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The Origin and Nature of Spurious Eigenvalues in the Spectral Tau Method[1]

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The Chebyshev–tau spectral method for approximating eigenvalues of boundary value problems may produce spurious eigenvalues with large positive real parts, even when all true eigenvalues of the problem are known to have negative real parts. We explain the origin and nature of the "spurious eigenvalues" in an example problem. The explanation will demonstrate that the large positive eigenvalues are an approximation of infinite eigenvalues in a nearby generalized eigenvalue problem.

Key Words: spectral methods, Chebyshev–tau method; spurious eigenvlaues; generalized eigenvalue problems.

1. INTRODUCTION

Spectral methods of numerical solution for some differential eigenvalue problems, including hydrodynamic stability problems may produce a set of "spurious eigenvalues" along with approximations to the true eigenvalues. An extensive literature that includes the early work of [11] and later in [3, 5, 9, 16, 21, 24, 25] documents this phenomenon. The intent of the present paper is to uncover the nature and origin of these "spurious eigenvalues" in the context of a typical model problem, proving that they exist at all orders of truncation in the Chebyshev–tau method, proving that "spurious eigenvalues" exist at all orders of truncation in a range of associated spectral methods, establishing how they behave under increases in truncation order for a range of spectral approximation methods, and explaining why they arise. Several authors have asserted that the spurious eigenvalues

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are a consequence of the "discretization" of the problem, while other authors have stated that the reason for the occurrence of the spurious eigenvalues is unknown. Our explanation will show that the spurious eigenvalues are an approximation of infinite eigenvalues in a generalized eigenvalue problem from a "nearby" Legendre spectral approximation of the boundary value problem. Our explanation of the origin of the spurious eigenvalues gives a reason *ad hoc* methods for eliminating the spurious eigenvalues work. Thus, this paper should give users of the Chebyshev–tau method, one of several spectral methods available, guidance in the method's use for approximating eigenvalues.

Previous authors usually define "spurious eigenvalues" as the positive or unstable eigenvalues when it is obvious that positive eigenvalues are not eigenvalues of the model problem under investigation. Here we show that some negative eigenvalues arising from the *ad hoc* methods for eliminating spurious eigenvalues share perturbation and growth characteristics with the spurious eigenvalues from the direct Chebyshev–tau method. This provides a clue about the nature and origin of the "spurious eigenvalues" as approximations of infinite eigenvalues in a generalized eigenvalue problem and permits a generalized definition of spurious eigenvalues.

The Chebyshev–tau method and other spectral methods applied to the model problem lead to a generalized eigenvalue problem of the form $A\mathbf{x} = \lambda B\mathbf{x}$. Stewart and Sun [20] have a complete theory for generalized eigenvalues that we use extensively. A more symmetric form of the generalized eigenvalue problem is $\beta A\mathbf{x} = \alpha B\mathbf{x}$, where a pair of complex numbers α, β with ratio $\lambda = \alpha/\beta$ becomes a generalized eigenvalue. More precisely, since pairs of complex numbers α, β with common ratio λ represent the same eigenvalue, lines through the origin in the complex plane $\mathbb{C}^2$ represent generalized eigenvalues. More simply, lines through the origin correspond to points on the unit circle. For the model problem we consider it is simpler yet, since we can take α, β to be real numbers, and so we can picture the generalized eigenvalues as points on the unit circle in $\mathbb{R}^2$. The important point to notice now is that if B has a nontrivial null-space while A is nonsingular, then $\alpha = 1$, $\beta = 0$ is a generalized eigenvalue. This pair $(1, 0)$ is an "infinite eigenvalue." The point $(1, 0)$ now acts as a "point at infinity." Perturbations can then move the eigenvalue into either the upper half-plane, or the lower half-plane, resulting in respectively a large-magnitude positive or negative ratio; see the schematic diagrams in Fig. 1.

Aside from the spurious eigenvalues, the Chebyshev–tau method computes the remaining eigenvalues accurately and efficiently, accounting for the method's popularity and utility.

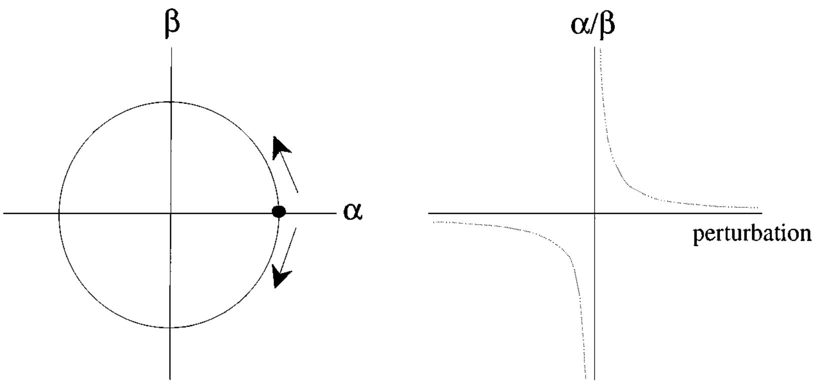

FIG. 1. Schematic diagram of perturbations of generalized eigenvalues.

The practical effect of the existence of "spurious eigenvalues" is to cast doubt on results obtained from the application of the Chebyshev–tau method to a stability analysis of a flow or structure. If positive eigenvalues, indicating exponential growth of a disturbance, are really spurious then the analyst may conclude incorrectly that the system is unstable. It is important to either alter the method to not compute spurious modes or to identify spurious modes so that they can be ignored in the analysis. Works addressing elimination of spurious modes include [9, 13, 16, 25] and those that simply state that spurious modes were computed and then ignored include [3, 22, 24]. The perturbation results in this paper give a more effective means of identifying spurious eigenvalues through their growth in magnitude as a function of truncation order.

We begin in Section 2 by defining the model problem that guides the explanation of the spurious eigenvalues in the spectral–tau method. Section 3 describes a parity reduction of the problem that simplifies later work. In Section 4 we then derive the characteristic polynomial, first in the Chebyshev–tau case, then in the more general Gegenbauer–tau case. This allows us to determine the sign and growth of the largest magnitude eigenvalues for the entire range of tau methods. Section 5 starts with a reduction to an equivalent basis of monomials instead of Gegenbauer polynomials to reduce the matrices to standard triangular-Hessenberg form. We can then apply the theory for generalized eigenvalues to show the model problem has an infinite generalized eigenvalue. For the related Gegenbauer–tau spectral methods, we show there is a generalized eigenvalue that is a perturbation of the infinite eigenvalue. We determine the size of the perturbation and find that it matches the growth of the magnitude of the eigenvalues from the characteristic polynomial method derived previously. Section 6 gives the explanation of the origin of infinite generalized eigenvalue in the Legendre–tau method. The boundary conditions and the form of the Legendre polynomials coincide, permitting the existence of a special solution corresponding to the infinite eigenvalue. Finally, we present some conclusions based on this paper's results. Some background facts are in an appendix.

2. THE MODEL PROBLEM AND THE TAU METHOD

We will consider the model problem

$$\begin{gathered} u^{(4)} = su'', \quad -1 < x < 1, \\ u(-1) = u(1) = u'(-1) = u'(1) = 0 \end{gathered} \tag{1}$$

for the occurrence of spurious eigenvalues when applying the Chebyshev–tau method to boundary value problems. The model problem occurs in [11, pp. 143–144] from a separation of variables applied to a one-dimensional model of the vorticity-streamfunction equations for low Reynolds number incompressible flow. This model problem is also considered in [9, 13, 16].

A similar boundary value problem occurs in hydrodynamic stability analysis in spherical coordinates,

$$\begin{gathered} D^2 u = sDu, \quad r_1 < r < r_2, \\ u(r_1) = u(r_2) = u'(r_1) = u'(r_2) = 0, \end{gathered}$$

where the second-order differential operator,

$$Du = u''(r) + \frac{2}{r}u' - \frac{l(l+1)u}{r^2},$$

occurs, instead of the second-derivative operator. The operator D arises from the spectral decomposition of the Laplacian in spherical coordinates. This problem also has spurious eigenvalues when applying the Chebyshev–tau method. See [9, 10, 23] for details. The structural similarity to the model problem (1) is obvious.

