CHEBYSHEV SPECTRAL COLLOCATION IN SPACE AND TIME FOR THE HEAT EQUATION*

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Abstract. Spectral methods can solve elliptic partial differential equations (PDEs) numerically with errors bounded by an exponentially decaying function of the number of modes when the solution is analytic. For time-dependent problems, almost all focus has been on low-order finite difference schemes for the time derivative and spectral schemes for the spatial derivatives. This mismatch destroys the spectral convergence of the numerical solution. Spectral methods that converge spectrally in both space and time have appeared recently. This paper shows that a Chebyshev spectral collocation method of Tang and Xu for the heat equation converges exponentially when the solution is analytic. We also derive a condition number estimate of the global spectral operator. Another space-time Chebyshev collocation scheme that is easier to implement is proposed and analyzed. This paper is a continuation of the first author's earlier paper in which two Legendre space-time collocation methods were analyzed.

Key words. spectral collocation, Chebyshev collocation, space-time, time-dependent partial differential equation

AMS subject classifications. 65M70, 65L05, 35K20, 35L20, 41A10

1. Introduction. Spectral methods have been successfully used for many decades to solve elliptic PDEs. If the solution is analytic, then the numerical solution converges exponentially as a function of the number of spectral modes. For time-dependent PDEs, the most common approach is to use a low-order finite difference approximation of the time derivative and a spectral approximation of the spatial derivatives. This is not ideal since the time discretization error overwhelms the spatial discretization error. In an earlier paper [9], a Legendre collocation method in both space and time based on the work of Tang and Xu [19] was proposed for the heat equation. The method was shown to converge spectrally when the solution is analytic. A condition number estimate for the global space-time operator of $O(N^4)$ was derived, where N is the number of spectral modes in each direction. This estimate is the same as that for the elliptic part of the operator. A second space-time method which is easier to implement and has similar performance was also proposed and analyzed. The purpose of this paper is to demonstrate spectral convergence and a $O(N^4)$ condition number estimate for the global space-time operator of the space-time Chebyshev collocation method. Although much of the basic framework of the theory for the methods based on the two different orthogonal polynomials are similar, the analysis for the Chebyshev case is much more difficult because of the presence of a singular weight function. In this paper, a simplified eigenvalue analysis paves the way for a condition number estimate of the Chebyshev space-time method and a similar analysis for other canonical linear PDEs ([10]). This paper and the earlier one [9] are the only ones in the literature to address the condition number of discrete global space-time operators.

Two additional contributions of this paper include sharp estimates of the eigenvalues of spectral integration and derivative matrices. It is shown that the real part of every eigenvalue of a spectral integration matrix is positive and the real part of every eigenvalue of a spectral derivative matrix is positive and bounded away from zero. See Propositions 3.4 and 4.1.

One drawback of these space-time spectral methods is that time stepping is no longer possible. The unknowns for all times must be solved simultaneously. This presents a serious problem for PDEs in three spatial dimensions and is particularly onerous for nonlinear PDEs.

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It should be made clear that due to spectral convergence, many fewer unknowns are needed compared to finite difference/element schemes for the same error tolerance.

An early work on spectrally accurate ordinary differential equation (ODE) solvers is [4]. Among the first works on space-time spectral methods for PDEs with periodic boundary conditions are [16, 17]. Other references include [5, 6, 7, 13, 15, 18, 20, 22, 23] and the references therein. Of course, this list is incomplete. See [9] for additional papers that address space-time spectral methods and papers that attempt to couple space and time components for faster computations. We wish to add one more reference [3] that provides a good survey of algorithms that are parallel in time.

In the next section, we state the notation used in this paper and recall some basic estimates used in the analysis. Following that, we demonstrate the spectral convergence of the space-time Chebyshev collocation method of Tang and Xu [19] for the 1D heat equation in Section 3. The condition number of the method is shown to be $O(N^4)$. In Section 4, a similar space-time spectral collocation method which is easier to implement for more general PDEs and which exhibits nearly identical characteristics is proposed and analyzed. Some simple numerical results are illustrated in Section 5. In the final section, a conclusion and some future work are outlined. Proofs of technical results needed for the condition number estimates are collected in Appendix A.

2. Notation and basic estimates. Below, we summarize our matrix notation to be followed by the notation pertaining to spectral methods. Let I_n denote the $n \times n$ identity matrix. For an $n \times n$ matrix M, let [M] denote the $(n - 1) \times (n - 1)$ matrix obtained from M by deleting the last column and row, while $[\![M]\!]$ denotes the $(n - 2) \times (n - 2)$ matrix obtained from M by deleting the first and last columns and rows. For any complex number a, its complex conjugate is denoted by \bar{a} , and its real and imaginary parts are denoted by $\Re a$ and $\Im a$, respectively. For any matrix M, let M^T and M^* denote the transpose and complex conjugate transpose of M, respectively. Let $|\cdot|_2$ denote the vector/matrix 2-norm and $|\cdot|_{\infty}$ the vector ∞ -norm. For positive integers m, n and any $a \in \mathbb{C}^{mn}$, let $A \in \mathbb{C}^{m \times n}$ be the matrix representation of a, that is, the columns of A, stacked on top of each other, form a. The notation is a = vec(A). Finally, \otimes denotes the tensor product. For matrices $X \in \mathbb{C}^{N \times N}$, $Y \in \mathbb{C}^{M \times M}$, and $z \in \mathbb{C}^{MN}$, recall that $(X \otimes Y)z = vec(YZX^T)$, where vec(Z) = z is the vector representation of Z. Throughout, C, c denote positive constants whose values may differ at different occurrences but are independent of N.

Fix a positive integer N. Let P_N denote the space of polynomials of degree at most N in x for a fixed t and degree at most N in t for a fixed x. Let x_0, \ldots, x_N denote the Chebyshev Gauss-Lobatto nodes with $x_0 = 1, x_N = -1$, and x_j the descending zeros of $T'_N(x)$, where $1 \le j \le N - 1$ and T_N is the Nth Chebyshev polynomial. The Chebyshev Gauss-Lobatto nodes along the t axis are denoted by $\{t_k\}$. Let

$$x_h = \begin{bmatrix} x_1 \\ \vdots \\ x_{N-1} \end{bmatrix}, \qquad t_h = \begin{bmatrix} t_0 \\ \vdots \\ t_{N-1} \end{bmatrix}.$$

Note that x_h excludes both boundary points, while t_h excludes only the initial point -1. For $0 \le j \le N$, let ℓ_j be the Lagrange interpolant, a polynomial of degree N of x_j so that $\ell_j(x_k) = \delta_{jk}$. Recall that the Chebyshev pseudospectral derivative matrix $D \in \mathbb{R}^{(N+1)\times(N+1)}$ has entries

$$D_{jk} = \frac{d\ell_k(x_j)}{dx}, \qquad 0 \le j, k \le N.$$

Let $d_h = D(0: N-1, N)$ be the first N entries of the last column of D. Define the Chebyshev interpolation operator as usual: for any continuous u,

(2.1)
$$\mathcal{I}_N u = \sum_{j=0}^N u(x_j)\ell_j.$$

The following is an important property of Chebyshev quadrature: for any polynomial v of degree at most 2N - 1,

$$\int_{-1}^{1} v(x) w(x) dx = \sum_{k=0}^{N} v(x_k) \rho_k, \qquad w(x) = \frac{1}{\sqrt{1-x^2}},$$

where $\{\rho_k\}$ is the set of weights associated with Chebyshev Gauss-Lobatto quadrature. Let W_h be the $(N + 1) \times (N + 1)$ diagonal matrix whose diagonal entries are $\{\rho_k\}$. Denote the weighted L^2 -norm of a continuous function v on $\Omega := (-1, 1)^2$ by

$$\|v\| := \left(\int_{\Omega} |v(x,t)|^2 w(x)w(t)dxdt\right)^{1/2}.$$

Also, define the corresponding discrete norm

$$\|v\|_N := \left(\sum_{j,k=0}^N \rho_j \rho_k |v(x_j, t_k)|^2\right)^{1/2}$$

It is well known ([2, Inequality (5.3.2)], for instance) that the weighted L^2 - and discrete norms are equivalent for all polynomials v of degree at most N:

(2.2)
$$||v|| \le ||v||_N \le 2||v||.$$

In case v is a function of one variable, we also write

$$||v|| = \left(\int_{-1}^{1} |v(x)|^2 w(x)\right)^{1/2}$$

An inverse estimate (see [2, (5.5.4)], for instance) states that there is some positive constant c so that

(2.3)
$$||v'|| \le cN^2 ||v||, \quad v \in P_N.$$

3. The space-time spectral collocation method of Tang-Xu. We treat the simplest case where the spatial and temporal domains are both (-1, 1). This is no loss of generality since this can always be accomplished by a simple change of variables. In cases where this may not be appropriate, the method can be repeatedly applied over several time intervals, for instance. Since the purpose of the paper is an analysis of the method, we shall not dwell on these and other refinements.

