x\phi)_\Lambda = 0, \qquad \forall \phi \in V_M. \tag{2.31}$$

As a specific case of Theorem 3.3 in [11], we have the following lemma.

Lemma 2.1 *If* $v \in {}_0H^1(\Lambda)$, $\partial_x^r(e^{\frac{\beta}{2}x}v) \in L^2_{\omega_{-1+r,\beta}}(\Lambda)$, *and integers* $1 \le r \le M+1$, *then*

$$\|\partial_x({}_0\pi^1_{M,\beta}v - v)\|_\Lambda \le c(\beta M)^{\frac{1-r}{2}}\|\partial_x^r(e^{\frac{\beta}{2}x}v)\|_{\omega_{-1+r,\beta},\Lambda}. \tag{2.32}$$

Following the same line of the proof of Theorem 3.3 in [11], we can derive that

$$\|{}_0\pi^1_{M,\beta}v - v\|_\Lambda \le c(\beta M)^{-\frac{r}{2}}\|\partial_x^r(e^{\frac{\beta}{2}x}v)\|_{\omega_{-1+r,\beta},\Lambda}. \tag{2.33}$$

We now introduce the orthogonal projection in time $P_N^{0,-1} : L^2_{\chi^{0,-1}}(I) \to S_N$, defined by

$$(P_N^{0,-1}v - v, \phi)_{\chi^{0,-1},I} = 0, \qquad \forall \phi \in S_N. \tag{2.34}$$

Denote

$$\hat{H}^1(I) = H^1(I) \cap L^2_{\chi^{0,-2}}(I).$$

It is clear that for any $\psi \in S_N^*$, we have $\chi^{0,1}\partial_t\psi \in S_N$. This, along with the definition (2.34), gives that for any $v \in \hat{H}^1(I)$ and $\psi \in S_N^*$,

$$\left(\partial_t\left(P_N^{0,-1}v - v\right), \psi\right)_I = -\left(P_N^{0,-1}v - v, \chi^{0,1}\partial_t\psi\right)_{\chi^{0,-1},I} = 0. \tag{2.35}$$

Consequently, we have the following approximation results from Theorem 1.1 in [10].

Lemma 2.2 *If* $v \in L^2_{\chi^{0,-1}}(I)$ *and* $\partial_t^s v \in L^2_{\chi^{s,s-1}}(I)$, *then*

$$||\partial_t^l\left(P_N^{0,-1}v - v\right)||_{\chi^{l,l-1},I} \lesssim N^{l-s}||\partial_t^s v||_{\chi^{s,s-1},I}, \quad l \le s, \quad l = 0, 1. \tag{2.36}$$

We next consider the convergence of the proposed scheme (2.29). Let u and u_{MN} be the solutions of (2.27) and (2.29), respectively, and

$$U_{MN} = P_N^{0,-1}{}_0\pi^1_{M,\beta}u = {}_0\pi^1_{M,\beta}P_N^{0,-1}u.$$

From (2.28) we obtain that

$$\begin{aligned}&(\partial_t U_{MN}, \varphi)_{\Omega_1} + (\partial_x U_{MN}, \partial_x\varphi)_{\Omega_1} + (U_{MN}, \varphi)_{\Omega_1} = (f, \varphi)_{\Omega_1}\\ &\quad + (\partial_t(U_{MN} - u), \varphi)_{\Omega_1} + (\partial_x(U_{MN} - u), \partial_x\varphi)_{\Omega_1} + (U_{MN} - u, \varphi)_{\Omega_1}.\end{aligned} \tag{2.37}$$

Set $e_{MN} = U_{MN} - u_{MN}$. By subtracting (2.37) from (2.29), we further derive that

$$\begin{aligned}&(\partial_t e_{MN}, \varphi)_{\Omega_1} + (\partial_x e_{MN}, \partial_x\varphi)_{\Omega_1} + (e_{MN}, \varphi)_{\Omega_1}\\ &\quad = (\partial_t(U_{MN} - u), \varphi)_{\Omega_1} + (\partial_x(U_{MN} - u), \partial_x\varphi)_{\Omega_1} + (U_{MN} - u, \varphi)_{\Omega_1}.\end{aligned} \tag{2.38}$$

Due to (2.35) and (2.31), we deduce readily that

$$\begin{aligned}(\partial_t(U_{MN}-u),\varphi)_{\Omega_1} &= (\partial_t({}_0\pi^1_{M,\beta}u-u),\varphi)_{\Omega_1},\\ (\partial_x(U_{MN}-u),\partial_x\varphi)_{\Omega_1} &= (\partial_x(P_N^{0,-1}u-u),\partial_x\varphi)_{\Omega_1}.\end{aligned}$$

Therefore, the equation (2.38) can be simplified to

$$\begin{aligned}&(\partial_t e_{MN},\varphi)_{\Omega_1}+(\partial_x e_{MN},\partial_x\varphi)_{\Omega_1}+(e_{MN},\varphi)_{\Omega_1}\\ &\quad=(\partial_t({}_0\pi^1_{M,\beta}u-u),\varphi)_{\Omega_1}+(\partial_x(P_N^{0,-1}u-u),\partial_x\varphi)_{\Omega_1}+(U_{MN}-u,\varphi)_{\Omega_1}.\end{aligned}\tag{2.39}$$

Taking $\varphi=\frac{1-t}{1+t}e_{MN}\in\tilde{Q}_{M,N}$ in the above equation, due to the fact

$$(\partial_t e_{MN},e_{MN})_{\chi^{1,-1},\Omega_1}=\frac{1}{2}\int_{\Omega_1}(\partial_t e^2_{MN})\chi^{1,-1}dtdx=||e_{MN}||^2_{\chi^{0,-2},\Omega_1},$$

we derive from the Cauchy–Schwartz inequality that

$$\begin{aligned}&||e_{MN}||_{\chi^{0,-2},\Omega_1}+||\partial_x e_{MN}||_{\chi^{1,-1},\Omega_1}+||e_{MN}||_{\chi^{1,-1},\Omega_1}\\ &\quad\lesssim||\partial_t\left({}_0\pi^1_{M,\beta}u-u\right)||_{\chi^{2,0},\Omega_1}+||\partial_x\left(P_N^{0,-1}u-u\right)||_{\chi^{1,-1},\Omega_1}\\ &\qquad+||U_{MN}-u||_{\chi^{1,-1},\Omega_1}.\end{aligned}\tag{2.40}$$

