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A PRACTICAL IMPLEMENTATION OF SPECTRAL METHODS RESISTANT TO THE GENERATION OF SPURIOUS EIGENVALUES

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SUMMARY

This work describes a practical way of constructing a spectral representation of linear boundary value problems (BVPs) using a tau method. All BVPs are treated as first-order systems, unlike most implementations which tend to view the problem in terms of a single high-order differential equation. For most applications this formulation will adhere more closely to the natural derivation of the original equations from, for example, a series of conservation laws. The technique is exemplified for Chebyshev polynomials in a variety of real applications, although detailed results are provided for any polynomial basis.

KEY WORDS Spectral Eigenvalues Tau

1. INTRODUCTION

This work aims to describe and exemplify a practical implementation of the spectral tau method for a selection of eigenvalue problems from mathematical physics. For our purposes, instability ensues whenever there is an eigenvalue with a positive real part and in practice this can happen via a stationary (real eigenvalue) or overstable (complex eigenvalue) mode, depending on the region of parameter space in which the problem is posed. On many occasions a principle of exchange of stabilities can be operative (i.e. instability can only ensue through stationary modes) and in this event tracking methods using inverse iteration or compound matrices are usually very effective, but otherwise the discontinuous dependence of critical eigenvalues on parametric variables can greatly reduce the effectiveness of these methods and it is in this latter environment that spectral techniques play an invaluable role.

The application of spectral methods (using Chebyshev polynomials) in the solution of differential equations is credited to Lanczos[1] and Clenshaw.[2] The Lanczos method has been developed and extensively applied to ordinary differential equations by Fox,[3] Fox and Parker[4] and others. Orszag[5,6] and Orszag and Kells[7] have shown that expansions in Chebyshev polynomials are better suited to the solutions of hydrodynamic stability problems than expansions in other sets of orthogonal functions. The method proposed in this work is valid for any polynomial basis provided that some basic requirements (to be detailed shortly) are satisfied, although in practice Chebyshev polynomials would be used over finite intervals unless errors are measured by some eccentric norm. Our experience suggests that within the gambit of eigenvalue problems the

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performance of Legendre polynomials is marginally inferior to that of Chebyshev polynomials and imposes more coding difficulties. In fact, both families of polynomials essentially satisfy the same difference equation for high orders and it seems reasonable that this property largely explains the comparable performance characteristics.

In more recent times, applications of spectral methods have been troubled by the emergence of spurious eigenvalues (with large positive real parts) in situations in which the mathematical solution is known to be stable. We mention the work of Gottlieb and Orszag,[8] Brenier *et al.*[9] and Zebib,[10] who all report this phenomenon in the context of hydrodynamic stability. More recently, Zebib[11] has developed a Galerkin scheme and Gardner *et al.*[12] have developed a 'modified tau' scheme which circumvent these difficulties, but noticeably at the expense of practicality. These works have made an important contribution to the development of spectral methods to the extent that they describe procedures to irradicate the occurrence of spurious eigenvalues. However, we believe that these ideas must be tempered by practical considerations and that there is a compromise position for an easily implementable scheme capable of handling systems of sizable order (say 12 or above) with variable coefficients but resistant to the occurrence of spurious eigenvalues.

It is appropriate to provide some further illumination on the meaning of 'practical' in the context of spectral techniques. There are two aspects to consider, namely the final formulation of the mathematical problem and its transformation into an equivalent numerical problem. Typically most eigenvalue problems are developed from a series of conservation laws such as mass conservation, momentum conservation, energy conservation, Maxwell's equations in the case of electromagnetically responsive materials, solute conservation in the case of salting or diffusion effects, etc. Hence in a real application it is often unnatural to formulate the problem in terms of a single high-order equation, not to mention the feasibility of doing this in any sensible fashion. On the other hand it is usually very easy to formulate the problem as a first-order system when it is derived from individual conservation equations and, as a bonus, this representation also simplifies the boundary conditions. In the following sections it will become clear that the construction of the spectral matrices for first-order systems is sufficiently straightforward that it can be done automatically by a utility programme.