Consider the linear heat equation

(3.1)
$$u_t = u_{xx} + f(x,t)$$
 on $(-1,1)^2$

with boundary conditions $u(\pm 1, t) = 0$ and initial condition $u(x, -1) = u_0(x)$. We seek a numerical solution $u \in P_N$ at t = 1.

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Fix an integer $N \ge 2$. We first derive the space-time Chebyshev spectral collocation method of [19]. Write

(3.2)
$$\ell_k(t) = \sum_{q=0}^N \alpha_{qk} T_q(t), \qquad 0 \le k \le N.$$

Let

$$c_k = \begin{cases} 2, & k = 0, \\ 1, & \text{otherwise.} \end{cases} \qquad d_k = \begin{cases} 2, & k = 0, N, \\ 1, & \text{otherwise.} \end{cases}$$

It is not difficult to show that

$$\alpha_{qk} = \begin{cases} \frac{2}{Nc_q d_k} \cos \frac{qk\pi}{N}, & 0 \le q < N, \\ \frac{(-1)^k}{Nd_k}, & q = N. \end{cases}$$

For any real t, define

$$u_h(t) = \begin{bmatrix} u(x_1, t) \\ \vdots \\ u(x_{N-1}, t) \end{bmatrix}, \qquad f_h(t) = \begin{bmatrix} f(x_1, t) \\ \vdots \\ f(x_{N-1}, t) \end{bmatrix}.$$

A semi-discrete approximation of the heat equation is

(3.3)
$$u'_{h}(t) = \sum_{k=0}^{N} \left(A u_{h}(t_{k}) + f_{h}(t_{k}) \right) \ell_{k}(t), \qquad u_{h}(-1) = u_{0h},$$

where $A = \llbracket D^2 \rrbracket$ and u_{0h} are the initial data evaluated at the vector of interior Chebyshev Gauss-Lobatto points x_h , i.e., $u_{0h} = u_0(x_h)$. Note that at the collocation point t_j , for $0 \le j < N$,

$$u_h'(t_j) = Au_h(t_j) + f_h(t_j),$$

which is precisely the system of collocation equations.

Using (3.2), it follows that

$$u_h'(t) = \sum_{q,k=0}^N \left(A u_h(t_k) + f_h(t_k) \right) \alpha_{qk} T_q(t).$$

Integrating in time from -1 to t_j for some $0 \le j < N$, we obtain

$$u_{h}(t_{j}) - u_{0h} = \sum_{k=0}^{N} \left(Au_{h}(t_{k}) + f_{h}(t_{k}) \right) \left[\alpha_{0k}(t_{j}+1) + \frac{\alpha_{1k}(t_{j}^{2}-1)}{2} + \sum_{q=2}^{N} \alpha_{qk} \left(\frac{T_{q+1}(t_{j})}{2(q+1)} - \frac{T_{q-1}(t_{j})}{2(q-1)} - \frac{(-1)^{q}}{q^{2}-1} \right) \right]$$

In the above formula, we used the identity

$$T_q(t) = \frac{T'_{q+1}(t)}{2(q+1)} - \frac{T'_{q-1}(t)}{2(q-1)}, \qquad q \ge 2.$$

The system can be represented as

(3.4)
$$u_h(t_j) = A \sum_{k=0}^{N-1} B_{kj} u_h(t_k) + g_j, \qquad 0 \le j < N,$$

where for $0 \le k \le N$,

$$B_{kj} = \alpha_{0k}(t_j + 1) + \frac{\alpha_{1k}(t_j^2 - 1)}{2} + \sum_{q=2}^{N} \alpha_{qk} \left(\frac{\cos\left((q+1)\pi j/N\right)}{2(q+1)} - \frac{\cos\left((q-1)\pi j/N\right)}{2(q-1)} - \frac{(-1)^q}{q^2 - 1} \right),$$

and

$$g_j = \sum_{k=0}^{N} B_{kj} f_h(t_k) + B_{Nj} A u_{0h} + u_{0h}.$$

We record the following identity for future reference:

$$B_{kj} = \int_{-1}^{t_j} \ell_k(t) \, dt = \sum_{q=0}^N \alpha_{qk} \int_{-1}^{t_j} T_q(t) \, dt.$$

Let $V_h, G_h \in \mathbb{R}^{(N-1) \times N}$ be the matrices whose *j*th column is $u_h(t_j)$ and $g_j, 0 \le j < N$, respectively. Then the system becomes

$$(3.5) V_h = AV_h B + G_h,$$

where $B \in \mathbb{R}^{N \times N}$ with entries B_{kj} , $0 \le k, j \le N - 1$. Let $v_h = vec(V_h)$, $g_h = vec(G_h)$, and

$$\mathcal{A}_h = (I_N \otimes I_{N-1}) - (B^T \otimes A).$$

Then (3.5) is equivalent to $A_h v_h = g_h$.

We begin with some preliminary results. The first two state that B^T is a discrete integration operator in two different senses: it exactly integrates polynomials of degree at most N evaluated at the collocation points and its inverse differs from [D] by a rank-one matrix. These facts are hardly surprising by the way B was derived in (3.4).

LEMMA 3.1. Let $N \ge 1$ and v be a complex polynomial of degree at most N so that v(-1) = 0. Then

$$B^T v(t_h) = \int_{-1}^{t_h} v(t) \, dt.$$

Proof. The proof is exactly the same as that for the Legendre case and is omitted. See [9].

LEMMA 3.2. Let $N \ge 1$. Then $B^T - [D]^{-1}$ is a rank-one matrix.

Proof. Let $\{a_k\}$ be arbitrary complex constants so that

$$u(t) = \sum_{k=0}^{N} a_k t^k, \qquad u(-1) = 0$$

Define $u_h = u(t_h)$. Let 1 be the vector of all ones. By the above lemma,

$$[D]B^{T}u_{h} = [D]\int_{-1}^{t_{h}}\sum_{k=0}^{N-1}a_{k}t^{k} dt + [D]\int_{-1}^{t_{h}}a_{N}t^{N} dt$$
$$=\sum_{k=0}^{N-1}a_{k}t_{h}^{k} + \frac{a_{N}}{N+1}[D]\left(t_{h}^{N+1} - (-1)^{N+1}\mathbf{1}\right)$$
$$=u_{h} + a_{N}\left(\frac{[D]}{N+1}\left(t_{h}^{N+1} + (-1)^{N}\mathbf{1}\right) - t_{h}^{N}\right)$$

Thus $[D]B^T - I_N$ is a rank-one matrix which depends on a_N but is independent of all other $a_j, 0 \le j < N$.

The third lemma states that when applied to an analytic function evaluated at the collocation points, the quadrature error is exponentially small.

LEMMA 3.3. Let $N \ge 1$ and z be analytic with z(-1) = 0. Then

$$\left| B^T z(t_h) - \int_{-1}^{t_h} z(t) \, dt \right|_2 \le c N^{1/2} e^{-CN},$$

where c depends on z but is independent of N.

Proof. Let L denote the quantity at the left-hand side of the inequality of the lemma. Then

$$L = \left| \left[B^T (\mathcal{I}_N z)(t_h) - \int_{-1}^{t_h} (\mathcal{I}_N z)(t) \, dt \right] + \int_{-1}^{t_h} (\mathcal{I}_N z - z)(t) \, dt \right|_2$$

$$\leq 0 + \sqrt{2N} \, \|\mathcal{I}_N z - z\|_{L^2(-1,1)}$$

$$< c N^{1/2} e^{-CN}.$$

Note that the term inside the square brackets is zero due to Lemma 3.1, while the last inequality is a Chebyshev interpolation error estimate for analytic functions. See [8, (5.45)], for instance.

The following results are needed to estimate the condition number of the method. The proof of the first one, one of the main technical results of this paper, is postponed to the appendix.

PROPOSITION 3.4. Let $N \ge 1$. The real part of every eigenvalue of B^T is positive.