Moreover, by Lemmas 2.1 and 2.2, we get that for integers $2\le r\le M+2$ and $s\ge 0$,

$$||\partial_t\left({}_0\pi^1_{M,\beta}u-u\right)||_{\chi^{2,0},\Omega_1}\lesssim(\beta M)^{\frac{1-r}{2}}||\partial_t\partial_x^{r-1}\left(e^{\frac{\beta x}{2}}u\right)||_{L^2_{\chi^{2,0}}(I;L^2_{\omega_{-2+r,\beta}}(\Lambda))},\tag{2.41}$$

$$||\partial_x\left(P_N^{0,-1}u-u\right)||_{\chi^{1,-1},\Omega_1}\lesssim||\partial_x\left(P_N^{0,-1}u-u\right)||_{\chi^{0,-1},\Omega_1}\lesssim N^{-s}||\partial_t^s\partial_x u||_{L^2_{\chi^{s,s-1}}(I;L^2(\Lambda))},\tag{2.42}$$

and

$$\begin{aligned}&||U_{MN}-u||_{\chi^{1,-1},\Omega_1}\\ &\quad\lesssim||P_N^{0,-1}({}_0\pi^1_{M,\beta}u-u)||_{\chi^{0,-1},\Omega_1}+||P_N^{0,-1}u-u||_{\chi^{0,-1},\Omega_1}\\ &\quad\lesssim||{}_0\pi^1_{M,\beta}u-u||_{\chi^{0,-1},\Omega_1}+||P_N^{0,-1}u-u||_{\chi^{0,-1},\Omega_1}\\ &\quad\lesssim(\beta M)^{\frac{1-r}{2}}||\partial_x^{r-1}(e^{\frac{\beta x}{2}}u)||_{L^2_{\chi^{0,-1}}(I;L^2_{\omega_{-2+r,\beta}}(\Lambda))}+N^{-s}||\partial_t^s u||_{L^2_{\omega^{s,s-1}}(I;L^2(\Lambda))}.\end{aligned}\tag{2.43}$$

For notional convenience, we introduce the spaces $A^r(\Omega_1)$ and $B^s(\Omega_1)$ associated with the norms as follows,

$$\begin{aligned}||u||_{A^r(\Omega_1)}=&\left(||\partial_t\partial_x^{r-1}\left(e^{\frac{\beta x}{2}}u\right)||^2_{L^2_{\chi^{2,0}}\left(I;L^2_{\omega_{-2+r,\beta}}(\Lambda)\right)}+||\partial_x^{r-1}\left(e^{\frac{\beta x}{2}}u\right)||^2_{L^2_{\chi^{0,-1}}\left(I;L^2_{\omega_{-2+r,\beta}}(\Lambda)\right)}\right.\\ &\left.+||\partial_x^{r}\left(e^{\frac{\beta x}{2}}u\right)||^2_{L^2_{\chi^{1,-1}}\left(I;L^2_{\omega_{-1+r,\beta}}(\Lambda)\right)}\right)^{\frac{1}{2}},\\ ||u||_{B^s(\Omega_1)}=&\left(||\partial_t^s\partial_x u||^2_{L^2_{\chi^{s,s-1}}(I;L^2(\Lambda))}+||\partial_t^s u||^2_{L^2_{\chi^{s,s-1}}(I;L^2(\Lambda))}\right)^{\frac{1}{2}}.\end{aligned}$$

Then, a combination of (2.40)–(2.43) leads to

$$||e_{MN}||_{\chi^{0,-2},\Omega_1}+||\partial_x e_{MN}||_{\chi^{1,-1},\Omega_1}\lesssim N^{-s}||u||_{B^s(\Omega_1)}+(\beta M)^{\frac{1-r}{2}}||u||_{A^r(\Omega_1)}.$$

On the other hand, using (2.42), Lemmas 2.1 and 2.2 again yields

$$\begin{aligned}||\partial_x(u-U_{MN})||_{\chi^{1,-1},\Omega_1} &\lesssim ||\partial_x({}_0\pi^1_{M,\beta}u-u)||_{\chi^{1,-1},\Omega_1}+||\partial_x {}_0\pi^1_{M,\beta}(P_N^{0,-1}u-u)||_{\chi^{1,-1},\Omega_1}\\ &\lesssim ||\partial_x({}_0\pi^1_{M,\beta}u-u)||_{\chi^{1,-1},\Omega_1}+||\partial_x(P_N^{0,-1}u-u)||_{\chi^{1,-1},\Omega_1}\\ &\lesssim (\beta M)^{\frac{1-r}{2}}||\partial_x^r(e^{\frac{\beta x}{2}}u)||_{L^2_{\chi^{1,-1}}\left(I;L^2_{\omega_{-1+r,\beta}}(\Lambda)\right)}\\ &\quad +N^{-s}||\partial_t^s\partial_x u||_{L^2_{\chi^{s,s-1}}(I;L^2(\Lambda))},\end{aligned}$$

and

$$\begin{aligned}||u-U_{MN}||_{\chi^{0,-1},\Omega_1} &\lesssim ||P_N^{0,-1}({}_0\pi^1_{M,\beta}u-u)||_{\chi^{0,-1},\Omega_1}+||P_N^{0,-1}u-u||_{\chi^{0,-1},\Omega_1}\\ &\lesssim (\beta M)^{\frac{1-r}{2}}||\partial_x^{r-1}(e^{\frac{\beta x}{2}}u)||_{L^2_{\chi^{0,-1}}\left(I;L^2_{\omega_{-2+r,\beta}}(\Lambda)\right)}\\ &\quad +N^{-s}||\partial_t^s u||_{L^2_{\chi^{s,s-1}}(I;L^2(\Lambda))}.\end{aligned}$$

The above estimates, together with the triangle inequality, lead to

Theorem 2.1 *For any* $u\in L^2_{\chi^{1,-1}}(I;{}_0H^1(\Lambda))\cap \hat{H}^1(I;L^2(\Lambda))\cap A^r(\Omega_1)\cap B^s(\Omega_1)$ *with integers* $2\le r\le M+1$ *and* $s\ge 0$,

$$||u-u_{MN}||_{\chi^{0,-1},\Omega_1}+||\partial_x(u-u_{MN})||_{\chi^{1,-1},\Omega_1}\lesssim N^{-s}||u||_{B^s(\Omega_1)}+(\beta M)^{\frac{1-r}{2}}||u||_{A^r(\Omega_1)}. \tag{2.44}$$