Another example is the Orr–Sommerfeld stability equation for plane Poiseuille flow

$$\left[u^{(4)} - 2\alpha^2 u'' + \alpha^4 u\right]/(-i\alpha R) + [(U - s)(u'' - \alpha^2 u) - U''u] = 0, \quad -1 < x < 1,$$

with boundary conditions

$$u(-1) = u(1) = u'(-1) = u'(1) = 0,$$

where u is the amplitude of the velocity disturbance, α is the wavenumber, R is the Reynolds number, the stability parameter for this problem, and $U(x) = 1 - x^2$ is the known steady base flow whose stability is being examined. It is important to know the value of R, where at least one eigenvalue first has a positive imaginary part as R is increased from zero, because for this eigenvalue the disturbance will grow exponentially in time, instead of being damped out. For more details see [9, 17, 24]. In this problem, $[u^{(4)} - 2\alpha^2 u'' + \alpha^4 u]/(-i\alpha R)$ is a fourth-order differential operator and $[(U - s)(u'' - \alpha^2 u) - U''u]$ is a second-order differential operator. The structural similarity to the model problem (1) is also obvious. Using the Chebyshev–tau spectral method produces two spurious eigenvalues with large positive imaginary parts; these spurious eigenvalues are clearly recognized by the large magnitudes of the values of at least one of the tau coefficients (see [9] for details).

The eigenvalues of the model problem (1) are all negative and satisfy either $s = -n^2\pi^2$ or $\tan(\sqrt{-s}) = \sqrt{-s}$. The first five eigenvalues are (numerically)

$$\begin{aligned} s_1 &= -\pi^2 \approx -9.869604401 \\ s_2 &\approx -20.19072856 \\ s_3 &= -4\pi^2 \approx -39.47841760 \\ s_4 &\approx -59.67951594 \\ s_5 &= -9\pi^2 \approx -88.826439612. \end{aligned} \tag{2}$$

The corresponding eigenfunctions are respectively

$$1 + (-1)^{n+1}\cos(n\pi x)$$

and

$$-\sqrt{-s}\cos(\sqrt{-s}x) + \sin(\sqrt{-s}x).$$

Lanczos [14, 15] first proposed the tau method as a means of solving boundary value problems without requiring basis functions to satisfy the boundary conditions. Fox [7, 8]

TABLE I
Eigenvalues, Including Spurious Eigenvalues, for the Model Problem (1) Computed with the Chebyshev–Tau Method

N	1	2	3	4	5	6
Eigenvalues	40	251.453	529.388	1331.132	2284.474	4272.17
	12	40.	251.453	529.388	1331.132	2284.47
		−11.453	−11.453	−9.892	−9.892	−9.870
			−25.388	−25.388	−20.338	−20.338
				−61.239	−61.239	−40.663
					−104.136	−104.136
						−189.638

later extensively developed its use with Chebyshev polynomials. Ortiz [18] extended the method with the use of canonical polynomials. Orszag [17] applied and advocated the Chebyshev–tau method for a wide variety of problems. See [9] for an example of applying the tau method to the model problem (1). Boyd [4, Chap. 18] has a useful and interesting overview of the history and philosophy of the tau method.

The tau method uses a truncated series expansion in a complete set of orthogonal functions as an approximation for the solution of an ordinary differential equation. We will use the family of Gegenbauer (or ultraspherical) polynomials as the complete orthonormal set of functions. The family of Gegenbauer polynomials include the Legendre polynomials and Chebyshev polynomials of the first and second kind as special cases. Chebyshev polynomials work well for this approximation technique because of their nearly optimal uniform approximation of continuous functions, their orthogonality and completeness, and other extremal properties [19]. In certain cases, the Chebyshev expansion is optimal among all expansions in terms of Gegenbauer polynomials (see [19] for a precise statement). This optimality accounts for the common use of Chebyshev polynomials for numerical approximations of all kinds.

Table I gives the eigenvalues from the various orders of Chebyshev–tau approximation of the boundary value problem (1). Note that two large positive eigenvalues result from the calculations and that they increase as the order of approximation increases. The negative eigenvalues appear to be converging to the values (2) of the boundary value problem (1). Note also that the eigenvalues "leap-frog," that is, the largest eigenvalue in column N becomes the second largest positive eigenvalue in column $N + 1$. Likewise the least eigenvalue in column N becomes the next-to-least eigenvalue in column $N + 1$. An abridged table of eigenvalues for higher truncation orders is given in [11, 16]. The entry for $N = 6$, common to the table above and to [11, 16], agree. However, the interest here is not in extending the table to high orders of approximation, but rather to explain the origin and nature of the two large positive eigenvalues that are spurious for the boundary value problem (1).

3. PARITY REDUCTION OF THE PROBLEM

The parity of the model problem (1) allows a reduction of the problem for theoretical purposes that exposes the more important and interesting phenomenon of the spurious eigenvalues in a clearer fashion. Recall that odd index Gegenbauer polynomials are odd polynomials and even index Gegenbauer polynomials are even [12, 19] for all values of the parameter ν. Since the derivatives in (1) are of even order, any odd index Gegenbauer polynomial inserted into the differential equation will remain odd after differentiations. This has the effect of partitioning the problem into odd and even portions. Such a parity reduction is common in spectral methods (see [4, Chap. 7]). It will suffice to examine only one subportion, say, the even portion of the problem.

Application of this reduction to the Chebyshev–tau method explains the "leap-frogging" of eigenvalues observed in Section 2. For, say, M odd, $M = 2N + 1$, the problem (1) factors into an "odd" equation of size $(N+1) \times (N+1)$ and an "even" equation of size $(N+1) \times (N+1)$. The odd portion comes from the odd Chebyshev polynomials $T_1(x)$, $T_3(x), \ldots, T_{2N+1}(x)$. Increasing the size of the approximation to $M+1$, we would partition the problem into an "odd" portion of size $(N+1) \times (N+1)$ and an "even" portion of size $(N+2) \times (N+2)$. The odd portion still comes from the odd Chebyshev polynomials $T_1(x), T_3(x), \ldots, T_{2N+1}(x)$ as in the previous problem. Those eigenvalues occurring in problem $M+1$ which also previously occurred in problem M are the recalculation of the eigenvalues from the subportion of the problem that was unchanged in passing from M to $M+1$. The leap-frogging occurs only for the model problem (1) and does not occur for more general eigenvalue problems containing mixed even and odd orders of differentiation (see [9]).

4. THE CHARACTERISTIC POLYNOMIAL AND THE LOWER BOUND FOR THE POSITIVE EIGENVALUE

We derive a general expression for the characteristic polynomial of the eigenvalue problem arising from a range of spectral–tau methods. In particular, we obtain the characteristic polynomials from the Chebyshev–tau method and the Legendre–tau method. The results will show that a range of spectral methods generate positive (or spurious) eigenvalues, increasing to an infinite eigenvalue from the Legendre–tau method. Professor Hans Weinberger suggested this derivation of the characteristic polynomial to us and we thank him for his assistance. We can also derive the same characteristic polynomial directly from determinants of the triangular-Hessenberg form of the matrix generalized eigenvalue problem through an intricate sequence of recursion arguments and reductions.