LEMMA 3.5. Let $N \ge 1$. Then $|B^T|_2 \le c$, with c a positive constant independent of N. Proof. Let z_h be a unit N-vector so that $|B^T z_h|_2 = |B^T|_2$. Let z be a polynomial of degree at most N with z(-1) = 0 and $z_h = z(t_h)$. By Lemma 3.1,

$$\begin{split} |B^{T}z_{h}|_{2}^{2} &= \left| \int_{-1}^{t_{h}} z(t) \, dt \right|_{2}^{2} = \sum_{k=0}^{N-1} \left(\int_{-1}^{t_{k}} z(t) w^{1/2}(t) \cdot w^{-1/2}(t) \, dt \right)^{2} \\ &\leq \sum_{k=0}^{N-1} \int_{-1}^{t_{k}} z^{2}(t) \, w(t) \, dt \, \int_{-1}^{1} \sqrt{1-t^{2}} \, dt \leq \frac{\pi N}{2} \int_{-1}^{1} z^{2}(t) \, w(t) \, dt \\ &\leq \frac{\pi N}{2} \, |[W_{h}^{1/2}] \, z_{h}|_{2}^{2} \leq c. \end{split}$$

The penultimate inequality is due to the equivalence of the discrete and weighted L^2 -norms (2.2), while the last inequality follows from the fact that the weights satisfy $\rho_k \leq cN^{-1}$ for all k. \Box

The next lemma is well known; see [2, Inequality (7.3.5)] or [21], for instance.

LEMMA 3.6. Let $N \ge 2$. Then the eigenvalues of $- \llbracket D^2 \rrbracket$ are real, bounded below by c and above by CN^4 , where c and C are positive and independent of N.

LEMMA 3.7. Let $N \ge 2$ and u be a function analytic in some open set in the complex plane containing the real interval [-1, 1] and $u(\pm 1) = 0$. Let $A = \llbracket D^2 \rrbracket$, where D is the Chebyshev pseudospectral derivative matrix. Then

$$\left| \left(Au(x_h) - u''(x_h) \right) \right|_{\infty} \le c N^3 e^{-CN}.$$

Proof. Recall the definition of the interpolation operator in (2.1). Observe that the identity $(\mathcal{I}_N u)''(x_h) = Au(x_h)$ holds. The result follows from the estimate ([12])

$$|(\mathcal{I}_N u - u)''(x_h)|_{\infty} \le cN^3 e^{-CN}. \qquad \Box$$

For any t, define the error vector

$$e_h(t) = u_h(t) - u(x_h, t),$$

where u is the solution of the heat equation (3.1) and u_h is the solution of (3.3). For $0 \le k < N$,

$$e'_{h}(t_{k}) = u'_{h}(t_{k}) - u_{t}(x_{h}, t_{k})$$

= $Au_{h}(t_{k}) + f(x_{h}, t_{k}) - (u_{xx}(x_{h}, t_{k}) + f(x_{h}, t_{k}))$
= $Au_{h}(t_{k}) - Au(x_{h}, t_{k}) + Au(x_{h}, t_{k}) - u_{xx}(x_{h}, t_{k})$
= $Ae_{h}(t_{k}) + r(t_{k}),$

where $r(t_k) = Au(x_h, t_k) - u_{xx}(x_h, t_k)$.

Let $E_h := E_h(t_h)$ be the long vector consisting of the vectors $e_h(t_k)$, for k = 0 to N - 1, stacked one on top of the other. Similarly, define \tilde{R}_h as the long vector consisting of the vectors $r(t_k)$:

(3.6)
$$E_h = \begin{bmatrix} e_h(t_0) \\ \vdots \\ e_h(t_{N-1}) \end{bmatrix}, \qquad \tilde{R}_h = \begin{bmatrix} r(t_0) \\ \vdots \\ r(t_{N-1}) \end{bmatrix}.$$

The system $e'_h(t_k) = Ae_h(t_k) + r(t_k)$ for all k can be more compactly represented as

$$E'_h(t_h) = (I_N \otimes A)E_h + \tilde{R}_h.$$

Applying $B^T \otimes I_{N-1}$ on both sides leads to

$$E_h = (B^T \otimes A)E_h + (B^T \otimes I_{N-1})\tilde{R}_h + \delta$$

where δ is a long vector with matrix representation Φ . Let Φ_j be the *j*th row of Φ . According to Lemma 3.3, $|\Phi_j|_2 \leq cN^{1/2}e^{-CN}$. The above equality can also be written as

(3.7)
$$\mathcal{A}_h E_h = R_h, \qquad R_h = (B^T \otimes I_{N-1})\tilde{R}_h + \delta.$$

See (3.5).

THEOREM 3.8. Let $N \geq 2$ and λ be an eigenvalue of A_h . Then

$$1 \le |\lambda| \le cN^4.$$

Proof. Let (v_h, λ) be an eigenpair of the matrix \mathcal{A}_h . Then it follows from (3.7) that $(\lambda - 1)v_h = -(B^T \otimes A)v_h$, or

$$\lambda - 1 = \gamma_j \mu_k,$$

where γ_j is some eigenvalue of B^T and μ_k is some eigenvalue of -A. The lower bound $|\lambda| > 1$ follows from Proposition 3.4 and Lemma 3.6. From (3.8), an upper bound of $|\lambda|$ follows from Lemmas 3.5 and 3.6:

$$|\lambda| \le 1 + |\gamma_j| \mu_k \le 1 + cN^4. \qquad \Box$$

We are able to derive the same upper bound for the magnitude of the eigenvalue using the technique of [9] but not the lower bound. The technique employed here is much simpler conceptually because the analysis reduces to an eigenvalue analysis of B^T and A.

THEOREM 3.9. For any integer $N \ge 2$, let u be the solution of the heat equation (3.1). Assume that u(x,t) is separately analytic in each variable. Let u_h be the solution of (3.4) and E_h be the long error vector defined in (3.6). Then

$$|W^{1/2}E_h|_2 \le cN^{3.5}e^{-CN}.$$

Proof. The proof uses Lemmas 3.7 and 3.5. It is similar to the proof given for the Legendre case in [9] and is not presented here. See [11]. \Box

We remark that for $f \in P_N$ and f_h , the long vector of f evaluated at the collocation points satisfies

$$\left(\int_{-1}^{1}\int_{-1}^{1}|f(x,t)|^{2}w(x)\,dx\,w(t)\,dt\right)^{1/2} \leq |W^{1/2}f_{h}|_{2}$$
$$\leq 2\left(\int_{-1}^{1}\int_{-1}^{1}|f(x,t)|^{2}w(x)\,dx\,w(t)\,dt\right)^{1/2},$$

using the equivalence of the weighted L^2 - and the discrete norms. This is the main reason for measuring the error in the discrete norm.

To measure the difficulty to solve a linear system with the coefficient matrix M, we sometimes use the spectral condition number, defined by

$$\kappa(M) = \frac{\max_{\lambda \in \Lambda(M)} |\lambda|}{\min_{\lambda \in \Lambda(M)} |\lambda|},$$

where $\Lambda(M)$ is the spectrum of M. Using the result of Theorem 3.8, it is easy to estimate the spectral condition number of the space-time spectral collocation method:

COROLLARY 3.10. Let $N \ge 2$. Then

$$\kappa(\mathcal{A}_h) \leq cN^4.$$

Note that a direct solver for (3.5) is the method of Bartels and Stewart [1].

4. A second space-time collocation method. We now give an alternate space-time spectral numerical method for the solution $u \in P_N$ of the heat equation (3.1). The spectral equations are

$$(I_{N+1} \otimes D)u_h = (D^2 \otimes I_{N+1})u_h + f_h,$$

where u_h and f_h are the vectors of u and f, respectively, evaluated at the collocation points. (The order of the variables is different from that of the first method for historical reasons.) Let \hat{u}_h denote the vector u_h obtained by deleting the components corresponding to boundary points and initial points, and similarly, \hat{f}_h is the vector f_h after removing the components corresponding to boundary points and initial points. The linear equation to be solved becomes

(4.1)
$$A_h \hat{u}_h = \hat{f}_h - (u_{0h} \otimes d_h), \qquad A_h = (I_{N-1} \otimes [D]) - (\llbracket D^2 \rrbracket \otimes I_N).$$

Let $vec(U_h) = \hat{u}_h$ and $vec(F_h) = \hat{f}_h - (u_{0h} \otimes d_h)$. Here U_h and F_h are $N \times (N-1)$ matrices. Then the above equation is equivalent to the Sylvester equation $[D]U_h - U_h [\![D^2]\!]^T = F_h$. This matrix system can be solved in $O(N^3)$ operations by the algorithm of Bartels and Stewart.