2.6 Numerical Results

We now describe the numerical implementation and present some numerical results for scheme (2.29). We choose the new basis functions $\{\varphi_k\}_{k=0}^{M-1}$ defined in (2.16) for the space discretization. As for the time discretization, we take $\{\xi_j\}_{j=0}^{N-1}$ and $\{\xi_j^*\}_{j=0}^{N-1}$ as the basis functions of S_N and S_N^*, stated below,

$$\xi_j(t)=L_j(t)+L_{j+1}(t)\in S_N,\qquad \xi_j^*(t)=L_j(t)-L_{j+1}(t)\in S_N^*, \tag{2.45}$$

where $L_j(x)$ is the Legendre polynomial of degree j. Accordingly, we define the following finite-dimensional spaces,

$$\begin{aligned}Q_{M,N}&=\mathrm{span}\{\varphi_k(x)\xi_j(t),\ k=0,1,\ldots,M-1,\ j=0,1,\ldots,N-1\},\\ \tilde{Q}_{M,N}&=\mathrm{span}\{\varphi_k(x)\xi_j^*(t),\ k=0,1,\ldots,M-1,\ j=0,1,\ldots,N-1\}.\end{aligned}$$

In actual computation, we expand the numerical solution as

$$u_{MN}(x,t)=\sum_{k=0}^{M-1}\sum_{j=0}^{N-1}\tilde{u}_{kj}\varphi_k(x)\xi_j(t)\in Q_{M,N}.$$

Substituting the above expression into the scheme (2.29) and taking $\varphi(x,t)=\varphi_{k'}(x)\xi^*_{j'}(t)$ with $k'=0,1,\ldots,M-1$ and $j'=0,1,\ldots,N-1$, we obtain

$$\sum_{k=0}^{M-1}\sum_{j=0}^{N-1}\left(a_{k'k}d_{j'j}+b_{k'k}c_{j'j}+a_{k'k}c_{j'j}\right)\tilde{u}_{kj}=f_{k'j'}, \tag{2.46}$$

where

$$a_{k'k} = (\varphi_k, \varphi_{k'})_\Lambda, \quad b_{k'k} = (\partial_x \varphi_k, \partial_x \varphi_{k'})_\Lambda, \quad c_{j'j} = (\xi_j, \xi^*_{j'})_I,$$
$$d_{j'j} = (\xi'_j, \xi^*_{j'})_I, \quad f_{k'j'} = (f, \varphi_{k'} \xi^*_{j'})_{\Omega_1}.$$

We can rewrite the system (2.46) in a compact matrix form. To do this, we introduce the matrices

$$\begin{aligned}
&\boldsymbol{A} = (a_{k'k})_{0\le k',k\le M-1}, \quad \boldsymbol{B} = (b_{k'k})_{0\le k',k\le M-1}, \quad \boldsymbol{C} = (c_{j'j})_{0\le j',j\le N-1},\\
&\boldsymbol{D} = (d_{j'j})_{0\le j',j\le N-1}, \quad \boldsymbol{F} = (f_{k'j'})_{0\le k'\le M-1, 0\le j'\le N-1},\\
&\boldsymbol{U} = (\tilde{u}_{kj})_{0\le k\le M-1, 0\le j\le N-1}.
\end{aligned}$$

Thus, the system (2.46) becomes

$$\boldsymbol{AUD}^t + \boldsymbol{BUC}^t + \boldsymbol{AUC}^t = \boldsymbol{F}, \tag{2.47}$$

which is also equivalent to the following form of tensor product,

$$(\boldsymbol{A} \otimes \boldsymbol{D}^t + \boldsymbol{B} \otimes \boldsymbol{C}^t + \boldsymbol{A} \otimes \boldsymbol{C}^t)\vec{u} = \vec{f}, \tag{2.48}$$

where

$$\begin{aligned}
\vec{u} &= (\tilde{u}_{00}, \tilde{u}_{10}, \dots, \tilde{u}_{M-1,0};\\
&\quad \tilde{u}_{01}, \tilde{u}_{11}, \dots \tilde{u}_{M-1,1}; \dots; \tilde{u}_{0,N-1}, \tilde{u}_{1,N-1}, \dots, \tilde{u}_{M-1,N-1})^t,\\
\vec{f} &= (f_{00}, f_{10}, \dots, f_{M-1,0};\\
&\quad f_{01}, f_{11}, \dots, f_{M-1,1}; \dots; f_{0,N-1}, f_{1,N-1}, \dots, f_{M-1,N-1})^t.
\end{aligned} \tag{2.49}$$

Remark 2.3 According to (2.17) and (2.18), the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ in the compact form (2.48) are diagonal with $\boldsymbol{A} = diag(\{\gamma_i\}_{i=0}^{M-1})$ and $\boldsymbol{B} = diag(\{\beta - \frac{\beta^2}{4}\gamma_i\}_{i=0}^{M-1})$. On the other hand, the matrices $\boldsymbol{C}$ and $\boldsymbol{D}$ can be derived explicitly from the properties of the Legendre polynomials (see Appendix of this paper), i.e.

$$c_{j'j} = \begin{cases} \frac{2}{2j+3}, & j = j' - 1,\\ \frac{4}{(2j+1)(2j+3)}, & j = j',\\ -\frac{2}{2j+1}, & j = j' + 1,\\ 0, & \text{otherwise}, \end{cases}$$

and $\boldsymbol{D} = 2\boldsymbol{I}_N$. Thus, the system (2.47) is reduced to

$$\left(2\gamma_k \boldsymbol{I}_N + \left(\beta + \left(1 - \frac{\beta^2}{4}\right)\gamma_k\right)\boldsymbol{C}^t\right)\vec{u}_k = \vec{f}_k, \quad k = 0, 1, \dots, M-1 \tag{2.50}$$

with

$$\vec{u}_k = (\tilde{u}_{k,0}, \tilde{u}_{k,1}, \dots, \tilde{u}_{k,N-1})^t, \quad \vec{f}_k = (f_{k,0}, f_{k,1}, \dots, f_{k,N-1})^t,$$

which can be solved efficiently.