4.1. *The Characteristic Polynomial for the General Gegenbauer–Tau Method*

Consider the residual problem of the spectral–tau method reduced by parity as in Section 3 applied to the model problem (1)

$$L\{u\} = u^{(4)} - su'' = \tau_1 f_{2N+2}(x) + \tau_2 f_{2N+4}(x).$$

Use the Gegenbauer polynomials as the set of orthogonal polynomials for the tau method. Specifically, we want to choose the coefficients of the even polynomial u of degree $2N+4$ in such a way that the residual of $L\{u\} = u^{(4)} - su''$ (which is an even polynomial of degree $2N+2$) is orthogonal to $G_0^\nu, G_2^\nu, G_4^\nu, \ldots, G_{2N}^\nu$. Then the residual will only be a multiple of G_{2N+2}^ν.

We write

$$L\{u\} = (D^2 - s)D^2\{u\} = (-D^2 + s)\{-u''\}, \tag{3}$$

where D is the derivative operator. Because $-u''$ is a polynomial, we use the Neumann series for the inverse of the operator $-D^2 + s$ to find that

$$-u'' = \tau_{2N+2} \sum_{k=0}^{N+1} s^{-k-1} D^{2k} T_{2(N+1)}. \tag{4}$$

This equation has a polynomial solution that satisfies the boundary conditions if and only if the integrals of 1 and of x times the right-hand side are zero. The integral of x times the right-hand side is zero by symmetry. Multiplying by s^{N+2} to create a polynomial, the condition for s to be an eigenvalue is that

$$s^{N+1} \int_{-1}^{1} G^{\nu}_{2(N+1)}(x)\, dx + 2 \sum_{k=1}^{N+1} s^{N+1-k} \left(G^{\nu}_{2(N+1)}\right)^{(2k-1)}(1) = 0.$$

We will deduce the special limiting case of $\nu = 0$, reducing to the Chebyshev–tau characteristic polynomial later.

The following lemmas derive the coefficients of the characteristic polynomial explicitly.

LEMMA 1. *Let $n \geq 0$ be an integer and $\nu \in (-\frac{1}{2}, \infty)$, $\nu \neq 0$. Then*

$$\int_{-1}^{1} G^{\nu}_{n}(x)\, dx = [(-1)^n + 1] \frac{(2\nu - 1)\Gamma(n + 2\nu - 1)}{(n+1)!\, \Gamma(2\nu)}.$$

A complete proof is in [6], or the reader can check the lemma by examining special cases. The proof proceeds by writing the integral in terms of hypergeometric functions and using hypergeometric function identities.

LEMMA 2. *Let $n, k \geq 0$ be integers and $\nu \in (-\frac{1}{2}, \infty)$, $\nu \neq 0$, then,*

$$\left.\frac{d^k}{dx^k} G^{\nu}_{n}(x)\right|_{x=1} = 2^k \binom{n + k + 2\nu - 1}{n - k} \prod_{j=0}^{k-1} (\nu + j).$$

A complete proof is in [6].

Notice that if the order of the differentiation, k, is greater than the order of the Gegenbauer polynomial, n, Lemma 2 will give the correct answer. In this case $n - k < 0$ and, since this term is in the bottom of the binomial coefficient, the binomial coefficient will be zero.

Lemmas 1 and 2 give the characteristic polynomial:

$$\begin{aligned} p(s) = {} & \frac{2}{\Gamma(2\nu)} \left(\frac{\Gamma(2N + 2\nu + 1)(2\nu - 1)}{(2N+3)!} \right) s^{N+1} \\ & + 2 \sum_{k=1}^{N+1} s^{N+1-k} 2^{2k-1} \binom{2N + 2k + 2\nu}{2N - 2k + 3} \prod_{j=0}^{2k-2} (\nu + j). \end{aligned} \tag{5}$$

Note that these lemmas do not cover the $\nu = 0$ case, when the Gegenbauer polynomials are the Chebyshev polynomials. In Lemma 1 there is a $\Gamma(2\nu)$ in the denominator of the formula. For $\nu = 0$, $\Gamma(2\nu)$ has a pole. A naive interpretation would then make the leading coefficient of the characteristic polynomial zero for all n. Similarly, for $\nu = 0$ the product

TABLE II
Sign Analysis on the Leading Coefficient of the Characteristic Polynomial

	$-\frac{1}{2}<\nu<0$	$0<\nu<\frac{1}{2}$	$\nu=\frac{1}{2}$	$\nu>\frac{1}{2}$
$\Gamma(2\nu)$	Negative	Positive	Positive	Positive
$2\nu-1$	Negative	Negative	Zero	Positive
Leading coefficient	Positive	Negative	Zero	Positive

in the formula from Lemma 2 yields 0 because of the $j=0$ factor. All coefficients of the characteristic polynomial would then be 0. To recover the Chebyshev–tau characteristic polynomial at $\nu=0$ from the general Gegenbauer–tau characteristic polynomial we must use a limiting argument.

4.2. *Spurious Eigenvalues from the Gegenbauer–Tau Method*

We can now use the characteristic polynomial (5) to prove the existence of a spurious eigenvalue for a range of ν's. We will examine the $\nu=0$ case corresponding to the Chebyshev polynomials of the first kind later (see Section 4.3).

First examine the leading coefficient. Since $N\geq 0$ and $\nu>-\frac{1}{2}$, then $\Gamma(2N+2\nu+1)>0$. Table II completes the sign analysis for the leading coefficient.

The sign analysis on the nonleading coefficients is simpler. The binomial coefficient is always positive since $2N+2k+2\nu>0$. The $j=0$ term of the product determines the sign of the nonleading coefficient. The nonleading coefficients will be negative for $-\frac{1}{2}<\nu<0$ and positive for $\nu>0$.

With these facts we have the following theorem.

THEOREM 1. *For* $-\frac{1}{2}<\nu<\frac{1}{2}$, $\nu\neq 0$, *the model problem* (1) *solved using the Gegenbauer–tau method and reduced by parity to the even portion will have a single positive eigenvalue*, λ_+, *where*

$$\lambda_+ > \frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2}.$$

Proof. First look at the case of $0<\nu<\frac{1}{2}$. For this case the leading coefficient is negative and the nonleading coefficients are all positive.

Define the polynomial

$$q(s) = \frac{2}{\Gamma(2\nu)}\left(\frac{\Gamma(2N+2\nu+1)(2\nu-1)}{(2N+3)!}\right)s^{N+1} + 4\nu\binom{2N+2\nu+2}{2N+1}s^N + 2^{2N+2}(4N+2\nu+2)\prod_{j=0}^{2N}(\nu+j).$$

Note that $q(0)=p(0)$ and that $q(s)<p(s)$ for $s>0$.

The polynomial $q(s)$ has only one critical point,

$$s_{\text{cr}} = \frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2};$$

$q(s_{\text{cr}})$ is a positive maximum value. Therefore $q(s)$ has a single root in the right-half line which is greater than s_{cr}.

Like $q(s)$ the characteristic polynomial $p(s)$ is positive at $s = 0$ and for sufficiently large s will be negative. Also, by definition, $p(s) > q(s)$. Therefore, the characteristic polynomial will have a root greater than the root of $q(s)$, which is, in turn, greater than s_{cr}. Hence, the Gegenbauer–tau approximation to the solution of the model problem will have an eigenvalue λ_+ such that

$$\lambda_+ > s_{\text{cr}} = \frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2}. \tag{6}$$

The characteristic polynomial has no other roots in the right-half line.

For the case $-\frac{1}{2} < \nu < 0$ the characteristic polynomial is simply the negative of the characteristic polynomial from the first case. Therefore, when $-\frac{1}{2} < \nu < 0$, the Gegenbauer–tau approximation to the solution of the model problem will also have an eigenvalue λ_+ such that

$$\lambda_+ > s_{\text{cr}} = \frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2}. \blacksquare \tag{7}$$

Note that as $\nu \to \pm\frac{1}{2}$ we have $s_{\text{cr}} \to \infty$ and so $\lambda_+ \to \infty$.