Let us see if there is any relation between this formulation and (3.5). Recall that $A = \llbracket D^2 \rrbracket$. If the two methods are equivalent, that is, they yield the same matrix equation and, of course, have the same solution (under exact arithmetic), then $V_h = U_h^T$. Taking the transpose of the second system results in $V_h[D]^T - AV_h = F_h^T$ or $V_h - AV_h[D]^{-T} = F_h^T[D]^{-T}$. Unfortunately, from Lemma 3.2, $[D]^{-T}$ is not identical to B (this can also be verified by an explicit computation for small values of N), and so the two methods are different.

In [9], it was mentioned that the second method for Legendre space-time collocation is easier to implement for more complicated PDEs. The same reasoning also applies here to the Chebyshev case.

Next we state two useful results, where the first one is a sharpening of a result proved in [14] in the context of stability theory of a linear hyperbolic PDE. The sharper result is not needed in this paper but is crucial in the upcoming work [10]. Its proof is postponed to the appendix.

PROPOSITION 4.1. Let $N \ge 1$. The real part of every eigenvalue of [D] is positive and bounded away from zero.

LEMMA 4.2. Let $N \ge 1$ and λ be an eigenvalue of [D]. Then $|\lambda| \le cN^2$.

Proof. An upper bound for the magnitude of an eigenvalue of D is well known and also equals cN^2 . Its proof is very similar to the proof of this lemma which is included here for completeness.

Let v_h be an eigenvector corresponding to λ and v be the unique polynomial of degree at most N so that v(-1) = 0 and $v(t_h) = v_h$. Note that $[D]v_h = \lambda v_h$ and $[D]v_h = v'(t_h)$, with the latter holding true due to the fact that v is a polynomial of degree at most N and the action of [D] on $v(t_h)$ gives its derivative exactly at the collocation points. It follows that $v'(t_i) = \lambda v(t_i)$, for $0 \le j < N$, and so

$$\sum_{j=0}^{N} v'(t_j) \overline{v(t_j)} \rho_j = \lambda \sum_{j=0}^{N} |v(t_j)|^2 \rho_j.$$

Note that the above two terms corresponding to j = N are both zero since v(-1) = 0. Since Chebyshev quadrature is exact for polynomials of degree at most 2N - 1, the left-hand side is equal to the integral

$$\int_{-1}^{1} v'(t)\overline{v(t)}w(t) \, dt \le \sqrt{\int_{-1}^{1} |v'|^2 w} \, \sqrt{\int_{-1}^{1} |\bar{v}|^2 w} \le cN^2 \int_{-1}^{1} |v|^2 w,$$

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with the last inequality holding true due to the inverse estimate (2.3). Thus,

$$|\lambda| = \frac{\left|\int_{-1}^{1} v' \bar{v} w\right|}{\sum_{j=0}^{N} |v(t_j)|^2 \rho_j} \le c N^2 \frac{\int_{-1}^{1} |v|^2 w}{\sum_{j=0}^{N} |v(t_j)|^2 \rho_j} \le C N^2$$

by the equivalence of the discrete and the weighted L^2 -norms.

The theorem below states that the spectral condition number of the discrete spectral differentiation operator scales like $O(N^4)$.

THEOREM 4.3. Let $N \ge 2$. Let A_h be the Chebyshev spectral collocation matrix defined above. Then

$$\kappa(A_h) \le CN^4.$$

Proof. Let $\{\gamma_j\}$ be the set of eigenvalues of [D] and $\{\mu_j\}$ be those of $-\llbracket D^2 \rrbracket$. From (4.1), it follows that for some j, k,

$$\lambda = \gamma_j + \mu_k.$$

From Proposition 4.1 and Lemma 3.6, $\Re \gamma_j$, $\mu_k \ge c$, for some positive constant c independent of N. Hence $\Re \lambda \ge 2c$, which implies that $|\lambda| \ge 2c$. From Lemmas 4.2 and 3.6, it follows that

$$|\lambda| \le CN^2 + cN^4 \le C_1 N^4.$$

Combine the above two inequalities to obtain

$$\kappa(A_h) \le cN^4$$
.

The convergence analysis is very similar to the one in the previous section. Let v be analytic in a region in the complex plane containing the real interval [-1, 1] and v(-1) = 0. Let $0 \le k < N$ and $\epsilon_k = (v - \mathcal{I}_N v)'(t_k)$. From [12], it is known that $|\epsilon_k|_{\infty} \le cN^2 e^{-CN}$. Observe that

$$v'(t_k) = (\mathcal{I}_N v)'(t_k) + (v - \mathcal{I}_N v)'(t_k)$$

= $([D] (\mathcal{I}_N)v(t_h))_k + \epsilon_k = ([D] v(t_h))_k + \epsilon_k.$

Recall the error equation

$$e'(t_k) = Ae(t_k) + r(t_k), \qquad 0 \le k < N,$$

where $r(t_k) = Au(x_h, t_k) - u_{xx}(x_h, t_k)$. Let $1 \le j \le N - 1$ and $e_j(t_k)$ refer to the *j*th component of $e(t_k)$, and define

$$e_j(t_h) = \begin{bmatrix} e_j(t_0) \\ \vdots \\ e_j(t_{N-1}) \end{bmatrix}, \qquad E_h = \begin{bmatrix} e_1(t_h) \\ \vdots \\ e_{N-1}(t_h) \end{bmatrix}, \qquad \tilde{R}_h = \begin{bmatrix} r_1(t_h) \\ \vdots \\ r_{N-1}(t_h) \end{bmatrix}.$$

Note that these vectors are the same as those defined in (3.6) except for a different ordering. Then, from the previous calculation, we have

$$([D]e_j(t_h))_k + \epsilon_{jk} = e'_j(t_k) = (Ae_h(t_k))_j + r_j(t_k),$$



FIG. 5.1. Convergence of the Chebyshev collocation method (A_h) for the heat equation.

where $|\epsilon_{jk}|_{\infty} \leq N^2 e^{-CN}$, or

$$A_h E_h = R_h := \tilde{R}_h - \epsilon,$$

where ϵ is a long vector formed by stacking together the vectors $\epsilon_j = [\epsilon_{j0}, \ldots, \epsilon_{j,N-1}]^T$. Using exactly the same analysis as before, the following convergence result can be shown:

THEOREM 4.4. For any integer $N \ge 2$, let u be the solution of the heat equation (3.1). Assume that u(x,t) is separately analytic in each variable. Then

$$|W^{1/2}E_h|_2 \le cN^{3.5}e^{-CN}$$

5. Numerical results. We have implemented a very simple Chebyshev collocation MAT-LAB program. First consider the heat equation

$$u_t = u_{xx} + f,$$

with boundary conditions $u(\pm 1, t) = 0$ and initial condition $u(x, -1) = u_0(x)$. Take f so that the exact solution is $u(x, t) = e^{x+t} \sin(\pi t/2) \sin \pi x$. For the method of Tang and Xu, the spectral convergence is clearly illustrated in Figure 5.1. Note that the error E_h is $O(10^{-14})$ at N = 18, which corresponds to a system with 306 unknowns. The spectrum of the discrete heat operator \mathcal{A}_h for the case N = 60 and a plot of the spectral condition numbers as a function of N are displayed in Figure 5.2. The corresponding figures for the second method (A_h) are given in Figures 5.3 and 5.4.

We also performed some numerical experiments for some nonlinear PDEs: the Allen-Cahn equation and the viscous Burgers' equations. Since the numerical results are very similar to the Legendre case, we do not include those in this paper. See [11].

It is straightforward to extend the methods to two spatial dimensions. As an illustration, take f so that the solution of the 2D heat equation $u_t = \Delta u + f$ on the spatial domain $(-1, 1)^2$ is

$$u(x, y, t) = e^{x+y+t+1} \sin \pi x \sin \pi y.$$

The convergence for the second method of Section 4 is illustrated in Figure 5.5.



FIG. 5.2. Spectrum (left) and spectral condition number (right) for the heat operator A_h .



FIG. 5.3. Convergence of the Chebyshev collocation method (A_h) for the heat equation.



FIG. 5.4. Spectrum (left) spectral condition number (right) for the heat operator A_h .



FIG. 5.5. Convergence of 2D heat equation. The error is the maximum error at the final time t = 1.

6. Discussion and conclusion. In this paper, we have shown that the space-time Chebyshev collocation method of Tang and Xu [19] converges spectrally in both space and time for the heat equation. The condition number of this method is shown to be bounded by $O(N^4)$. We have also proposed another space-time spectral collocation which is easier to implement and has similar characteristics as the first one. The analysis relies on new sharp estimates of the spectra of [D] and B^T . Some simple numerical experiments verify the theoretical results: the space-time spectral convergence and an $O(N^4)$ condition number of both methods. Numerical results for the viscous Burgers' and the Allen-Cahn equations demonstrate the potential of this method for nonlinear PDEs.