Next, let $\{x_k\}_{k=0}^M$ be the Laguerre-Gauss-Radau quadrature points on the interval Λ, and $\{t_j\}_{j=0}^N$ be the Legendre-Gauss-Lobatto quadrature points on the interval I. We measure the numerical accuracy by the maximum error, which is defined by

$$||u - u_{MN}||_{M,N,\max} = \max_{0\le k\le M, 0\le j\le N} |u(x_k, t_j) - u_{MN}(x_k, t_j)|.$$

Table 1 The numerical errors of scheme (2.47) with fixed $N = 14$

	$M = 20$	$M = 40$	$M = 60$	$M = 80$	$M = 100$
$\beta = 1$	1.08e−03	1.24e−05	1.16e−07	1.19e−09	2.70e−11
$\beta = 2$	3.32e−05	1.15e−08	6.10e−12	3.83e−15	5.61e−15
$\beta = 3$	3.49e−06	2.16e−10	2.01e−14	2.78e−15	3.61e−15

Table 2 The numerical errors of scheme (2.47) with fixed $M = 70$

	$N = 4$	$N = 6$	$N = 8$	$N = 10$	$N = 12$	$N = 14$
$\beta = 1$	8.86e−03	7.87e−05	3.35e−07	1.68e−08	1.68e−08	1.68e−08
$\beta = 2$	9.05e−03	7.70e−05	3.35e−07	8.70e−10	1.51e−12	1.24e−13
$\beta = 3$	9.08e−03	7.75e−05	3.36e−07	8.68e−10	1.51e−12	2.16e−15

Table 3 The numerical comparisons of two different schemes in time

	Crank–Nicolson scheme in time			Scheme (2.47) with $N = 14$		
	$M = 20$	$M = 60$	$M = 100$	$M = 20$	$M = 60$	$M = 100$
$\beta = 1$	1.06e−03	2.33e−07	2.32e−07	1.08e−03	1.16e−07	2.70e−11
$\beta = 2$	3.29e−05	2.39e−07	2.36e−07	3.32e−05	6.10e−12	5.61e−15
$\beta = 3$	3.48e−06	2.39e−07	2.39e−07	3.49e−06	2.01e−14	3.61e−15

We first take the test function

$$u(x,t) = e^{-x} \sin 2x \sin(1+t), \quad (x,t) \in \Omega_1,$$

which decays exponentially as x goes to infinity. To examine the errors of space discretization, we fix $N = 14$ in time. In Table 1, we list the errors with various M (the degree of basis functions in space) and β. The results indicate that the errors decay exponentially as M increases. Also, a suitable choice of parameter β leads to more accurate numerical results. These facts coincide well with our theoretical analysis. On the other hand, in order to examine the errors of time discretization, we fix $M = 70$ in space. In Table 2, we present the values of $||U - u_{MN}||_{M,N,\max}$ versus N (the degree of basis functions in time) and β, which also indicates an exponential convergence.

For numerical comparisons, we also employ second order Crank–Nicolson scheme for time discretization with time step size 0.001. In Table 3, we list the values of $||u - u_{MN}||_{M,N,\max}$. They demonstrate that scheme (2.47) with $N = 14$ provides more accurate numerical results than the Crank–Nicolson scheme in time.

We next take the test function

$$u(x,t) = \frac{\sin x}{(1+x)^3} \sin(1+t), \quad (x,t) \in \Omega_1,$$

which decays algebraically as x goes to infinity.

In Table 4, we fix $N = 14$ in time and list the numerical errors in different M and β. They indicate that the errors decay algebraically, which also coincide well with our theoretical analysis. Besides, for examining the errors of time discretization, we fix $M = 60$ in space.

Table 4 The numerical errors of scheme (2.47) with fixed $N = 14$

	$M = 20$	$M = 60$	$M = 100$	$M = 140$	$M = 180$
$\beta = 1$	7.02e−04	1.06e−06	2.70e−07	9.39e−08	4.43e−08
$\beta = 2$	1.74e−05	8.74e−07	2.03e−07	7.90e−08	3.83e−08
$\beta = 3$	2.83e−05	1.76e−06	3.18e−07	1.45e−07	6.27e−08

Table 5 The numerical errors of scheme (2.47) with fixed $M = 60$

	$N = 4$	$N = 6$	$N = 8$	$N = 10$	$N = 12$	$N = 14$
$\beta = 1$	2.68e−03	2.92e−05	1.06e−06	1.06e−06	1.06e−06	1.06e−06
$\beta = 2$	2.71e−03	2.84e−05	8.74e−07	8.74e−07	8.74e−07	8.74e−07
$\beta = 3$	2.77e−03	2.83e−05	1.76e−06	1.76e−06	1.76e−06	1.76e−06

Table 6 The numerical comparisons of two different schemes in time

	Crank–Nicolson scheme			Scheme (2.47) with $N = 14$		
	$M = 20$	$M = 60$	$M = 100$	$M = 20$	$M = 60$	$M = 100$
$\beta = 1$	1.16e−03	8.14e−05	2.00e−05	7.02e−04	1.06e−06	2.70e−07
$\beta = 2$	3.29e−04	2.32e−05	5.22e−06	1.74e−05	8.74e−07	2.03e−07
$\beta = 3$	3.48e−04	1.94e−05	4.65e−06	2.83e−05	1.76e−06	3.18e−07

In Table 5, we make a list of the errors versus N and β, which indicates again an algebraical rate of convergence.

For numerical comparisons, we use second order Crank–Nicolson scheme in time again with time step size 0.001. In Table 6, we list the maximum errors with the same values of M in the two cases. They show that scheme (2.47) with $N = 14$ provides more accurate numerical results than the Crank–Nicolson scheme in time.

3 Simultaneously Orthogonal Hermite Functions on the Whole Line and Their Applications

Let $\mathbb{R} = (-\infty, +\infty)$ and $\Omega_2 = I \times \mathbb{R}$. We define as usual $L^2_\omega(\mathbb{R})$ ($L^2_\omega(\Omega_2)$), with the inner product $(u, v)_{\omega,\mathbb{R}}$ ($(u, v)_{\omega,\Omega_2}$).