4.3. *Reduction of the Gegenbauer–Tau Characteristic Polynomial to the Chebyshev–Tau Characteristic Polynomial ($\nu = 0$)*

Recall the definition of the Chebyshev polynomials in terms of Gegenbauer polynomials [1, 2],

$$T_n(x) = \frac{n}{2} \lim_{\nu\to 0} \frac{G_n^\nu(x)}{\nu}.$$

The convergence of the limit in the Gegenbauer polynomial definition of the Chebyshev polynomials is uniform [6]. Uniform convergence allows this limit to be interchanged with integrals and derivatives.

First calculate the leading coefficient in the limit case,

$$\begin{aligned}\int_{-1}^{1} T_{2N+2}(x)\,dx &= \int_{-1}^{1} \frac{2N+2}{2} \lim_{\nu\to 0} \frac{G_{2N+2}^\nu(x)}{\nu}\,dx \\ &= (N+1) \lim_{\nu\to 0} \frac{1}{\nu} \int_{-1}^{1} G_{2N+2}^\nu\,dx \\ &= -\frac{2}{(2N+3)(2N+1)}.\end{aligned}$$

Likewise we can calculate the remaining coefficients.

$$\left.\frac{d^{2k-1}}{dx^{2k-1}} T_{2N+2}(x)\right|_{x=1} = \frac{\prod_{j=0}^{2k-2}\left((2N+2)^2 - j^2\right)}{\prod_{j=0}^{2k-2}(2j+1)}.$$

Thus, we can recover the Chebyshev–tau characteristic polynomial from the Gegenbauer–tau characteristic polynomial.

As in Section 4.2 the Chebyshev–tau approximation to the solution of the model problem has a spurious positive eigenvalue, λ_+, such that

$$\lambda_+ > 2N(2N+1)(2N+2)(2N+3).$$

Notice that this is precisely the lower bound found in Theorem 1 with $\nu = 0$. We have the following theorem.

THEOREM 2. *For* $-\frac{1}{2} < \nu < \frac{1}{2}$ *the model problem* (1) *reduced by parity and solved using the Gegenbauer–tau method will have a single positive eigenvalue,* λ_+, *where*

$$\lambda_+ > \frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2}.$$

5. MATHEMATICAL REDUCTIONS AND REFORMULATIONS

The usual matrix formulation of the tau method is inconvenient for theoretical analysis for two reasons. The matrices A and B are dense, with a partial "checkerboard" structure (see [9]). Furthermore, because of the "boundary bordering" (see [4]) the matrix B is singular. The singularity of B requires a partitioning process for the determination of the eigenvalues; see [9].

In this section, we describe an alternative but equivalent spectral formulation of the problem (1). The alternative formulation results in a nonsingular matrix system with a triangular-Hessenberg structure that is convenient for theoretical analysis.

In the following subsections we briefly describe the steps that lead to the triangular-Hessenberg form. The modifications do not alter the problem or its eigenvalues, but they do take advantage of various properties to eliminate unnecessary or obscuring information from the problem. First, we have already shown in Section 3 how to factor the original procedure into odd and even parts, reducing by half the size of the problem to be solved. Next, we show how to automatically incorporate the boundary conditions into the process to eliminate the singular rows of the matrix eigenvalue problem. Finally, we show that the original problem leads to a special triangular-Hessenberg form by using monomial basis functions, instead of the (equivalent) Chebyshev or Gegenbauer polynomials. It is in this final context that the origin of the spurious eigenvalues is understood.

5.1. *Galerkin–Gegenbauer Bases, Monomial Bases, Galerkin–Monomial Bases*

Finding a polynomial of degree $N+4$ which satisfies the differential equation and boundary conditions in the sense of having residual orthogonal to $G_0^\nu(x), \ldots, G_N^\nu(x)$ approximately solves the model problem (1). Of course, users most commonly apply this approximation with $\nu = 0$, the Chebyshev polynomials, because the Chebyshev polynomials are optimal in several respects. However, investigation of the spurious eigenvalues requires increased generality with the full range of Gegenbauer polynomials.

The boundary conditions imply that the approximating polynomial has a root of multiplicity 2 at $x = 1$ and $x = -1$ so $(1 - x^2)^2$ factors from the polynomial solution. Thus we may solve for the approximation in terms of the basis functions,

$$(1 - x^2)^2 G_k^\nu(x). \tag{8}$$

This is a "basis recombination" as in [4, Section 6.5]. That is, for the model problem (1) we are able to recast the Gegenbauer–tau method (or more commonly, the Chebyshev–tau method) into a Galerkin–Gegenbauer–tau method (see also the discussion of nomenclature in [4, Chap. 18]). The eigenvalues of the system using the Galerkin–Chebyshev basis functions (8) (with $\nu = 0$) are the same as the eigenvalues of the system using the Chebyshev polynomials and the subsequent reduction (see [9]) with the boundary conditions.

One final theoretical consideration will also simplify the problem. We will use an even polynomial incorporating the boundary conditions $(1-x^2)^2 p_N(x) = (1-x^2)^2 \sum_{k=0}^{N} a_k x^{2k}$ as the approximation to the solution of the boundary value problem. This is a "Petrov–Galerkin method" (see [4, Chap. 18, p. 598]). This amounts to a change of basis using the change of basis from the Gegenbauer polynomials to the monomials. We will denote the resulting matrix equation as

$$L_{N+1}^\nu \mathbf{a} = s R_{N+1}^\nu \mathbf{a}. \tag{9}$$

The superscript indicates the index of the Gegenbauer polynomials used, and the subscript indicates the order of approximation. When it is clear from context, or unnecessary, we will omit the indices. Formulas for the entries of L and R are

$$\begin{aligned} L_{i,j}^{(0)} = \pi \Bigg[&(2j)(2j-1)(2j-2)(2j-3)2^{4-2j} \binom{2j-4}{j-2-i} \\ &- 2(2j+2)(2j+1)(2j)(2j-1)2^{2-2j} \binom{2j-2}{j-1-i} \\ &+ (2j+4)(2j+3)(2j+2)(2j+1)2^{-2j} \binom{2j}{j-i} \Bigg] \end{aligned}$$

and

$$\begin{aligned} R_{i,j}^{(0)} = \pi \Bigg[&(2j)(2j-1)2^{2-2j} \binom{2j-2}{j-1-i} - 2(2j+2)(2j+1)2^{-2j} \binom{2j}{j-i} \\ &+ (2j+4)(2j+3)2^{-2-2j} \binom{2j+2}{j+1-i} \Bigg] \end{aligned}$$

for the Chebyshev case, and

$$\begin{aligned} L_{i,j}^{(\nu)} = {} & \frac{\pi 2^{-2\nu+1} \Gamma(2i+2\nu)}{\Gamma(\nu)\Gamma(2i+1)} \\ & \times \Bigg[(2j)(2j-1)(2j-2)(2j-3)2^{-2j+4} \binom{2j-4}{j-i-2} \frac{\Gamma(j+i-1)}{\Gamma(j+i+\nu-1)} \\ & - 2(2j+2)(2j+1)(2j)(2j-1)2^{-2j+2} \binom{2j-2}{j-i-1} \frac{\Gamma(j+i)}{\Gamma(j+i+\nu)} \\ & + (2j+4)(2j+3)(2j+2)(2j+1)2^{-2j} \binom{2j}{j-i} \frac{\Gamma(j+i+1)}{\Gamma(j+i+\nu+1)} \Bigg] \end{aligned}$$

and

$$R_{i,j}^{(\nu)} = \frac{\pi 2^{-2\nu+1}\Gamma(2i+2\nu)}{\Gamma(\nu)\Gamma(2i+1)} \times \left[(2j)(2j-1)2^{-2j+2}\binom{2j-2}{j-i-1}\frac{\Gamma(j+i)}{\Gamma(j+i+\nu)} - 2(2j+2)(2j+1)2^{-2j}\binom{2j}{j-i}\frac{\Gamma(j+i+1)}{\Gamma(j+i+\nu+1)} + (2j+4)(2j+3)2^{-2j-2}\binom{2j+2}{j-i+1}\frac{\Gamma(j+i+2)}{\Gamma(j+i+\nu+2)}\right]$$

for the general Gegenbauer case.