It is important to notice that both numerically and mathematically the first-order system representation of the problem differs subtly from that associated with the single high-order equation. In the former, derivatives are treated as independent variables and enjoy their individual expansion, whereas in the latter, derivatives are generated from the basic solution by differentiating the spectral expansions and thus are relegated to the status of dependent variables. This latter approach potentially creates an unstable representation of the problem which manifests itself through spurious eigenvalues, whereas in the case of the first-order system it is reasonable to attribute the increased suppression of spurious eigenvalues to the superior numerical representation of high derivatives. Similar benefits are enjoyed in the treatment of boundary conditions, which essentially consist of a series of linearly independent relationships connecting the independent variables, and in particular it is no longer necessary to compute higher derivatives of the spectral polynomials on the boundaries.

The main drawback of this new approach lies in the fact that the spectral matrices are considerably larger than those generated by the techniques of Orszag[5] or Gardner *et al.*[12] It is conceivable that in very extreme cases RAM limitations may be a fatal handicap, but for the vast majority of applications the exceptional convergence qualities of spectral methods usually guarantee that 20 or so polynomials are more than adequate. Thus for most purposes this drawback is more than counterbalanced by the ease of coding and the resilience to the generation of spurious eigenvalues.

2. SOME GENERAL REMARKS ON ORTHOGONAL POLYNOMIALS

Let $\pi_0(x), \pi_1(x), \pi_2(x), \ldots,$ be a family of real polynomials orthogonal with respect to the weight function $w(x)$ over the real interval $\mathscr{I}$ and such that $\pi_r(x)$ has degree r. The inner product $\langle f, g\rangle$ over $\mathscr{I}$ is defined by the rule

$$\langle f, g\rangle = \int_{\mathscr{I}} w(x) f(x) g(x)\, dx \tag{1}$$

and with respect to this inner product the polynomials $\pi_r(x)$, $r \geqslant 0$, satisfy

$$\langle \pi_n, \pi_m\rangle = \int_{\mathscr{I}} w(x)\pi_n(x)\pi_m(x)\, dx = \begin{cases} 0, & n \neq m, \\ \mu_n, & n = m. \end{cases} \tag{2}$$

Although the weight function $w(x)$ and interval $\mathscr{I}$ uniquely define the family members up to a multiplicative constant, traditionally such families are viewed as the polynomial solution of some second-order differential equation or are constructed from a generating function. For the purposes of this work it is most profitable to regard the πs as solutions of the second-order difference equation

$$\pi_0 = 1, \qquad \pi_{r+1} = (x - \delta_{r+1})\pi_r(x) - \gamma_{r+1}^2 \pi_{r-1}(x), \tag{3}$$

where conventionally, $\pi_{-1}(x) = 0$ and δ_{r+1} and γ_{r+1}^2 are defined by

$$\delta_{r+1} = \frac{\langle x\pi_r, \pi_r\rangle}{\mu_r} \quad \text{for } r \geqslant 0, \qquad \gamma_{r+1}^2 = \begin{cases} 0 & \text{for } r = 0, \\ \mu_r/\mu_{r-1} & \text{for } r \geqslant 1. \end{cases} \tag{4}$$

Spectral analyses with polynomial bases rely critically on the fact that the set of all polynomials is closed under differentiation and multiplication. In the context of the π-family the derivative of $\pi_r(x)$ is expressible as a linear combination of $\pi_0(x), \ldots, \pi_{r-1}(x)$ and the product $\pi_r(x)\,\pi_s(x)$ is expressible as a linear combination of $\pi_0(x), \ldots, \pi_{|r+s|}(x)$. In fact, the construction of the πs from (2) attributes them with the property that $\pi_r(x)\pi_s(x)$ is a linear combination of $\pi_{|r-s|}(x), \ldots, \pi_{r+s}(x)$. This feature of orthogonal polynomials is not widely known and is proved by induction. To sum up, it is always possible to find D_{nm} and β_{nmk} such that whenever $n \geqslant m$

$$\frac{d\pi_{n-1}(x)}{dx} = \sum_{s=1}^{n-1} D_{ns}\phi_{s-1}(x), \qquad \pi_{n-1}(x)\pi_{m-1}(x) = \sum_{s=1}^{2m-1} \beta_{nms}\pi_{n+m-s-1}(x). \tag{5}$$