3.1 The Generalized Hermite Functions

Let $H_l(x)$ be the standard Hermite polynomial of degree l. For any $\beta > 0$, the generalized Hermite functions are given by (cf. [30])

$$H_l^\beta(x) = \frac{1}{\sqrt{2^l l!}} e^{-\frac{1}{2}\beta^2 x^2} H_l(\beta x), \qquad l \geq 0.$$

They are the eigenfunctions of the following singular Sturm–Liouville problem,

$$e^{\frac{1}{2}\beta^2 x^2}\partial_x(e^{-\beta^2 x^2}\partial_x(e^{\frac{1}{2}\beta^2 x^2} v(x))) + \lambda_l^\beta v(x) = 0, \qquad \lambda_l^\beta = 2\beta^2 l, \qquad l \geq 0. \tag{3.1}$$

The set of $H_l^\beta(x)$ forms a complete $L^2(\mathbb{R})$-orthogonal system, i.e.

$$\int_{\mathbb{R}} H_l^\beta(x) H_m^\beta(x) dx = \frac{\sqrt{\pi}}{\beta}\delta_{l,m}. \tag{3.2}$$

They also satisfy the following relation,

$$\int_{\mathbb{R}} \partial_x H_l^\beta(x)\partial_x H_m^\beta(x) dx = \begin{cases} -\frac{\beta}{2}\sqrt{\pi(l+1)(l+2)}, & l = m-2, \\ \sqrt{\pi}\beta(l+\frac{1}{2}), & l = m, \\ -\frac{\beta}{2}\sqrt{\pi l(l-1)}, & l = m+2, \\ 0, & \text{otherwise}. \end{cases} \tag{3.3}$$

For any $v \in L^2(\mathbb{R})$, we have

$$v(x) = \sum_{l=0}^{\infty} v_l^\beta H_l^\beta(x) \tag{3.4}$$

with

$$v_l^\beta = \frac{\beta}{\sqrt{\pi}} \int_{\mathbb{R}} v(x) H_l^\beta(x) dx.$$

Consider the following problem on the whole line,

$$\begin{cases} -\partial_x^2 u(x) + u(x) = f(x), \quad x \in \mathbb{R}, \\ \lim\limits_{x\to\pm\infty} u(x) = 0, \end{cases} \tag{3.5}$$

where f is given such that the above problem is well-posed. Let

$$V_M = \text{span}\{H_l^\beta(x),\ 0 \le l \le M\}.$$

The Hermite spectral-Galerkin approximation to (3.5) is to find $u_M \in V_M$ such that

$$(\partial_x u_M, \partial_x \psi)_{\mathbb{R}} + (u_M, \psi)_{\mathbb{R}} = (f, \psi)_{\mathbb{R}}, \quad \forall \psi \in V_M. \tag{3.6}$$

Denote

$$a_{jk} = (H_k^\beta, H_j^\beta)_{\mathbb{R}}, \quad b_{jk} = (\partial_x H_k^\beta, \partial_x H_j^\beta)_{\mathbb{R}},$$

and introduce the matrices

$$\boldsymbol{A} = (a_{jk})_{0\le k,j\le M}, \quad \boldsymbol{B} = (b_{jk})_{0\le k,j\le M}.$$

Then we have from (3.2) and (3.3) that $\boldsymbol{A} = \frac{\sqrt{\pi}}{\beta}\boldsymbol{I}_{M+1}$ and $\boldsymbol{B}$ is a symmetric penta-diagonal matrix.

3.2 Simultaneously Orthogonal Hermite Functions on the Whole Line

We shall construct simultaneously orthogonal Hermite functions on the whole line according to the structure of the mass and stiffness matrices.

Since the matrix $\boldsymbol{B}$ is a symmetric penta-diagonal matrix, we can easily compute its eigenpairs, which are all real and positive. Let $\boldsymbol{E} = (e_{kj})_{k,j=0,\dots,M}$ be the matrix formed by the orthogonal eigenvectors of $\boldsymbol{B}$ and $\boldsymbol{\Lambda} = diag(\{\lambda_i\}_{i=0}^M)$ be the diagonal matrix with main diagonal being the corresponding eigenvalues, i.e.

$$\boldsymbol{BE} = \boldsymbol{E\Lambda}, \qquad \boldsymbol{E}^t\boldsymbol{E} = \boldsymbol{I}_{M+1},$$

where $\boldsymbol{I}_{M+1}$ stands for the identity matrix of order $M+1$. Let

$$\psi_k(x) = \sum_{j=0}^{M} e_{jk} H_j^\beta(x), \qquad 0 \le k \le M. \tag{3.7}$$

Since the matrix $\boldsymbol{E}$ is nonsingular, the functions $\{\psi_k\}_{k=0}^M$ form a new basis of V_M satisfying the following simultaneously orthogonal properties,

$$(\psi_l, \psi_i)_{\mathbb{R}} = \sum_{k,j=0}^{M} e_{kl} e_{ji} \left(H_k^\beta, H_j^\beta\right)_{\mathbb{R}} = \sum_{k,j=0}^{M} e_{ji} a_{jk} e_{kl} = (\boldsymbol{E}^t\boldsymbol{AE})_{il} = \frac{\sqrt{\pi}}{\beta}\delta_{il}, \tag{3.8}$$

$$(\partial_x\psi_l, \partial_x\psi_i)_{\mathbb{R}} = \sum_{k,j=0}^{M} e_{kl} e_{ji} \left(\partial_x H_k^\beta, \partial_x H_j^\beta\right)_{\mathbb{R}} = \sum_{k,j=0}^{M} e_{ji} b_{jk} e_{kl} = (\boldsymbol{E}^t\boldsymbol{BE})_{il} = \lambda_i\delta_{il}. \tag{3.9}$$

From (3.8) and (3.9), we find that the new basis functions $\{\varphi_k\}_{k=0}^{M-1}$ is mutually orthogonal in both L^2 and H^1 inner products. In other words, the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ under this new basis $\{\psi_k\}_{k=0}^M$ are both diagonal. An immediate consequence of (3.8)–(3.9) is that

$$(\partial_x\psi_l, \partial_x\psi_i)_{\mathbb{R}} = \frac{\lambda_l\beta}{\sqrt{\pi}}(\psi_l, \psi_i)_{\mathbb{R}},$$

which implies

$$(\partial_x\psi_l, \partial_x v)_{\mathbb{R}} = \frac{\lambda_l\beta}{\sqrt{\pi}}(\psi_l, v)_{\mathbb{R}}, \quad \forall v \in V_M. \tag{3.10}$$

3.3 An Efficient Space-Time Hermite–Legendre Spectral Method

In this subsection, we propose an efficient space-time spectral method for Black–Scholes-type equation based on Hermite–Legendre Galerkin method using simultaneously orthogonal Hermite functions (3.7) in space and a dual-Petrov-Legendre-Galerkin formulation in time.