Note that L is an upper triangular matrix and R is an upper Hessenberg matrix. This is another simplification in the problem, since the standard QZ algorithm for the solution of generalized eigenvalue problems first reduces the problem to the triangular-Hessenberg form (which is always possible) and then proceeds to solve the resulting generalized eigenvalue problem, [20]. Although the monomial basis is ill-conditioned for numerical computation, using the monomial basis for reduction to triangular-Hessenberg form does help expose the central point of this theoretical investigation which is the nature and origin of the spurious eigenvalues.

Increasing the order of approximation from $2N$ to $2(N+1)$ by using the polynomial $(1-x^2)^2\sum_{k=0}^{N+1} a_k x^{2k}$ adds a column to both L and R corresponding to the inner products of the derivatives of $(1-x^2)^2 x^{2(N+1)}$ with $G_{2j}^{\nu}(x)$ and a row corresponding to the inner products of derivatives of $(1-x^2)^2 x^{2i}$ with $G_{2(N+1)}^{\nu}(x)$. This means that as the size of the approximation increases, the matrices L and R need not be completely recalculated. It also means that for a given degree $2N$ of approximation, the principal submatrices of L and R contain the lesser degrees of approximation. Both properties are useful for the theoretical analysis in this paper.

5.2. *The Gegenbauer–Tau Method Yields a Regular Generalized Eigenvalue Problem*

For generalized eigenvalue problems, we follow the discussion and notation of [20, Chap. VI]. For $\alpha, \beta \in \mathbb{C}$ consider $(\alpha, \beta) \neq (0, 0)$. Then for any complex scalar γ, $\langle\alpha, \beta\rangle \stackrel{\text{def}}{=} \{\gamma(\alpha, \beta)^{\mathrm{T}} : \gamma \in \mathbb{C}\}$. Write $\langle\lambda\rangle = \langle\lambda, 1\rangle$ and define $\langle\infty\rangle = \langle 1, 0\rangle$.

For vector spaces V_1 and V_2, $\mathbf{x} \in V_1$, and operators A, B with $A, B : V_1 \to V_2$, if

$$\beta A\mathbf{x} = \alpha B\mathbf{x}$$

for $(\alpha, \beta) \neq (0, 0)$ and $\mathbf{x} \neq \mathbf{0}$, then $\langle\alpha, \beta\rangle$ is a (generalized) eigenvalue of the pair (A, B) with (right) (generalized) eigenvector $\mathbf{x}$.

The matrix pair (A, B), with both matrices square of the same dimensions, is *singular* if for all (α, β), $\det(\beta A - \alpha B) = 0$. Otherwise the pair is *regular*. If either $\det(A) \neq 0$ or $\det(B) \neq 0$, then the pair (A, B) is regular. If the pair of $N \times N$ matrices (A, B) is regular, then there are precisely N generalized eigenvalues.

In triangular-Hessenberg form it is simple to show that the matrix generalized eigenvalue problem (9) resulting from the Gegenbauer–tau method is regular. Since $L^{(\nu)}$ is upper triangular, it suffices to show that the diagonal entries are nonzero. From Section 5.1 the

jth diagonal entry of $L^{(\nu)}$ is

$$(2j+4)(2j+3)(2j+2)(2j+1)2^{-2j}\frac{(2j+\nu)\Gamma(\nu)\Gamma(2j+1)}{\Gamma(2j+\nu+1)}.$$

Thus, there are $N+1$ (generalized) eigenvalues for the matrix pair. We may find the eigenvalues as the roots of the characteristic polynomial

$$\det\bigl(L^{(\nu)}-\lambda R^{(\nu)}\bigr).$$

From Section 5.1 we can show that for Legendre polynomials, when $\nu=1/2$, the first row of the matrix $R^{(1/2)}_{N+1}$ is zero (see also Section 5.4). Hence, $R^{(1/2)}_{N+1}$ is singular, with a rank of N. Therefore, there is only one linearly independent right null vector for $R^{(1/2)}_{N+1}$. Then we have

THEOREM 3. *The matrix pair* $(L^{(1/2)}_{N+1}, R^{(1/2)}_{N+1})$ *has one infinite generalized eigenvalue* $\langle 1,0\rangle=\langle\infty\rangle$.

5.3. *Generalized Eigenvalue Perturbation Theory*

We use generalized eigenvalue perturbation theory to show that for $0\le\nu<1$ the system (9) has an eigenvalue that approaches $\langle\infty\rangle$ as the order of approximation increases. We first need more background from [20].

Let $A_{(N+1)}$ be an $(N+1)\times(N+1)$ matrix. Define

$$\left\|A_{(N+1)}\right\| = \sup_{0\le i,j\le N} e^{i+j-2N}|a_{i,j}|.$$

Let (A, B) be a regular matrix pair with simple generalized eigenvalue $\langle\alpha,\beta\rangle$ and left and right eigenvectors $\mathbf{y}$ and $\mathbf{x}$. Let $(\tilde{A},\tilde{B})=(A+E, B+F)$ be a regular matrix pair and a perturbation of (A, B) with corresponding generalized eigenvalue $\langle\tilde{\alpha},\tilde{\beta}\rangle$. Let $\epsilon=\|E\|+\|F\|$.

The chordal metric $\chi(\langle\cdot,\cdot\rangle,\langle\cdot,\cdot\rangle)$ for generalized eigenvalues is

$$\chi(\langle\alpha,\beta\rangle,\langle\gamma,\delta\rangle)=\frac{|\alpha\delta-\beta\gamma|}{\sqrt{|\alpha|^2+|\beta|^2}\sqrt{|\gamma|^2+|\delta|^2}}.$$

Let (A, B) be a regular pair, and let its eigenvalues be $\langle\lambda_1\rangle,\ldots,\langle\lambda_n\rangle$. Then there is an ordering $\langle\tilde{\lambda}_1\rangle,\ldots,\langle\tilde{\lambda}_n\rangle$ of the eigenvalues of $(\tilde{A},\tilde{B})$ such that

$$\lim_{\epsilon\to 0}\chi(\langle\lambda_i\rangle,\langle\tilde{\lambda}_i\rangle)=0,\quad i=0,\ldots,n$$

(see [20, Theorem 2.1, p. 293]). No eigenvalues are lost in perturbing the original matrix pair for small enough perturbations.

From [20, Theorem 2.2, p. 293] we get

$$\chi(\langle\tilde{\alpha},\tilde{\beta}\rangle,\langle\mathbf{y}^H\tilde{A}\mathbf{x},\mathbf{y}^H\tilde{B}\mathbf{x}\rangle)<O(\epsilon^2).$$

For convenience, we will indicate the size of the matrices with a subscript. We will find a matrix pair (E, F) so that $(L^{(\nu)}_{(N+1)}, R^{(\nu)}_{(N+1)})=(L^{(1/2)}_{(N+1)}+E_{(N+1)}, R^{(1/2)}_{(N+1)}+F_{(N+1)})$. We will show that $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ has an infinite generalized eigenvalue $\langle\infty\rangle$ for each N. Defining $\epsilon = \|E\| + \|F\|$ as the size of the perturbation as in [20], the matrix pair $(L^{(\nu)}_{(N+1)}, R^{(\nu)}_{(N+1)})$ will be an $O(\epsilon)$ perturbation of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$. If $\langle\alpha, \beta\rangle$ is the generalized eigenvalue of $(L^{(\nu)}_{(N+1)}, R^{(\nu)}_{(N+1)})$ corresponding to the infinite eigenvalue of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ the perturbation Theorem 2.2 of Stewart and Sun gives the asymptotic behavior of $\langle\alpha, \beta\rangle$.