In [10], we have extended our analysis to other standard linear PDEs (Schrödinger, Airy, wave, and beam equations) and conducted numerical experiments for common nonlinear PDEs (nonlinear reaction diffusion equation from combustion, nonlinear Schrödinger, KdV, Sine-Gordon, Kuramoto-Shivashinsky and Cahn-Hilliard) with similar results. It is remarkable that space-time spectral methods work so well for these different classical PDEs with different features: diffusion, dispersion, nonlinear advection, etc.

Space-time spectral methods are extremely robust methods, which converge spectrally for most standard linear PDEs with standard boundary conditions. They deserve more investigations, especially more sophisticated algorithms to speed up the linear algebra.

Appendix A. Proofs of the propositions. In this appendix, we prove Propositions 3.4 and 4.1.

First, the following preliminary result due to [14] is useful. Since no proof was given there, we include it here for completeness.

LEMMA A.1. Let $N \ge 1$. If $f = \sum_{k=0}^{4N-1} b_k T_k$ for some complex constants b_k , then

$$\sum_{j=0}^{N} \rho_j f(t_j) = \int_{-1}^{1} f(t) w(t) dt + \pi b_{2N}.$$

Proof. Using the definition of f,

$$\begin{split} \sum_{j=0}^{N} \rho_{j} f(t_{j}) &- \int_{-1}^{1} f(t) w(t) dt = \sum_{j=0}^{N} \rho_{j} \sum_{k=0}^{4N-1} b_{k} T_{k}(t_{j}) - \int_{-1}^{1} \sum_{k=0}^{4N-1} b_{k} T_{k}(t) w(t) dt \\ &= \sum_{k=0}^{2N-1} b_{k} \bigg[\sum_{j=0}^{N} \rho_{j} T_{k}(t_{j}) - b_{k} \int_{-1}^{1} T_{k}(t) w(t) dt \bigg] \\ &+ b_{2N} \bigg[\sum_{j=0}^{N} \rho_{j} T_{2N}(t_{j}) - \int_{-1}^{1} T_{2N}(t) w(t) dt \bigg] \\ &+ \sum_{k=2N+1, \, k \text{ even}}^{4N-1} b_{k} \bigg[\sum_{j=0}^{N} \rho_{j} T_{k}(t_{j}) - \int_{-1}^{1} T_{k}(t) w(t) dt \bigg] \\ &+ \sum_{k=2N+1, \, k \text{ odd}}^{4N-1} b_{k} \bigg[\sum_{j=0}^{N} \rho_{j} T_{k}(t_{j}) - \int_{-1}^{1} T_{k}(t) w(t) dt \bigg] \\ &=: S_{1} + S_{2} + S_{3} + S_{4}. \end{split}$$

 $S_1 = 0$ since Chebyshev-Gaussian quadrature is exact for any polynomial of degree at most 2N - 1. Using the identity

(A.1)
$$2T_m T_n = T_{m+n} + T_{|m-n|},$$

 $T_{2N} = 2T_N^2 - 1$ follows immediately. Then, for the term S_2 , we find

$$\begin{split} \sum_{j=0}^{N} \rho_j T_{2N}(t_j) &- \int_{-1}^{1} T_{2N}(t) w(t) dt = \sum_{j=0}^{N} \rho_j (2T_N^2(t_j) - 1) - \int_{-1}^{1} (2T_N^2(t) - 1) w(t) dt \\ &= 2 \left(\sum_{j=0}^{N} \rho_j T_N^2(t_j) - \int_{-1}^{1} T_N^2(t) w(t) dt \right) - \left(\sum_{j=0}^{N} \rho_j - \int_{-1}^{1} w(t) dt \right) \\ &= 2 \left(\pi - \frac{\pi}{2} \right) - 0 = \pi. \end{split}$$

In the above formulas, the definition of the Chebyshev Gauss–Lobatto points $t_j = \cos(j\pi/N)$ has been used to evaluate the penultimate sum:

$$\sum_{j=0}^{N} \rho_j T_N^2(t_j) = \sum_{j=0}^{N} \rho_j \cos^2\left(N \cos^{-1}\left[\cos\left(\frac{\pi j}{N}\right)\right]\right)$$
$$= \sum_{j=0}^{N} \rho_j \cos^2(\pi j) = \sum_{j=0}^{N} \rho_j = \int_{-1}^{1} w(t) dt = \pi.$$

Therefore $S_2 = \pi b_{2N}$. For S_3 , assume k = 2N + 2p, for $1 \le p \le N - 1$. Then,

$$\sum_{j=0}^{N} \rho_j T_{N+p}^2(t_j) = \sum_{j=0}^{N} \rho_j \cos^2\left((N+p)\frac{\pi j}{N}\right)$$
$$= \sum_{j=0}^{N} \rho_j \cos^2\left(\pi j + p\frac{\pi j}{N}\right) = \int_{-1}^{1} T_p^2(t)w(t)dt.$$

From (A.1), $T_{2N+2p} = 2T_{N+p}^2 - 1$, and so

$$\begin{split} \sum_{j=0}^{N} \rho_j T_{2N+2p}(t_j) &- \int_{-1}^{1} T_{2N+2p}(t) w(t) dt \\ &= \sum_{j=0}^{N} \rho_j (2T_{N+p}^2(t_j) - 1) - \int_{-1}^{1} (2T_{N+p}^2(t) - 1) w(t) dt \\ &= 2 \left(\sum_{j=0}^{N} \rho_j T_p^2(t_j) - \int_{-1}^{1} T_p^2(t) w(t) dt \right) - \left(\sum_{j=0}^{N} \rho_j - \int_{-1}^{1} w(t) dt \right) \\ &= 0. \end{split}$$

Consequently, $S_3 = 0$.

Finally, assume k = 2N + 2p + 1, for $0 \le p \le N - 1$. Then,

$$\sum_{j=0}^{N} \rho_j T_{2N+2p+1}(t_j) = \sum_{j=0}^{N} \rho_j \cos\left((2N+2p+1)\frac{\pi j}{N}\right)$$
$$= \sum_{j=0}^{N} \rho_j \cos\left(\frac{(2p+1)\pi j}{N}\right) = \int_{-1}^{1} T_{2p+1}(t)w(t)dt = 0,$$

since T_{2p+1} is an odd function. By the same reason,

$$\int_{-1}^{1} T_{2N+2p+1}(t)w(t) = 0.$$

Therefore

$$\sum_{j=0}^{N} \rho_j T_{2N+2p+1}(t_j) - \int_{-1}^{1} T_{2N+2p+1}(t) w(t) dt = 0,$$

implying that $S_4 = 0$. This completes the proof. \Box

Next we give a proof of Proposition 4.1. As mentioned before, it is an improvement of a result due to [14] which showed that the real part of every eigenvalue of [D] is positive. The technique of proof is directly relevant for the proof of Proposition 3.4.

Proof of Proposition 4.1. Let λ be an eigenvalue of [D] and v be a polynomial of degree N so that v(-1) = 0:

(A.2)
$$v = \sum_{k=0}^{N} a_k T_k,$$

where a_k are complex numbers. Suppose v satisfies the ODE

(A.3)
$$v'(t) = \lambda v(t) + \frac{\lambda a_N}{N} (1-t) T'_N(t).$$

Note that the left-hand side of the above equation is a polynomial of degree N - 1, while the first term at the right-hand side is a polynomial of degree N. The second term at the right-hand

side is a polynomial of degree N and has a constant factor chosen so that the right-hand side is a polynomial of degree N - 1. Observe that

(A.4)
$$v'(t_j) = \lambda v(t_j), \qquad 0 \le j < N.$$

When 0 < j < N, this is true because $T'_N(t_j) = 0$ by definition of the Chebyshev–Lobatto points. When j = 0, then $t_0 = 1$, and the equality is obvious. (A.4) is equivalent to the relation

$$[D]v(t_h) = \lambda v(t_h).$$

Using (A.2), equate the coefficient of t^{N-1} on both sides of (A.3) to obtain

(A.5)
$$a_{N-1} = 2a_N \left(\frac{N}{\lambda} - 1\right).$$

Note that $\lambda \neq 0$ since otherwise, from (A.3) and the initial condition v(-1) = 0, it would follow that $v \equiv 0$ and so $v(t_h)$ is the zero vector which cannot be an eigenvector. If $a_N = 0$, then the left-hand side of (A.3) is a polynomial of degree one less than that at the right-hand side, which is impossible. Henceforth assume $a_N \neq 0$.