Black–Scholes-type equation plays an important role in option pricing. In the classical Black–Scholes–Merton framework, the stock price dynamics follows a geometric Brownian motion, which has a continuous sample path,

$$ds = \mu s dt + \sigma s dB_t.$$

Here, s is the stock price at time t, μ is the instantaneous expected return on the stock, σ is the instantaneous volatility of the return, dB_t is the standard Brownian motion or Weiner process.

Let $V(s,t)$ denote the price of a derivative security contingent at time t, T be the time of expiration and K be the strike price. The standard Black–Scholes equation with terminal condition is

$$\begin{cases} \partial_t V(s,t)+\frac{1}{2}\sigma^2 s^2 \partial_s^2 V(s,t)+rs\partial_s V(s,t)-rV(s,t)=0, & (s,t)\in(0,+\infty)\times(0,T), \\ V(s,T)=\max(s-K,0), & s\in(0,+\infty). \end{cases} \tag{3.11}$$

In this subsection, we consider the general problems as follows,

$$\begin{cases} \partial_t V(s,t)+\frac{1}{2}\sigma^2 s^2 \partial_s^2 V(s,t)+rs\partial_s V(s,t)-rV(s,t)=F(s,t), & (s,t)\in(0,+\infty)\times(0,T), \\ V(0,t)=0, \ \lim\limits_{s\to+\infty} V(s,t)=0, & t\in(0,T), \\ V(s,T)=u_T(s), & s\in(0,+\infty), \end{cases} \tag{3.12}$$

where F is a given function. Taking the transformation

$$x=\ln s, \quad \tau=-\frac{2}{T}t+1,$$

the problem (3.12) becomes the following equation with constant coefficients,

$$\begin{cases} \frac{T}{2}\partial_\tau u(x,\tau)-a\partial_x^2 u(x,\tau)-b\partial_x u(x,\tau)+cu(x,\tau)=f(x,\tau), & (x,\tau)\in\Omega_2=\mathbb{R}\times I, \\ \lim\limits_{x\to\pm\infty} u(x,\tau)=0, & \tau\in\bar{I}, \\ u(x,-1)=\tilde{u}_T(x), & x\in\mathbb{R}, \end{cases} \tag{3.13}$$

where $a=\frac{\sigma^2}{2}$, $b=r-\frac{\sigma^2}{2}$ and $c=r$. For simplicity, we assume that $\tilde{u}_T(x)=0$. Let

$$Q=H^1(\mathbb{R})\otimes S, \qquad \tilde{Q}=H^1(\mathbb{R})\otimes S^*,$$

where S and S^* are defined as before. The weak formulation of the problem (3.13) is to find $u\in Q$ such that

$$\frac{T}{2}(\partial_\tau u, v)_{\Omega_2}+a(\partial_x u,\partial_x v)_{\Omega_2}-b(\partial_x u, v)_{\Omega_2}+c(u,v)_{\Omega_2}=(f,v)_{\Omega_2}, \quad \forall v\in\tilde{Q}. \tag{3.14}$$

We introduce the following finite-dimensional spaces,

$$Q_{M,N}=V_M\otimes S_N, \qquad \tilde{Q}_{M,N}=V_M\otimes S_N^*.$$

The spectral scheme of the problem (3.13) is to seek $u_{MN}\in Q_{M,N}$ such that

$$\begin{aligned} &\frac{T}{2}(\partial_\tau u_{MN},\varphi)_{\Omega_2}+a(\partial_x u_{MN},\partial_x\varphi)_{\Omega_2}-b(\partial_x u_{MN},\varphi)_{\Omega_2}+c(u_{MN},\varphi)_{\Omega_2} \\ &\quad=(f,\varphi)_{\Omega_2}, \quad \forall\varphi\in\tilde{Q}_{M,N}. \end{aligned} \tag{3.15}$$

Remark 3.1 Since the error analysis of scheme (3.15) is quite similar to that of scheme (2.29), we omit the details here.

We now describe the numerical implementation for scheme (3.15). We choose the simultaneously orthogonal Hermite basis functions $\{\psi_k\}_{k=0}^M$ in (3.7) for the space discretization. As for the time discretization, we take $\{\xi_j\}_{j=0}^{N-1}$ and $\{\xi_j^*\}_{j=0}^{N-1}$ as the basis functions of S_N and S_N^* defined in (2.45). Accordingly, we denote the finite-dimensional spaces,

$$\begin{aligned} Q_{M,N}&=\text{span}\{\psi_k(x)\xi_j(\tau),\ k=0,1,\ldots,M,\ j=0,1,\ldots,N-1\}, \\ \tilde{Q}_{M,N}&=\text{span}\{\psi_k(x)\xi_j^*(\tau),\ k=0,1,\ldots,M,\ j=0,1,\ldots,N-1\}. \end{aligned}$$

In actual computation, we expand the numerical solution as

$$u_{MN}(x,\tau) = \sum_{k=0}^{M} \sum_{j=0}^{N-1} \tilde{u}_{kj} \psi_k(x) \xi_j(\tau) \in Q_{M,N}.$$