5.4. *Infinite Eigenvalues in the Legendre–Tau Method ($\nu = 1/2$)*

The first step in proving the existence of spurious eigenvalues for the Gegenbauer–tau method is to examine the case of $\nu = 1/2$ corresponding to Legendre polynomials. For $\nu = 1/2$ the Gegenbauer–tau method yields an infinite generalized eigenvalue.

THEOREM 1. *Let $N > 0$ be an integer. The matrix pair $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ is regular and has a simple infinite generalized eigenvalue.*

Proof. From Section 5.2 we know that $L^{(1/2)}_{(N+1)}$ is upper triangular and nonsingular so the matrix pair is regular.

From Section 5.1 $R^{(1/2)}_{(N+1)}$ is upper Hessenberg so $R^{(1/2)}_{(N+1)}$ has rank of at least N. It is easy to show the elements of the first row of $R^{(1/2)}_{(N+1)}$ are zero, so $R^{(1/2)}_{(N+1)}$ is singular and has rank N [6].

The matrix pair $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ has at least one infinite generalized eigenvalue $\langle 1, 0\rangle$. It is not hard to see that this is a simple generalized eigenvalue. The associated right eigenvector of this infinite generalized eigenvalue is a right null vector for $R^{(1/2)}_{(N+1)}$ and the null space of $R^{(1/2)}_{(N+1)}$ is of dimension one. Therefore, the infinite generalized eigenvalue must be simple. ■

In Section 5.5 we will need the right and left eigenvectors of the matrix pair $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ associated with the infinite generalized eigenvalue.

THEOREM 2. *The left eigenvector of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ is*

$$\mathbf{y}_{(N+1)} = (1, 0, \ldots, 0),$$

where there are $N + 1$ entries in the vector. The right eigenvector, $\mathbf{x}_{(N+1)}$, is

$$x_j = \frac{(-1)^{N-j}}{2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)}$$

for $0 \le j \le N$

The proof is in [6, Section 5.3].

Now that we know that the matrix pair $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ is regular and has a simple infinite generalized eigenvalue we can use this to show that for a range of ν's around $\nu = 1/2$ the Gegenbauer–tau approximation to the solution of the model problem will give a spurious eigenvalue.

5.5. *Perturbation Analysis*

With the technical lemmas from Appendix A we can prove that a spurious eigenvalue will arise from the application of the Gegenbauer–tau approximation method to the model problem for $0 \le \nu < \frac{1}{2}$ and $1/2 < \nu \le 1$. From Section 5.3, if a matrix pair (A, B) of

$(N+1) \times (N+1)$ matrices is "close" to $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ then there will be a generalized eigenvalue $\langle \alpha_{(N+1)}, \beta_{(N+1)} \rangle$ of (A, B) that corresponds to the infinite generalized eigenvalue of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$. The corresponding eigenvalue is approximately

$$\langle \alpha_{(N+1)}, \beta_{(N+1)} \rangle = \langle \mathbf{y}^H L^{(1/2)}_{(N+1)} \mathbf{x}, \mathbf{y}^H R^{(1/2)}_{(N+1)} \mathbf{x} \rangle + O(\epsilon^2),$$

where $\mathbf{y}$ and $\mathbf{x}$ are the left and right eigenvectors of the pair $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$ and ϵ is

$$\epsilon = \left\| L^{(\nu)}_{(N+1)} - L^{(1/2)}_{(N+1)} \right\| + \left\| R^{(\nu)}_{(N+1)} - R^{(1/2)}_{(N+1)} \right\|.$$

Using the norm defined in Appendix A and Lemma 3 we can make, for sufficiently large N, $R^{(\nu)}_{(N+1)}$ as close to $R^{(1/2)}_{(N+1)}$ as we want and similarly for $L^{(\nu)}_{(N+1)}$ and $L^{(1/2)}_{(N+1)}$.

THEOREM 3. *Let $0 \le \nu \le 1$, $\nu \ne 1/2$ be given. Let $\langle \alpha^{(\nu)}, \beta^{(\nu)} \rangle$ be the generalized eigenvalue of $(L^{(\nu)}_{(N+1)}, R^{(\nu)}_{(N+1)})$ that corresponds to the infinite generalized eigenvalue $\langle \infty \rangle = \langle 1, 0 \rangle$ of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$. Then*

$$\langle \alpha^{(\nu)}, \beta^{(\nu)} \rangle = \left\langle 1, \frac{2(2\nu-1)(2\nu-3)}{(2N+3)(2N+2)(2N-2\nu+3)(2N+2\nu+2)} \right\rangle + O(\epsilon^2),$$

where

$$\epsilon^2 < e^{-N+4} \left(A_{N,\nu} + A_{N,\frac{1}{2}} \right) (64N^4 + 64N^3 + 192N^2 + 104N + 40)^2.$$

The constants $A_{N,\nu}$ are defined in Appendix A.

Proof. First, establish the upper bound on ϵ^2. From Lemma 3 we get

$$\left\| L^{(\nu)}_{(N+1)} \right\| < e^{-N/2+2} A_{N,\nu} (64N^4 + 64N^3 + 176N^2 + 80N + 24).$$

and

$$\left\| R^{(\nu)}_{(N+1)} \right\| < e^{-N/2+2} A_{N,\nu} (16N^2 + 24N + 16).$$

Hence,

$$\begin{aligned} \epsilon^2 &= \left(\left\| L^{(\nu)}_{(N+1)} - L^{(1/2)}_{(N+1)} \right\| + \left\| R^{(\nu)}_{(N+1)} - R^{(1/2)}_{(N+1)} \right\| \right)^2 \\ &\le \left(\left\| L^{(\nu)}_{(N+1)} \right\| + \left\| L^{(1/2)}_{(N+1)} \right\| + \left\| R^{(\nu)}_{(N+1)} \right\| + \left\| R^{(1/2)}_{(N+1)} \right\| \right)^2 \\ &= e^{-N+4} \left(A_{N,\nu} + A_{N,\frac{1}{2}} \right)^2 (64N^4 + 64N^3 + 192N^2 + 104N + 40)^2. \end{aligned}$$

Recall that $A_{N,\nu} = (2N+\nu)\Gamma(\nu)$. Therefore, $\epsilon^2 \to 0$ at least as $N^{10} e^{-N}$.

Now we can calculate the approximation to $\langle \alpha_{(N+1)}, \beta_{(N+1)} \rangle$. Recall that

$$\langle \alpha^{(\nu)}, \beta^{(\nu)} \rangle = \langle \mathbf{y}^H L^{(\nu)}_{(N+1)} \mathbf{x}, \mathbf{y}^H R^{(\nu)}_{(N+1)} \mathbf{x} \rangle + O(\epsilon^2),$$

where the right and left eigenvectors of $(L^{(1/2)}_{(N+1)}, R^{(1/2)}_{(N+1)})$, $\mathbf{x}$ and $\mathbf{y}$, respectively, are given by Theorem 2. Evaluating and simplifying gives (see [6] for details)

$$\mathbf{y}^H L^{(\nu)}_{(N+1)}\mathbf{x} = \frac{AB_\nu\left(\frac{5}{2}-\nu\right)_N(2N+4)(2N+3)(2N+2)(2N+1)}{\Gamma(\nu+1)(\nu+1)_N}$$
$$\mathbf{y}^H R^{(\nu)}_{(N+1)}\mathbf{x} = -\frac{AB_\nu(2\nu-1)\left(\frac{3}{2}-\nu\right)_N(N+2)(2N+1)}{\Gamma(\nu+2)(\nu+2)_N}.$$

Therefore, we get

$$\left\langle\alpha^{(\nu)},\beta^{(\nu)}\right\rangle \approx \left\langle\mathbf{y}^H L^{(\nu)}_{(N+1)}\mathbf{x}, \mathbf{y}^H R^{(\nu)}_{(N+1)}\mathbf{x}\right\rangle = \left\langle 1, \frac{\mathbf{y}^H R^{(\nu)}_{(N+1)}\mathbf{x}}{\mathbf{y}^H L^{(\nu)}_{(N+1)}\mathbf{x}}\right\rangle.$$

Substituting and canceling wherever possible we get

$$\left\langle\alpha^{(\nu)},\beta^{(\nu)}\right\rangle \approx \left\langle 1, \frac{(2\nu-1)(2\nu-3)}{(2N+3)(2N+2)(2N-2\nu+3)(2N+2\nu+2)}\right\rangle.$$

See [6] for details. ■

This theorem leads to the following results.