Let $\beta \in (0,1)$, whose value will be determined later. Multiply (A.4) by the factor $\rho_j(1-t_j)(1+\beta t_j)\overline{v(t_j)}$, then add the result to the complex conjugate of (A.4) multiplied by $\rho_j(1-t_j)(1+\beta t_j)v(t_j)$, and then sum the equation to obtain

(A.6)
$$\sum_{j=0}^{N} \rho_j f(t_j) = 2R \sum_{j=0}^{N} \rho_j (1-t_j) (1+\beta t_j) |v(t_j)|^2 := C_1 R,$$

where $f(t) = (1-t)(1+\beta t)(|v|^2)'(t)$ is a polynomial of degree 2N+1 and $\lambda = R+iS$ for real R, S. Note that we can extend the above sums to j = N because both terms corresponding to j = N vanish. Note also that C_1 is positive since otherwise $v(t_j) = 0$, for $1 \le j \le N$. From (A.3), $v'(t_j) = 0$, for $1 \le j \le N$, and these conditions imply that $v \equiv 0$. In particular $v(t_h) = 0$, and so it cannot be an eigenvector.

The goal is to show that the left-hand side of (A.6) is positive. To that end, write the left-hand side as F + E, where

$$F = \int_{-1}^{1} f(t) w(t) dt, \qquad E = \sum_{j=0}^{N} \rho_j f(t_j) - F.$$

After integration by parts and some algebra,

$$F = \int_{-1}^{1} \frac{1 - \beta + \beta t + \beta t^2}{1 + t} |v(t)|^2 w(t) dt.$$

It is easy to see that $1 - \beta + \beta t + \beta t^2 \ge c$, which is a positive constant for $\beta \in (0, 4/5)$. Let $z(t) = v(t)/\sqrt{1+t}$, which is continuous on [-1, 1] since v(-1) = 0. Thus

$$F \ge c \int_{-1}^{1} |z(t)|^2 w(t) \, dt =: C_2$$

Write

$$f(t) = \sum_{k=0}^{2N+1} b_k T_k(t),$$

for some coefficients b_k . Then from Lemma A.1, $E = \pi b_{2N}$. Thus $F + E \ge C_2 + \pi b_{2N}$. Since the leading coefficient of T_k is 2^{k-1} and the coefficient of t^{k-1} of T_k is zero, it follows that the coefficient of t^{2N} of f is $2^{2N-1}b_{2N}$, which is equal to the coefficient of t^{2N} of the polynomial

$$-2\Re(a_N\overline{a_{N-1}})(T_{N-1}T_N)'\,\beta t^2 - 2(1-\beta)|a_N|^2T_NT_N'\,t.$$

From (A.2),

$$b_{2N}2^{2N-1} = -2^{2N-2}\Re(a_N\overline{a_{N-1}})(2N-1)\beta - 2^{2N-1}|a_N|^2(1-\beta)N,$$

or

$$b_{2N} = -\beta \Re \left(a_N \overline{a_{N-1}} \right) \frac{2N-1}{2} - |a_N|^2 (1-\beta) N.$$

Substitute (A.5) to get

(A.7)
$$b_{2N} = |a_N|^2 \left(-\beta N(2N-1) \frac{R}{|\lambda|^2} + \beta (2N-1) - (1-\beta)N \right).$$

Now (A.6) becomes

$$C_1 R = E + F \ge C_2 + \pi b_{2N}.$$

Substitute (A.7) into the above inequality to obtain

$$\left(\frac{C_1}{\pi} + \frac{|a_N|^2 \beta N(2N-1)}{|\lambda|^2}\right) R \ge \frac{C_2}{\pi} + |a_N|^2 \left(\beta(3N-1) - N\right).$$

For any value of β satisfying

$$\frac{N}{3N-1} < \beta < \frac{4}{5},$$

it is possible to deduce that

(A.8)
$$\left(\frac{C_1}{\pi} + \frac{2|a_N|^2 N^2}{|\lambda|^2}\right) R \ge C_3,$$

for some positive constant C_3 independent of N. It can be concluded that R > 0.

To show that R is bounded away from zero, first note that from (A.2), for $0 \le k \le N$,

$$a_k ||T_k||_{0,w}^2 = \int_{-1}^1 v T_k w, \qquad ||u||_{0,w}^2 = \int_{-1}^1 u^2 w,$$

leading to

$$|a_k| \le \frac{\|v\|_{0,w} \, \|T_k\|_{0,w}}{\|T_k\|_{0,w}^2} < 1,$$

if we assume the normalization $||v||_{0,w} = 1$. From (A.5), it follows that

$$|a_{N-1}|^2 = 4 \left| \frac{N}{\lambda} - 1 \right|^2 |a_N|^2,$$

or

(A.9)
$$\frac{|a_N|^2 N^2}{|\lambda|^2} = \frac{|a_{N-1}|^2 N^2}{4 |N-\lambda|^2} < \frac{1}{4 \left|1 - \frac{\lambda}{N}\right|^2} = \frac{1}{4 \left[\left(1 - \frac{R}{N}\right)^2 + \frac{S^2}{N^2}\right]}.$$

If N = 1, then [D] = 1/2 = R. Henceforth, assume $N \ge 2$. If R > 1, then we are done. Otherwise, assume $R \le 1$. Then (A.9) becomes

$$\frac{|a_N|^2 N^2}{|\lambda|^2} < \frac{1}{4\left(1 - \frac{1}{N}\right)^2} \le 1$$

since $N \ge 2$. Inserting this inequality into (A.8) immediately yields that $R \ge C_4$ with a positive constant independent of N. \Box

Finally, we prove the remaining proposition.

Proof of Proposition 3.4. When N = 1, 2, the eigenvalues of B^T are 1 and $(1 \pm i/\sqrt{3})/2$, respectively, and they have a positive real part. Henceforth, assume $N \ge 3$. Suppose $\{a_k\}$ is a set of complex constants so that

(A.10)
$$v = \sum_{k=0}^{N} a_k T_k, \quad v(-1) = 0,$$

with $||v||_{0,w} = 1$, and where v satisfies

(A.11)
$$\int_{-1}^{t} v(\tau) d\tau = \lambda v(t) + \frac{a_N}{N(N+1)} (t^2 - 1) T'_N(t),$$

for λ an eigenvalue of B^T . Note that the coefficient $a_N/(N(N+1))$ at the right-hand side of (A.11) has been chosen so that the coefficients of T_{N+1} on both sides of (A.11) agree. It is easy to verify that $B^T v(t_h) = \lambda v(t_h)$. Using the identity

$$\int_{-1}^{t} T_k(\tau) d\tau = \frac{1}{2} \left(\frac{T_{k+1}(t)}{k+1} - \frac{T_{k-1}(t)}{k-1} \right) + \frac{(-1)^{k+1}}{k^2 - 1}, \qquad k \ge 2,$$

and on equating the coefficients of T_N, T_{N-1} , and T_{N-2} on both sides of (A.11), we obtain (details will be given later)

(A.12)
$$\frac{a_{N-1}}{2N} = \lambda a_N,$$

(A.13)
$$\frac{a_{N-2} - a_N}{2(N-1)} = \lambda a_{N-1} - \frac{a_N}{2(N+1)},$$

(A.14)
$$\frac{a_{N-3} - a_{N-1}}{2(N-2)} = \lambda a_{N-2}.$$

(A.11) evaluated at $t = t_j$ reads

(A.15)
$$\int_{-1}^{t_j} v(\tau) d\tau = \lambda v(t_j), \qquad 0 \le j \le N.$$

Let $\beta \in (0,1)$, whose value will be determined later. Multiply (A.15) by the factor $\rho_j(1-t_j)(1-\beta t_j)\overline{v(t_j)}$, then add the result to the complex conjugate of (A.15) multiplied by $\rho_j(1-t_j)(1-\beta t_j)v(t_j)$, and then sum the equations to obtain

(A.16)
$$\sum_{j=0}^{N} \rho_j f(t_j) = 2R \sum_{j=0}^{N} \rho_j (1-t_j) (1-\beta t_j) |v(t_j)|^2 := C_2 R,$$

where

$$f(t) = (1-t)(1-\beta t) \left(\left| \int_{-1}^{t} v(\tau) d\tau \right|^2 \right)'$$

is a polynomial of degree 2N + 3, $R = \Re \lambda$, and C_2 is positive. Note that each term corresponding to j = N in (A.16) vanishes since v(-1) = 0. Write

$$f(t) = \sum_{k=0}^{2N+3} b_k T_k(t)$$

for some complex b_k . By applying Lemma A.1, we have

$$\int_{-1}^{1} f(t)w(t)dt + \pi b_{2N} = C_2 R.$$

After integration by parts, the above identity becomes

(A.17)
$$\int_{-1}^{1} \frac{1+\beta-\beta t-\beta t^2}{1+t} \left| \int_{-1}^{t} v(\tau) d\tau \right|^2 w(t) dt + \pi b_{2N} = C_2 R.$$