Substituting the above expression into the scheme (3.15), and taking $\varphi(x,\tau) = \psi_{k'}(x)\xi^*_{j'}(\tau)$ with $k' = 0, 1, \ldots, M$ and $j' = 0, 1, \ldots, N-1$, we obtain

$$\sum_{k=0}^{M} \sum_{j=0}^{N-1} \big(\frac{T}{2} a_{k'k} h_{j'j} + a c_{k'k} d_{j'j} - b b_{k'k} d_{j'j} + c a_{k'k} d_{j'j}\big) \tilde{u}_{kj} = f_{k'j'}, \tag{3.16}$$

where

$$\begin{aligned} &a_{k'k} = (\psi_k, \psi_{k'})_{\mathbb{R}}, \quad b_{k'k} = (\partial_x \psi_k, \psi_{k'})_{\mathbb{R}}, \quad c_{k'k} = (\partial_x \psi_k, \partial_x \psi_{k'})_{\mathbb{R}}, \\ &d_{j'j} = (\xi_j, \xi^*_{j'})_I, \quad h_{j'j} = (\xi'_j, \xi^*_{j'})_I, \quad f_{k'j'} = (f, \psi_{k'} \xi^*_{j'})_{\Omega_2}. \end{aligned}$$

We can rewrite the system (3.16) in a compact matrix form. To do this, we introduce the matrices

$$\begin{aligned} &\boldsymbol{A} = (a_{k'k})_{0 \le k',k \le M}, \quad \boldsymbol{B} = (b_{k'k})_{0 \le k',k \le M}, \quad \boldsymbol{C} = (c_{k'k})_{0 \le k',k \le M}, \\ &\boldsymbol{D} = (d_{j'j})_{0 \le j',j \le N-1}, \quad \boldsymbol{H} = (h_{j'j})_{0 \le j',j \le N-1}, \quad \boldsymbol{F} = (f_{k'j'})_{0 \le k' \le M, 0 \le j' \le N-1}, \\ &\boldsymbol{U} = (\tilde{u}_{kj})_{0 \le k \le M, 0 \le j \le N-1}. \end{aligned}$$

Thus, the system (3.16) becomes

$$\frac{T}{2} \boldsymbol{A}\boldsymbol{U}\boldsymbol{H}^t + a\boldsymbol{C}\boldsymbol{U}\boldsymbol{D}^t - b\boldsymbol{B}\boldsymbol{U}\boldsymbol{D}^t + c\boldsymbol{A}\boldsymbol{U}\boldsymbol{D}^t = \boldsymbol{F}, \tag{3.17}$$

which is also equivalent to the following form of tensor product,

$$\left(\frac{T}{2} \boldsymbol{A} \otimes \boldsymbol{H}^t + a\boldsymbol{C} \otimes \boldsymbol{D}^t - b\boldsymbol{B} \otimes \boldsymbol{D}^t + c\boldsymbol{A} \otimes \boldsymbol{D}^t\right) \vec{u} = \vec{f}, \tag{3.18}$$

where

$$\begin{aligned} &\vec{u} = (\tilde{u}_{00}, \tilde{u}_{10}, \ldots, \tilde{u}_{M,0}; \tilde{u}_{01}, \tilde{u}_{11}, \ldots \tilde{u}_{M,1}; \ldots; \tilde{u}_{0,N-1}, \tilde{u}_{1,N-1}, \ldots, \tilde{u}_{M,N-1})^t, \\ &\vec{f} = (f_{00}, f_{10}, \ldots, f_{M,0}; f_{01}, f_{11}, \ldots, f_{M,1}; \ldots; f_{0,N-1}, f_{1,N-1}, \ldots, f_{M,N-1})^t. \end{aligned} \tag{3.19}$$

Remark 3.2 According to (3.8) and (3.9), the matrices $\boldsymbol{A}$ and $\boldsymbol{C}$ in the compact form (3.18) are diagonal with $\boldsymbol{A} = diag(\{\frac{\sqrt{\pi}}{\beta}\})$ and $\boldsymbol{C} = diag(\{\lambda_i\}_{i=0}^{M})$. On the other hand, the matrices $\boldsymbol{D}$ and $\boldsymbol{H}$ can be derived explicitly from the properties of the Legendre polynomials (see Appendix of this paper), i.e.

$$d_{j'j} = \begin{cases} \frac{2}{2j+3}, & j = j'-1, \\ \frac{4}{(2j+1)(2j+3)}, & j = j', \\ -\frac{2}{2j+1}, & j = j'+1, \\ 0, & \text{otherwise}, \end{cases}$$

and $\boldsymbol{H} = 2\boldsymbol{I}_N$. The system (3.18) can be solved efficiently.

3.4 Numerical Results

In this subsection, we present some numerical results to show the efficiency of the proposed method for (3.13).

Let $\{x_k\}_{k=0}^{M}$ be the Hermite-Gauss quadrature points, and $\{t_j\}_{j=0}^{N}$ be the Legendre-Gauss-Lobatto quadrature points on the interval I. We measure the numerical accuracy by the maximum error, which is defined by

$$||u - u_{MN}||_{M,N,\max} = \max_{0\le k\le M, 0\le j\le N} |u(x_k, t_j) - u_{MN}(x_k, t_j)|.$$

In actual computation, let $a = c = 1$ and $b = 0$. We first take the exact solution

$$u(x, \tau) = e^{-x^2} \sin 2x \sin(1 + \tau), \quad (x, \tau) \in \Omega_2,$$

which decays exponentially as x goes to infinity. To examine the errors of space discretization, we fix $N = 16$ in time. In Table 7, we list the errors with different M and β. The results indicate that the errors decay exponentially as M increases. We note that higher accuracy is achieved with a suitable choice of parameter β. Next, in order to measure the errors of time discretization, we fix $M = 30$ in space. In Table 8, we present the values of $||u-u_{MN}||_{M,N,\max}$ versus N and β, which also shows an exponential convergence.

For numerical comparisons, we also employ second order Crank–Nicolson scheme for time discretization with time step size 0.001. In Table 9, we list the values of $||u - u_{MN}||_{M,N,\max}$. They demonstrate that scheme (3.17) with $N = 16$ provides more accurate numerical results than the Crank–Nicolson scheme in time.