For completeness, the specific forms of (5) for Chebyshev polynomials $T_n(x)$, Hermite polynomials $H_n(x)$, Laguerre polynomials $L_n(x)$ and Legendre polynomials $P_n(x)$ are now recorded and specific forms of D can be extracted from these results for a particular application. Most comprehensive accounts of the functions of mathematical physics reference the derivative results and it is well known that

$$T_n'(x) = \begin{cases} \displaystyle\sum_{r=0}^{n/2-1} 2nT_{n-2r-1}(x), & n \text{ even}, \\ \displaystyle\sum_{r=0}^{(n-3)/2} 2nT_{n-2r-1}(x) + nT_0(x), & n \text{ odd}, \end{cases}$$

$$H_n'(x) = 2nH_{n-1}(x), \qquad L_n'(x) = -\sum_{r=0}^{n-1} L_r(x), \tag{6}$$

$$P'_n(x)=\begin{cases}\sum_{r=0}^{n/2-1}(2n-4r-1)P_{n-2r-1}(x), & n \text{ even},\\ \sum_{r=0}^{(n-1)/2}(2n-4r-1)P_{n-2r-1}(x), & n \text{ odd}.\end{cases}$$

However, except for Chebyshev polynomials, forms for $\pi_n(x)\pi_m(x)$ are obscure. It can be shown that

$$T_n(x)T_m(x)=\tfrac{1}{2}(T_{m+n}(x)+T_{n-m}(x)), \qquad L_n(x)L_m(x)=\sum_{r=0}^{2m} a_{nmr}L_{n+m-r}(x),$$

$$H_n(x)H_m(x)=n!m!\sum_{r=0}^{m}\frac{2^r H_{n+m-2r}(x)}{r!(n-r)!(m-r)!}, \tag{7}$$

$$P_n(x)P_m(x)=\sum_{r=0}^{m}\frac{A_{m-r}A_rA_{n-r}}{A_{n+m-r}}\left(\frac{2n+2m-4r+1}{2n+2m-2r+1}\right)P_{n+m-2r}(x),$$

where it is assumed that $n\geqslant m$ and a_{nmr} and A_r are given by the expressions

$$a_{nmr}=(-1)^r\sum_{s=\max(0,r-m)}^{\min(m,r)}\binom{n}{s}\binom{m}{s}\binom{n}{r-s}\binom{m}{r-s}s!(r-s)!, \qquad A_r=\frac{1}{2^r}\binom{2r}{r}.$$

Future sections of this work will assume approximate representations of functions in terms of a finite series of spectral polynomials. This is therefore an opportune point to discuss this problem in some detail. Suppose that

$$f(x)\approx\sum_{r=1}^{n}c_r\pi_{r-1}(x); \tag{8}$$

then the orthogonality of $\pi_0(x),\ldots,\pi_{n-1}(x)$ leads to the immediate conclusion that

$$c_r=\frac{1}{\mu_{r-1}}\int_{\mathscr{I}}w(x)f(x)\pi_{r-1}(x)\,\mathrm{d}x$$

and this is approximated by the Gaussian quadrature of maximum precision to obtain

$$c_r=\frac{1}{\mu_{r-1}}\sum_{k=1}^{n}a_kf(x_k)\pi_{r-1}(x_k), \tag{9}$$

where $x_1,\ldots,x_n$ are the zeros of $\pi_n(x)$ and are all guaranteed to lie in the interval $\mathscr{I}$. Essentially Gaussian quadratures provide a mechanism for constructing discrete orthogonality relations. Clearly this procedure is only sensible once the $x_1,\ldots,x_n$ and $a_1,\ldots,a_n$ are known. It is relatively straightforward to verify that $\pi_n(x)$ is the characteristic polynomial of the real, symmetric, tridiagonal $n\times n$ matrix

$$\begin{bmatrix}\delta_1 & \gamma_2 & \cdot & & \\ \gamma_2 & \delta_2 & \gamma_3 & \cdot & \\ & \cdot & \cdot & \cdot & \\ & & & \gamma_n & \delta_n\end{bmatrix}.$$

Thus the zeros of $\pi_n(x)$ are the eigenvalues of this matrix and can be determined accurately using the QR algorithm. Moreover, suppose that $\mathbf{v}^{(j)}=v_k^{(j)}\mathbf{e}_k$ is the eigenvector associated with the eigenvalue x_j; then the quadrature weight a_j is given by

$$a_j = \frac{v_1^{(j)} v_1^{(j)}}{\sum_{k=1}^{n} v_k^{(j)} v_k^{(j)}} \mu_0 = \frac{v_1^{(j)} v_1^{(j)}}{\sum_{k=1}^{n} v_k^{(j)} v_k^{(j)}} \int_{\mathscr{I}} w(x)\, \mathrm{d}x.$$

These latter results are presented without any justification and the reader is referred to Reference 13 for further details. In conclusion, the coefficients $c_1, \ldots, c_n$ are thus determined for any choice of polynomial basis.