Use (A.10), (A.12), (A.13), (A.14) to obtain (details will be given later)

$$\begin{aligned} \text{(A.18)} \qquad b_{2N} &= \frac{1}{2} \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N} + \frac{1}{N+1} \right) \\ &\quad - \frac{(1+\beta)}{4} \left[\Re(\overline{a_N} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N+1} \right) \right. \\ &\quad + \frac{1}{N} |a_{N-1}|^2 - \frac{1}{N-1} |a_N|^2 \right] \\ &\quad + \frac{\beta}{8} \left[\Re(\overline{a_N} a_{N-3}) \left(\frac{1}{N-2} + \frac{1}{N+1} \right) \right. \\ &\quad + \Re(\overline{a_{N-1}} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N} \right) \\ &\quad - \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N-2} + \frac{1}{N-1} \right) \right] \\ &\quad - (1+\beta) |a_N|^2 \left(\frac{c_{N+1}}{(N+1)2^N} + \frac{c_N}{(N+1)2^{N-1}} \right) \\ &\quad + \beta \Re(\overline{a_N} a_{N-1}) \left(\frac{c_{N+1}}{(N+1)2^{N+1}} + \frac{c_N}{N2^{N-1}} + \frac{c_{N-1}}{(N+1)2^{N-1}} \right) \end{aligned}$$

Here $c_k = -2^{k-3}k$ is the second leading coefficient of T_k :

(A.19)
$$T_k(t) = 2^{k-1}t^k + c_k t^{k-2} + \cdots, \qquad k \ge 2.$$

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Substitute the expression for b_{2N} into (A.17) to obtain

(A.20)
$$\int_{-1}^{1} \frac{1+\beta-\beta t-\beta t^2}{1+t} \left| \int_{-1}^{t} v(\tau) d\tau \right|^2 w(t) dt + S_1 = (S_2 + C_2)R,$$

where

$$S_{1} = \pi \frac{(1+\beta)}{4} \frac{N-1}{(N+1)^{2}} |a_{N}|^{2} + \pi \frac{(1+\beta)}{4} \frac{N-1}{N(N+1)} |a_{N-1}|^{2} -\pi (1+\beta) \left(\frac{c_{N+1}}{(N+1)2^{N}} + \frac{c_{N}}{(N+1)2^{N-1}}\right) |a_{N}|^{2} > 0,$$

$$S_{2} = \pi S_{3} |a_{N}|^{2} + \frac{\pi \beta}{2} \frac{(2N-1)(N-2)}{N(N+1)} |a_{N-1}|^{2} -2\pi \beta N |a_{N}|^{2} \left[\frac{c_{N+1}}{(N+1)2^{N+1}} + \frac{c_{N}}{N2^{N-1}} + \frac{c_{N-1}}{(N+1)2^{N-1}}\right],$$

and

$$S_3 = -4\beta \frac{N(2N-1)(N-1)}{N+1}R^2 + 4(1+\beta)\frac{N^2}{N+1}R - \frac{3\beta}{2}\frac{1}{(N+1)^2} - \frac{2N+1}{N+1}R$$

Note that the last term of the expression for S_2 is positive since $c_k < 0$ and the coefficient of $|a_{N-1}|^2$ is positive. Note also that the integral at the left-hand side of (A.20) is positive for $\beta \in (0, 1)$. Hence the remaining goal is to choose β so that S_3 , a quadratic in R, is positive. Toward that end, the maximum of S_3 occurs at

$$R = \frac{1+\beta}{2\beta} \frac{N}{(2N-1)(N-1)}$$

with maximum value

$$\frac{(1+\beta)^2}{\beta} \frac{N^3}{(2N-1)(N^2-1)} - \frac{3\beta}{2} \frac{N}{(N+1)^2} - \frac{2N+1}{N+1}$$

Hence we require

$$\frac{(1+\beta)^2}{\beta} \frac{N^3}{(2N-1)(N-1)} - \frac{3\beta}{2} \frac{N}{N+1} > 2N+1.$$

Notice that for $N \geq 3$,

$$\frac{N^2}{(2N-1)(N-1)} > \frac{1}{2}, \qquad \frac{3}{N+1} < 1.$$

Assume that $\beta < 1/3$, then $1 + \beta > 4\beta$ and

$$\frac{(1+\beta)^2}{\beta} \frac{N^3}{(2N-1)(N-1)} - \frac{\beta}{2} \frac{3N}{N+1} > \frac{15}{2}\beta N.$$

Therefore it is enough to choose β so that

$$\frac{4N+2}{15N}<\beta<\frac{1}{3}.$$

With this choice of β , it follows from (A.20) that R > 0.

Next we supply some details of the above calculations. First we prove (A.12)–(A.14). Apply (A.10) in (A.11) to obtain

(A.21)
$$\sum_{k=0}^{N} a_k \int_{-1}^{t} T_k(\tau) d\tau = \lambda \sum_{k=0}^{N} a_k T_k(t) + \frac{a_N}{N(N+1)} (t^2 - 1) T'_N(t).$$

The left-hand side of this equation is

$$\begin{split} \sum_{k=0}^{N} a_k \int_{-1}^{t} T_k(\tau) d\tau &= a_N \int_{-1}^{t} T_N(\tau) d\tau + a_{N-1} \int_{-1}^{t} T_{N-1}(\tau) d\tau \\ &\quad + a_{N-2} \int_{-1}^{t} T_{N-2}(\tau) d\tau + a_{N-3} \int_{-1}^{t} T_{N-3}(\tau) d\tau + \cdots \\ &= \frac{1}{2} a_N \left[\frac{T_{N+1}}{N+1} - \frac{T_{N-1}}{N-1} \right] + \frac{1}{2} a_{N-1} \left[\frac{T_N}{N} - \frac{T_{N-2}}{N-2} \right] \\ &\quad + \frac{1}{2} a_{N-2} \left[\frac{T_{N-1}}{N-1} - \frac{T_{N-3}}{N-3} \right] + \frac{1}{2} a_{N-3} \left[\frac{T_{N-2}}{N-2} - \frac{T_{N-4}}{N-4} \right] + \cdots \\ &= \frac{a_N}{2(N+1)} T_{N+1} + \frac{a_{N-1}}{2N} T_N + \left(\frac{a_{N-2}}{2(N-1)} - \frac{a_N}{2(N-1)} \right) T_{N-1} \\ (A.22) \qquad \qquad + \left(\frac{a_{N-3}}{2(N-2)} - \frac{a_{N-1}}{2(N-2)} \right) T_{N-2} + \cdots . \end{split}$$

The second term at the right-hand side of (A.21) is

$$\begin{aligned} \frac{a_N}{N(N+1)}(t^2-1)T'_N(t) &= \frac{a_N}{(N+1)}(t^2-1) \left[\frac{T'_N(t)}{N} - \frac{T'_{N-2}(t)}{N-2} + \frac{T'_{N-2}(t)}{N-2} - \frac{T'_{N-4}(t)}{N-4} + \frac{T'_{N-4}(t)}{N-4} \right] \\ &= \frac{a_N}{(N+1)} 2(t^2-1) \left[T_{N-1} + T_{N-3} + \frac{T'_{N-4}(t)}{2(N-4)} \right] \\ &= \frac{a_N}{(N+1)} \left[2t^2 T_{N-1} + 2t^2 T_{N-3} - 2T_{N-1} - 2T_{N-3} + \cdots \right] \\ &= \frac{a_N}{(N+1)} \left[t(T_N + T_{N-2}) + t(T_{N-2} + T_{N-4}) - 2T_{N-1} - 2T_{N-3} + \cdots \right] \\ &= \frac{a_N}{(N+1)} \left[\frac{1}{2} (T_{N+1} + T_{N-1} + T_{N-3} + T_{N-3} + T_{N-3} + T_{N-1} + T_{N-3} + \cdots \right]. \end{aligned}$$

So the right-hand side of (A.21) becomes

$$\lambda \sum_{k=0}^{N} a_k T_k(t) + \frac{a_N}{N(N+1)} (t^2 - 1) T'_N(t)$$

= $\lambda a_N T_N(t) + \lambda a_{N-1} T_{N-1}(t) + \lambda a_{N-2} T_{N-2}(t) + \dots$
+ $\frac{a_N}{(N+1)} \left[\frac{1}{2} (T_{N+1} + 3T_{N-1} + 4T_{N-3} + \dots) - 2T_{N-1} - 2T_{N-3} + \dots \right]$
(A.23) = $\frac{a_N}{2(N+1)} T_{N+1} + \lambda a_N T_N(t) + \left[\lambda a_{N-1} - \frac{a_N}{2(N+1)} \right] T_{N-1}(t)$
+ $\lambda a_{N-2} T_{N-2}(t) + \dots$

Therefore by equating the coefficients of equations (A.22) and (A.23), we arrive at (A.12)–(A.14).