THEOREM 4. *The Chebyshev–tau method applied to the model problem,* (1), *will yield a positive spurious eigenvalue of magnitude at least* $O(N^4)$.

THEOREM 5. *Let* $0 \le \nu \le 1$ *be given. The Gegenbauer–tau approximation to the model problem* (1) *will yield*

1. *a positive spurious eigenvalue for* $0 \le \nu < 1/2$,
2. *an infinite generalized eigenvalue for* $\nu = 1/2$,
3. *a negative spurious eigenvalue for* $1/2 < \nu \le 1$

for all truncation orders.

6. INFINITE EIGENVALUES IN THE LEGENDRE–TAU METHOD

This section explains how the boundary conditions act together with the Legendre–tau method to allow the existence of an infinite eigenvalue. The Gegenbauer–tau method for values of ν near the Legendre case $\nu = 1/2$ will have an eigenvalue that is a perturbation of the infinite eigenvalue. For $0 \le \nu < 1/2$ the perturbation moves the infinite eigenvalue into the regime where it is positive. For $1/2 < \nu \le 1$ the perturbation moves the eigenvalue into the regime where it is negative. The origin of the infinite eigenvalue in the Legendre–tau method together with the perturbation theory for generalized eigenvalues explains the origin of the spurious eigenvalues.

We need to show that the Legendre–tau method of all orders applied to the model problem (1) yields an infinite generalized eigenvalue. For a given order $N+4$ an infinite generalized eigenvalue would be the pair $\langle\alpha_{(N+1)}, \beta_{(N+1)}\rangle = \langle 1, 0\rangle$ for which there is a polynomial of degree $N+4$ whose residual for the model problem

$$\beta D^4 u = \alpha D^2 u$$
$$u(-1) = u(1) = u'(-1) = u'(1) = 0$$

is orthogonal to the Legendre polynomials $P_0(x), \dots P_N(x)$. As in Section 5.1, because we seek polynomial solutions we may incorporate the boundary conditions directly into the equation

$$-D^2\left(\sum_{j=0}^{N} a_j(1-x^2)^2 P_j(x)\right) = \tau P_{N+2}(x).$$

We can rescale and slightly simplify the problem by dividing through by $-\tau$ and incorporating it into the unknown coefficients a_j.

To simplify and eliminate the consideration of cases, consider only even $N = 2M$. Solve by expanding in the linearly independent even Legendre polynomials as basis functions. Equation (6) is now rewritten as

$$\sum_{j=0}^{M} a_j D^2\left[(1-x^2)^2 P_{2j}(x)\right] = P_{N+2}(x).$$

Now expand the polynomial $D^2[(1-x^2)^2 P_j(x)]$ in even Legendre polynomials as

$$D^2\left[(1-x^2)^2 P_{2j}(x)\right] = \sum_{k=0}^{j+1} K_{j,k} P_{2k}(x).$$

From the orthogonality relation, the coefficients $K_{j,k}$ for $k = 0, \dots, j+1$ are

$$K_{j,k} = \frac{2k+1}{2}\int_{-1}^{+1} D^2\left[(1-x^2)^2 P_{2j}(x)\right] P_{2k}(x)\,dx.$$

Integrating by parts twice and rearranging, the coefficients are

$$K_{j,k} = \frac{2k+1}{2}\int_{-1}^{+1} P_{2j}(x)(1-x^2)^2 P''_{2k}(x)\,dx.$$

For a given j, by orthogonality only the even Legendre polynomials $P_{2k}(x)$ of degrees $2j+2$, $2j$, and $2j-2$ can contribute nonzero terms. That is,

$$D^2\left[(1-x^2)^2 P_{2j}(x)\right] = K_{j,j-1}P_{2j-2}(x) + K_{j,j}P_{2j}(x) + K_{j,j+1}P_{2j+2}(x)$$

Using this information, we must show the $M+2$ equations in the $M+1$ unknowns $a_0 \dots a_M$ generated from (6) by equating coefficients of $P_k(x)$, $k = 0, \dots, M+1$ on left and right are consistent.

The first of these equations, equating coefficients of $P_0(x)$, would have all coefficients 0. The equation from the coefficients for P_{2k}, $k = 1, \dots, M-1$, will involve a_{k-1}, a_k, a_{k+1}. Finally, the equation from the coefficients of P_{2M+2} will only involve a_M. Clearly, the system is tridiagonal. The rank of the coefficient matrix is $M+1$, and the rank of the augmented matrix is also $M+1$. The system is consistent and there is a solution. The implication is that the Legendre–tau method allows an infinite eigenvalue.

The Legendre polynomials can be expressed by the Rodriguez formula [1]

$$P_j(x) = \frac{(-1)^j}{j!\,2^j}\frac{d^j}{dx^j}(1-x^2)^j.$$

The Rodriguez formula for the Gegenbauer polynomials is, for comparison,

$$G_j^{(\nu)}(x) = \frac{1}{e_j(1-x^2)^{\nu-1/2}} \frac{d^j}{dx^j}\left[(1-x^2)^{\nu-1/2}(1-x^2)^j\right],$$

where the normalizing constant e_j is in [1, Eq. (22.11.2), p. 785].

Using the Rodriguez formula in (6), we want to show that

$$\frac{d^2}{dx^2}\left(\sum_{j=0}^{N} a_j(1-x^2)^2 \frac{d^j}{dx^j}\frac{(-1)^j}{j!\,2^j}(1-x^2)^j\right) = \frac{d^{N+2}}{dx^{N+2}}\frac{(-1)^{N+2}}{(N+2)!\,2^{N+2}}(1-x^2)^{N+2}. \quad (10)$$

has a solution. Of course, from the argument in the previous paragraph, we know that (10) has a solution. The expression in terms of the Rodriguez expansion makes it plausible that a solution exists. It is plausible that solution would *not* exist for the Gegenbauer polynomials because the derivatives of the term $(1-x^2)^{\nu-1/2}$ in the denominator and under the derivative will introduce terms which cannot be matched on the right side of the expression.

The expansion in terms of the Rodriguez formula explains why the Legendre–tau spectral method has an infinite eigenvalue for the boundary-value problem (1). The similarity of the boundary conditions to the form of the Legendre polynomial solution permits a solution where none would ordinarily be expected. For the Gegenbauer polynomials, the boundary conditions do not match the form of the basis polynomials because of the presence of the term $(1-x^2)^{\nu-1/2}$ in the Rodriguez formula.

7. CONCLUSIONS

In prior sections, we have an explanation for the origin and a description of the nature of the spurious eigenvalues in spectral methods for a differential eigenvalue problem. In particular, we have an explanation for the widely reported positive spurious eigenvalues in the Chebyshev–tau method. The analysis of the spurious eigenvalues was in terms of a simplified model problem; a problem that is simple enough to have an explicit solution to validate the spectral methods, yet still contains the essence of more general problems. Many other investigators have used the model problem as an example of the use of spectral methods. Finally, the model problem occurs naturally in the investigation of some fluid dynamics problems. From that analysis we observe that:

1. The model problem factors into odd and even problems, each generating a spurious eigenvalue. The factoring simplifies the analysis but is not essential to the analysis.
2. The popular Chebyshev–tau and Legendre–tau methods are each instances in a family of spectral methods using the Gegenbauer polynomials, $G_n^{\nu}(x)$, as basis functions.
3. One member of the family of Gegenbauer–tau methods, namely the Legendre–tau method when $\nu = 1/2$, applied to the model problem has an infinite eigenvalue in the sense of generalized eigenvalue theory.
4. Positive spurious eigenvalues occurring for $0 \le \nu < 1/2$ are approximations to infinite eigenvalues in a generalized eigenvalue problem for $\nu = 1/2$.
5. Large magnitude negative eigenvalues occur when $1/2 \le \nu \le 1$, prompting us to enlarge the definition of spurious eigenvalues to include all large-magnitude eigenvalues that are perturbations of an infinite eigenvalue, regardless of sign.