Table 7 The numerical errors of scheme (3.17) with fixed $N = 16$

	$M = 20$	$M = 40$	$M = 60$	$M = 80$	$M = 100$
$\beta = 0.5$	3.29e−01	1.95e−02	1.89e−03	2.00e−04	2.22e−05
$\beta = 1$	8.66e−05	1.18e−08	1.36e−12	2.00e−15	2.66e−15
$\beta = 1.5$	7.12e−14	3.22e−15	2.22e−15	2.89e−15	2.82e−15

Table 8 The numerical errors of scheme (3.17) with fixed $M = 30$

	$N = 4$	$N = 6$	$N = 8$	$N = 10$	$N = 12$	$N = 14$
$\beta = 0.5$	9.33e−02	7.96e−02	8.09e−02	8.03e−02	8.07e−02	8.06e−02
$\beta = 1$	1.56e−02	1.63e−04	1.04e−06	9.53e−07	9.55e−07	9.53e−07
$\beta = 1.5$	1.63e−02	1.66e−04	7.78e−07	2.11e−09	3.78e−12	5.66e−15

Table 9 The numerical comparisons of two different schemes in time

	Crank–Nicolson scheme in time			Scheme (3.17) with $N = 16$		
	$M = 20$	$M = 60$	$M = 100$	$M = 20$	$M = 60$	$M = 100$
$\beta = 1$	7.96e−05	3.05e−07	2.94e−07	8.66e−05	1.36e−12	2.66e−15
$\beta = 1.5$	2.95e−07	3.04e−07	3.03e−07	7.12e−14	2.22e−15	2.82e−15
$\beta = 2$	3.14e−06	3.04e−07	3.05e−07	3.32e−06	4.66e−5	5.94e−15

Table 10 The numerical errors of scheme (3.17) with fixed $h = 3$ and $N = 16$

	$M = 20$	$M = 60$	$M = 100$	$M = 140$	$M = 180$
$\beta = 1$	1.87e−02	1.67e−04	6.85e−06	5.44e−07	6.21e−08
$\beta = 1.5$	6.22e−04	2.38e−06	5.69e−08	2.41e−07	1.67e−08
$\beta = 2$	6.58e−05	1.11e−05	3.11e−06	1.35e−06	8.20e−08

Table 11 The numerical errors of scheme (3.17) with fixed $h = 5$ and $N = 16$

	$M = 20$	$M = 60$	$M = 100$	$M = 140$	$M = 180$
$\beta = 1$	5.72e−02	1.07e−03	5.23e−05	5.53e−06	7.31e−07
$\beta = 1.5$	3.46e−03	6.42e−06	9.19e−08	2.75e−09	1.30e−10
$\beta = 2$	1.40e−04	4.25e−08	1.16e−09	2.57e−10	1.08e−11

Table 12 The numerical errors of scheme (3.17) with fixed $h = 5$ and $M = 140$

	$N = 4$	$N = 6$	$N = 8$	$N = 10$	$N = 12$
$\beta = 1$	2.17e−03	1.94e−05	5.53e−06	5.52e−06	5.51e−06
$\beta = 1.5$	2.36e−03	1.84e−05	7.06e−08	2.74e−09	2.75e−09
$\beta = 2$	2.34e−03	1.80e−05	7.04e−08	2.57e−10	2.57e−10

Table 13 The numerical comparisons of two different schemes in time

	Crank–Nicolson scheme			New scheme with $N = 16$		
	$M = 20$	$M = 60$	$M = 100$	$M = 20$	$M = 60$	$M = 100$
$\beta = 1$	6.74e−02	1.03e−03	4.72e−05	5.72e−02	1.07e−03	5.23e−05
$\beta = 1.5$	3.44e−03	5.93e−06	1.65e−07	3.46e−03	6.42e−06	9.19e−08
$\beta = 2$	1.30e−04	1.22e−07	8.88e−08	1.40e−04	4.25e−08	1.16e−09

We next take the exact solution

$$u(x,\tau) = \frac{\sin x}{(1+x^2)^h}\sin(1+\tau), \quad (x,\tau) \in \Omega_2,$$

which decays algebraically as x goes to infinity.

In Table 10, we take $h = 3$, $N = 16$ and list the numerical errors in different M and β. They indicate that the errors decay algebraically. In Table 11, we take $h = 5$, $N = 16$ and list the numerical errors in different M and β. They also indicate that the errors decay algebraically. From Tables 10 and 11, we find that higher accuracy can be achieved as h increases. In addition, for examining the errors of time discretization, we fix $M = 140$ in space. In Table 12, we make a list of the errors versus N and β, which also indicates an algebraical rate of convergence.

For numerical comparisons, we use second order Crank–Nicolson scheme in time again with time step size 0.001 and $h = 5$. In Table 13, we list the maximum errors with the

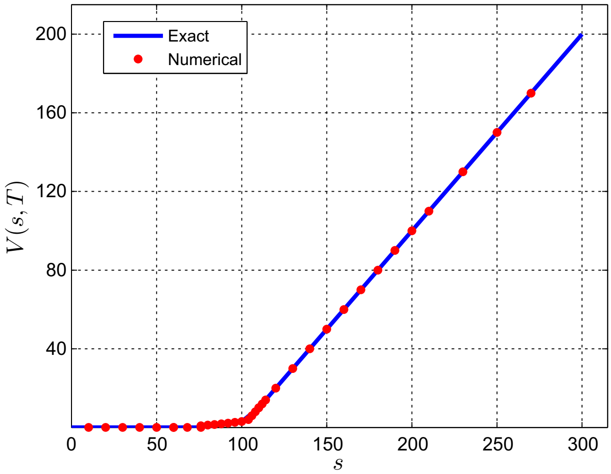

Fig. 1 The graph of the numerical solution and the exact solution at $t = T$

same values of M in the two cases. They indicate that scheme (3.17) provides more accurate numerical results than the Crank–Nicolson scheme in time.

Finally, we present some numerical results for European call options under the Black–Scholes model (3.11) with the following benchmark parameters (see [5])

$$T = 0.25, \quad K = 100, \quad r = 0.05, \quad \sigma = 0.15.$$

Fig. 1 shows the agreement between the numerical solution and the theoretical one and thus demonstrates the effectiveness of our method for the benchmark problem.

4 Conclusion Remarks

In this paper, we constructed two series of simultaneously orthogonal basis functions on the half/whole line by matrix decomposition techniques, which lead to diagonal systems for second order problems with constant coefficients. We proposed efficient space-time spectral methods based on the simultaneously orthogonal Laguerre/Hermite-Galerkin scheme in space and a dual-Petrov-Galerkin formulation in time for problems defined on unbounded domains. Using these suggested methods, higher accuracy was achieved. Particularly, the use of the simultaneously orthogonal basis functions in space may greatly simplify the implementation of the space-time spectral methods.

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