Next we show that the following equalities follow from (A.12)–(A.14):

(A.24)
$$\frac{1}{2N}\Re(a_{N-1}\overline{a_N}) = R |a_N|^2,$$

(A.25)
$$\frac{1}{2(N-1)}\Re(a_{N-2}\overline{a_{N-1}}) = R\left(|a_{N-1}|^2 + \frac{2N}{N^2 - 1}|a_N|^2\right),$$

(A.26)
$$\frac{1}{N-1}\Re(a_{N-2}\overline{a_N}) = \left(8NR^2 + \frac{2}{N^2 - 1}\right)|a_N|^2 - \frac{1}{N}|a_{N-1}|^2,$$

(A.27)
$$\frac{1}{N-2}\Re(a_{N-3}\overline{a_N}) = \left(32N(N-1)R^3 + \left[\frac{4}{N+1} + \frac{2N}{N-2}\right]R\right)|a_N|^2 - \frac{6(N-1)}{N}R|a_{N-1}|^2.$$

Observe that (A.24) follows directly from (A.12). From (A.13), we find

$$\frac{1}{2(N-1)}a_{N-2} = \lambda a_{N-1} + \frac{1}{N^2 - 1}a_N.$$

Use this equation and (A.12) to arrive at (A.25) and

(A.28)
$$\frac{1}{N-1}\Re(a_{N-2}\overline{a_N}) = \lambda a_{N-1}\overline{a_N} + \overline{\lambda}\overline{a_{N-1}}a_N + \frac{2}{N^2-1}|a_N|^2.$$

Also from (A.12)

(A.29)
$$\frac{1}{N}|a_{N-1}|^2 = \lambda a_N \overline{a_{N-1}} + \overline{\lambda} \overline{a_N} a_{N-1}.$$

Add (A.28) and (A.29), and use (A.24) to recover (A.26). The following equations follow from (A.14) and (A.12), respectively:

(A.30)
$$\frac{1}{N-2}\Re(a_{N-3}\overline{a_N}) = \lambda a_{N-2}\overline{a_N} + \overline{\lambda}\overline{a_{N-2}}a_N + \frac{1}{N-2}\Re(a_N\overline{a_{N-1}}),$$

and

(A.31)
$$\frac{1}{N}\Re(a_{N-1}\overline{a_{N-2}}) = \lambda a_N\overline{a_{N-2}} + \overline{\lambda}\overline{a_N}a_{N-2}.$$

Add (A.30) and (A.31) to get

$$\frac{1}{N-2}\Re(a_{N-3}\overline{a_N}) + \frac{1}{N}\Re(a_{N-1}\overline{a_{N-2}}) = 4R\,\Re(a_N\overline{a_{N-2}}) + \frac{1}{N-2}\Re(a_N\overline{a_{N-1}}).$$

Combine the above, (A.24), (A.25), and (A.26) to get (A.27).

Finally we derive the expression for b_{2N} . Apply (A.10) and performing some calculations leads to

$$\begin{split} \bar{v} \int v + v \int \bar{v} \\ &= 2|a_N|^2 (T_N \int T_N) + 2|a_{N-1}|^2 (T_{N-1} \int T_{N-1}) \\ &+ 2\Re(\overline{a_N}a_{N-1}) \left(T_N \int T_{N-1} + T_{N-1} \int T_N \right) \\ &+ 2\Re(\overline{a_N}a_{N-2}) \left(T_N \int T_{N-2} + T_{N-2} \int T_N \right) \\ &+ 2\Re(\overline{a_N}a_{N-3}) \left(T_N \int T_{N-3} + T_{N-3} \int T_N \right) \\ &+ 2\Re(\overline{a_{N-1}}a_{N-2}) \left(T_{N-1} \int T_{N-2} + T_{N-2} \int T_{N-1} \right) + \cdots \\ &= |a_N|^2 \left(T_N \left[\frac{T_{N+1}}{N+1} - \frac{T_{N-1}}{N-1} \right] \right) + |a_{N-1}|^2 \left(T_{N-1} \left[\frac{T_N}{N} - \frac{T_{N-2}}{N-2} \right] \right) \\ &+ \Re(\overline{a_N}a_{N-1}) \left(T_N \left[\frac{T_N}{N} - \frac{T_{N-2}}{N-2} \right] + T_{N-1} \left[\frac{T_{N+1}}{N+1} - \frac{T_{N-1}}{N-1} \right] \right) \\ &+ \Re(\overline{a_N}a_{N-2}) \left(T_N \left[\frac{T_{N-2}}{N-2} - \frac{T_{N-4}}{N-4} \right] + T_{N-3} \left[\frac{T_{N+1}}{N+1} - \frac{T_{N-1}}{N-1} \right] \right) \\ &+ \Re(\overline{a_{N-1}}a_{N-2}) \left(T_{N-1} \left[\frac{T_{N-1}}{N-1} - \frac{T_{N-3}}{N-3} \right] + T_{N-2} \left[\frac{T_N}{N} - \frac{T_{N-2}}{N-2} \right] \right) + \cdots , \end{split}$$

where \cdots denotes the remaining parts in the expansion. By (A.19),

$$\begin{split} \bar{v}(t) \int_{-1}^{t} v(\tau) d\tau + v(t) \int_{-1}^{t} \bar{v}(\tau) d\tau \\ &= \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N} + \frac{1}{N+1} \right) 2^{2N-2} t^{2N} \\ &+ \left[\Re(\overline{a_N} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N+1} \right) \right. \\ &+ \frac{1}{N} |a_{N-1}|^2 - \frac{1}{N-1} |a_N|^2 \right] 2^{2N-3} t^{2N-1} \\ &+ \left[\Re(\overline{a_N} a_{N-3}) \left(\frac{1}{N-2} + \frac{1}{N+1} \right) + \Re(\overline{a_{N-1}} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N} \right) \right. \\ &- \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N-2} + \frac{1}{N-1} \right) \right] 2^{2N-4} t^{2N-2} \end{split}$$

$$+ |a_N|^2 \left(\frac{c_{N+1}}{N+1} 2^{N-1} + \frac{c_N}{N+1} 2^N \right) t^{2N-1} + \Re(\overline{a_N}a_{N-1}) \left(\frac{c_{N+1}}{N+1} 2^{N-2} + \frac{c_N}{N} 2^N + \frac{c_{N-1}}{N+1} 2^N \right) t^{2N-2} + \cdots .$$

Then

$$\begin{split} f(t) &= \left(1 - (1+\beta)t + \beta t^2\right) \left(\bar{v}(t) \int_{-1}^{t} v(\tau) d\tau + v(t) \int_{-1}^{t} \bar{v}(\tau) d\tau\right) \\ &= \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N} + \frac{1}{N+1}\right) 2^{2N-2} t^{2N} \\ &- (1+\beta) \left[\Re(\overline{a_N} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N+1}\right) \right. \\ &+ \frac{1}{N} |a_{N-1}|^2 - \frac{1}{N-1} |a_N|^2 \right] 2^{2N-3} t^{2N} \\ &+ \beta \left[\Re(\overline{a_N} a_{N-3}) \left(\frac{1}{N-2} + \frac{1}{N+1}\right) + \Re(\overline{a_{N-1}} a_{N-2}) \left(\frac{1}{N-1} + \frac{1}{N}\right) \right. \\ &- \Re(\overline{a_N} a_{N-1}) \left(\frac{1}{N-2} + \frac{1}{N-1}\right) \right] 2^{2N-4} t^{2N} \\ &- (1+\beta) |a_N|^2 \left(\frac{c_{N+1}}{N+1} 2^{N-1} + \frac{c_N}{N+1} 2^N\right) t^{2N} \\ &+ \beta \Re(\overline{a_N} a_{N-1}) \left(\frac{c_{N+1}}{N+1} 2^{N-2} + \frac{c_N}{N} 2^N + \frac{c_{N-1}}{N+1} 2^N\right) t^{2N} \\ &= 2^{2N-1} b_{2N} t^{2N} + \cdots, \end{split}$$

where b_{2N} is given by (A.18).

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