3. THE CHEBYSHEV SPECTRAL REPRESENTATION

This work aims to develop a spectral representation of the general linear eigenvalue problem

$$\frac{\mathrm{d}Y}{\mathrm{d}z} = AY + \lambda BY, \quad z \in (a, b), \tag{10}$$

where Y is an N-vector with components $y_1, \ldots, y_N$ and A and B are complex matrices whose entries only depend on the real variable x. The technique will be described in detail for the Chebyshev representation since this is the scenario for the vast majority of applications. Equivalent results will be stated for any polynomial basis on the assumption that the coefficients arising in (5) are known. System (10) must be supplemented by N boundary conditions, which need to be linearly independent on any given boundary. The eigenvalue itself may occur linearly in these conditions and indeed this happens with Stekloff problems which typically arise in variational problems containing a transversality condition. Such conditions often appear in energy analytic methods.

The Chebyshev polynomials $T_n(x)$ are orthogonal over the interval $[-1, 1]$ with respect to the weight function $w(x) = (1 - x^2)^{-1/2}$. Let us observe that the formula $x = -1 + 2(z - a)/(b - a)$ maps $[a, b]$ into $[-1, 1]$ and in the process derivatives with respect to z and x are related through the constant multiplying factor $2/(b - a)$. Similarly, all non-constant entries of A and B are mapped into equivalent forms in $[-1, 1]$. Hence it is convenient to assume from the outset that equation (10) is already formulated in the interval $[-1, 1]$. Suppose now that the components of Y are each approximated by a series of M polynomials so that

$$y_r(x) = \sum_{j=1}^{M} \alpha_{jr} T_{j-1}(x), \quad 1 \leqslant r \leqslant N. \tag{11}$$

In fact, (11) is not an exact solution of (10) but instead satisfies the differential equation

$$\frac{\mathrm{d}Y}{\mathrm{d}x} = (A(x) + \lambda B(x))\, Y + R_M(x),$$

where R_M is an N-dimensional vector describing the remainder term and whose nature will depend on the form of A and B. The strategy is based on the expectation that $R_M \to 0$ as $M \to \infty$. In view of (5), each component of Y can be differentiated and the result expressed in terms of the original basis functions to obtain

$$\frac{\mathrm{d}y_r}{\mathrm{d}x} = \sum_{j=1}^{M} \alpha_{jr} \left(\sum_{s=1}^{M} D_{sj} T_{s-1}(x) \right) = \sum_{s=1}^{M} \left(\sum_{j=1}^{M} D_{sj} \alpha_{jr} \right) T_{s-1}(x), \tag{12}$$

where

$$D_{1,2j} = 2j - 1, \quad j \geqslant 1, \qquad D_{i,i+2j-1} = 4j + 2i - 4, \quad i \geqslant 2 \quad j \geqslant 1. \tag{13}$$

Although the right-hand side of (10) contains two terms, it is sufficient to treat AY and recognize that the discussion of BY is identical. The rth component of AY is

$$\sum_{s=1}^{N} A_{rs} y_s = \sum_{s=1}^{N} A_{rs}\left(\sum_{i=1}^{M} \alpha_{is} T_{i-1}(x)\right) = \sum_{s=1}^{N}\sum_{i=1}^{M} \alpha_{is}\left(\sum_{k=1}^{\infty} \Omega_{rsk} T_{k-1}(x)\right) T_{i-1}(x), \tag{14}$$

where $\sum_{k=1}^{\infty} \Omega_{rsk} T_{k-1}(x)$ is the Chebyshev expansion of the (r, s)th entry of A. If any entry of A or B requires an infinite Chebyshev expansion (i.e. is not a polynomial), then the remainder term R_M is an infinite sequence of Chebyshev polynomials.