However, note that our enlarged sense of spurious eigenvalues does not emphasize the potential effect of the spurious eigenvalues on a dynamic calculation based on a spectral tau formulation. If a time-dependent version of a problem with spurious eigenvalues were integrated in time, there is a large difference between problems with positive and negative spurious eigenvalues. Positive spurious eigenvalues are catastrophic to the calculation, leading to erroneous blowup of the solution in time, whereas negative spurious eigenvalues are innocuous. A family of related spectral methods can produce both positive and negative spurious eigenvalues, so users must be aware how results can change as the method is varied.

6. The boundary conditions, when incorporated into a polynomial solution, match the form of the Legendre polynomials. The similarity of the boundary conditions to the form of the Legendre polynomials permits the infinite eigenvalue.

7. Spurious eigenvalues from the Gegenbauer–tau method grow at least as fast as

$$\frac{(2N)(2N+2\nu+1)(2N+2\nu+2)(2N+3)}{1-4\nu^2}$$

in the truncation order N. In particular, the spurious eigenvalues from the Chebyshev–tau method are larger than $(2N)(2N+1)(2N+2)(2N+3)$.

For a schematic diagram of the results, consider the Legendre–tau method on the model problem with infinite eigenvalues (along with good approximations to the true eigenvalues) as a point in a space of approximation methods. Other approximation methods are perturbations away from this point. These perturbations change the infinite eigenvalue by perturbing it away from infinity into the positive eigenvalue regime. Some other spectral methods that are seldom used perturb the eigenvalue into the negative eigenvalue regime. *Ad hoc* methods for removing spurious eigenvalues may change either the problem or the method for the Chebyshev–tau method, perturbing the large eigenvalues into the negative eigenvalue regime. We intend further research to make this precise with perturbation results from generalized eigenvalue theory.

Finally, we observe that a now established diagnostic tool for use in showing that a problem has eigenvalues that are approximations to infinite eigenvalues (i.e., are spurious) is to observe the growth rate for dominant eigenvalues computed with truncation order, N in the spectral series. If the magnitude of the eigenvalue grows faster than N^n, $n \approx 3$ or 4, it is probably spurious in the sense we have explained in this paper.

APPENDIX A: DEFINITION OF THE MATRIX NORM

This section contains several facts for the generalized eigenvalue analysis. All proofs are technical and are omitted. Detailed proofs are in [6].

The first detail is the definition of the matrix norm defining the size of the perturbation ϵ in Section 5.3. Let $A_{(N+1)}$ be an $(N+1)\times(N+1)$ matrix. Then define

$$\left\|A_{(N+1)}\right\| = \sup_{0\le i,j\le N} e^{i+j-2N}|a_{i,j}|.$$

It is easy to show that this is indeed a norm.

The rest of this section consists of technical lemmas that will help with the analysis in Section 5.5. These lemmas, while important to the analysis, detract from the actual analysis.

The next lemma gives an upper bound on the norm of the matrices $L^{(\nu)}_{(N+1)}$ and $R^{(\nu)}_{(N+1)}$ under the norm defined in this section.

LEMMA 3. *Let $\nu \geq 0$ be given. Then*

$$\left\|L^{(\nu)}_{(N+1)}\right\| < e^{-N/2+2} A_{N,\nu}(64N^4 + 64N^3 + 176N^2 + 80N + 24)$$

and

$$\left\|R^{(\nu)}_{(N+1)}\right\| < e^{-N/2+2} A_{N,\nu}(16N^2 + 24N + 16)$$

where

$$A_{i,\nu} = \begin{cases} 1, & \nu = 0, \\ (2i+\nu)\Gamma(\nu), & \nu \neq 0. \end{cases}$$

The last two lemmas in this section will be used in Section 5.5 to estimate perturbed eigenvalues. The first lemma gives the evaluations of several summations.

LEMMA 4. *Let $N > 0$ be an integer. Then*

1.

$$\sum_{j=0}^{N} \left[\frac{2^{-2j}(2j)!\,(-1)^{N-j}}{j!\,\Gamma(j+\nu+2)2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)} \right] = \frac{A\left(\frac{3}{2}-\nu\right)_N}{\Gamma(\nu+2)(\nu+2)_N},$$

2.

$$\sum_{j=0}^{N} \left[\frac{j2^{-2j}(2j)!\,(-1)^{N-j}}{j!\,\Gamma(j+\nu+2)2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)} \right]$$
$$= \frac{A\left(N^2+\frac{5}{2}N\right)\left(\frac{3}{2}-\nu\right)_N}{\left(\frac{3}{2}-\nu\right)\Gamma(\nu+2)(\nu+2)_N},$$

3.

$$\sum_{j=0}^{N} \left[\frac{2^{-2j}(2j)!\,(-1)^{N-j}}{j!\,\Gamma(j+\nu+1)2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)} \right] = \frac{A\left(\frac{5}{2}-\nu\right)_N}{\Gamma(\nu+1)(\nu+1)_N},$$

4.

$$\sum_{j=0}^{N} \left[\frac{j2^{-2j}(2j)!\,(-1)^{N-j}}{j!\,\Gamma(j+\nu+1)2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)} \right]$$
$$= \frac{A\left(N^2+\frac{5}{2}N\right)\left(\frac{5}{2}-\nu\right)_N}{\left(\frac{5}{2}-\nu\right)\Gamma(\nu+1)(\nu+1)_N},$$

5.

$$\sum_{j=0}^{N} \left[\frac{j^2 2^{-2j}(2j)!\,(-1)^{N-j}}{j!\,\Gamma(j+\nu+1)2^{N-j}(N-j)!} \frac{\prod_{k=0}^{2N-2j-1}(2N-k)}{\prod_{k=0}^{N-j-1}(4N+3-2k)} \right]$$
$$= \frac{A\left(N^2+\frac{5}{2}N\right)\left(\frac{5}{2}-\nu\right)_N}{\left(\frac{5}{2}-\nu\right)\Gamma(\nu+1)(\nu+1)_N}\left(1+\frac{(N-1)\left(N+\frac{7}{2}\right)}{\left(\frac{7}{2}-\nu\right)}\right),$$

where

$$A = \frac{(2N)!}{2^N N! \prod_{k=0}^{N-1}(4N+3-2k)}$$

The last lemma in this section gives simplified formulas for $R_{0,j}^{(\nu)}$ and $L_{0,j}^{(\nu)}$ for $\nu \geq 0$

LEMMA 5. *Let* $N > 0$ *be an integer*, $0 \leq j \leq N$ *and* $\nu \geq 0$ *then,*

$$R_{0,j}^{(\nu)} = B_\nu(2\nu - 1)\frac{2^{-2j}(2j)!}{j!\,\Gamma(j+\nu+2)}\,(((2\nu-3)j-2))$$

$$L_{0,j}^{(\nu)} = B_\nu\frac{2^{-2j}(2j)!}{j!\,\Gamma(j+\nu+1)}\big((16\nu^2-96\nu+140)j^2-(16\nu^2-100)j+24\big),$$

where

$$B_\nu = \begin{cases} 2, & \nu = 0, \\ \nu\Gamma(\nu), & \nu \neq 0. \end{cases}$$

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