The apparent complexity of (14) suggests that this is a suitable point to look ahead and anticipate the nature of the mathematical problem this approach will generate. Let V be the MN-dimensional vector whose components are formed from N blocks, each of dimension M and in which the rth block has components $\alpha_{1r}, \ldots, \alpha_{Mr}$. From (12) the component y'_r of Y' depends linearly on the coefficients $\alpha_{1r}, \ldots, \alpha_{Mr}$, and when this observation is extended to Y itself, it is clear that the differentiation of Y can be viewed in terms of the matrix premultiplication of V by an $MN \times MN$ matrix E whose general form can be thought of in terms of N^2 blocks where each block is an $M \times M$ matrix. In fact, E is block diagonal with form diag$(D, \ldots, N$ times).

In a similar way the right-hand side of equation (14) can be interpreted in terms of this block notation and effectively states that the (r, s)th block of the $MN \times MN$ matrix representing AY has the form

$$\sum_{i=1}^{M}\left(\sum_{k=1}^{\infty} \Omega_{rsk} T_{k-1}(x) T_{i-1}(x)\right)\alpha_{is} = \frac{1}{2}\sum_{i=1}^{M}\sum_{k=1}^{\infty} \Omega_{rsk}(T_{k+i-2}(x) + T_{|k-i|}(x)) \tag{15}$$

in view of property (7). In this double sum there are two cases of interest: either A_{rs} is constant so that Ω_{rs1} is the only non-zero term in its Chebyshev expansion or A_{rs} is a function of x with a potentially infinite Chebyshev expansion. In the former case it is clear that the (r, s)th block is filled by

$$\sum_{i=1}^{M} \Omega_{rs1} T_{i-1} \alpha_{is}$$

or in matrix terms by $A_{rs} I_M$, where I_M is the identity $M \times M$ matrix. In fact, this result is true for every polynomial basis. Let us now suppose that A_{rs} is not constant. In order to handle $T_{|k-i|}(x)$, it is convenient to subdivide the second sum into the cases $k \leqslant i$ and $k > i$ and then treat each separately. After adjusting the summation index, it is easily verified that expression (15) can be rewritten in the form

$$\frac{1}{2}\sum_{i=1}^{M}\left(\sum_{j=i}^{\infty} \Omega_{rs(j-i+1)} T_{j-1}(x)\right)\alpha_{is} + \frac{1}{2}\sum_{i=1}^{M}\left(\sum_{j=2}^{\infty} \Omega_{rs(i+j-1)} T_{j-1}(x)\right)\alpha_{is}$$
$$+ \frac{1}{2}\sum_{i=1}^{M}\left(\sum_{j=1}^{i} \Omega_{rs(i-j+1)} T_{j-1}(x)\right)\alpha_{is}. \tag{16}$$

Suppose that this block is represented by the $M \times M$ matrix Q. It transpires that the structural symmetry of Q is masked by the contents of its first row and column. It is a matter of algebra to verify that the components of expression (16) pertaining to the first row and column of Q are

$$\alpha_{1s}\sum_{j=1}^{\infty} \Omega_{rsj} T_{j-1}(x) + \frac{1}{2}\sum_{i=2}^{M} \alpha_{is}\Omega_{rsi} T_0(x),$$

and since the first column is derived from the coefficient of α_{1s} and the first row is derived from the coefficient of $T_0(x)$, then clearly

$$Q_{1j} = \tfrac{1}{2}\Omega_{rsj}, \quad j \geq 2, \qquad Q_{i1} = \Omega_{rsi}, \quad i \geq 1. \tag{17}$$

The remaining elements of Q describe the expression

$$\frac{1}{2}\sum_{i=2}^{M}\left(\sum_{j=i}^{\infty}\Omega_{rs(j-i+1)}T_{j-1}(x)\right)\alpha_{is} + \frac{1}{2}\sum_{i=2}^{M}\left(\sum_{j=2}^{\infty}\Omega_{rs(i+j-1)}T_{j-1}(x)\right)\alpha_{is} + \frac{1}{2}\sum_{i=2}^{M}\left(\sum_{j=2}^{i}\Omega_{rs(i-j+1)}T_{j-1}(x)\right)\alpha_{is}. \tag{18}$$

The terms in (18) contributing to the diagonal entries of Q are readily seen to be

$$\sum_{i=2}^{M}\alpha_{is}\Omega_{rs1}T_{i-1}(x) + \frac{1}{2}\sum_{i=2}^{M}\alpha_{is}\Omega_{rs(2i-1)}T_{i-1}(x)$$

and hence $Q_{ii} = \Omega_{rs1} + \frac{1}{2}\Omega_{rs(2i-1)}$, $i \geq 2$. Whenever $j > i$, the contributing terms from (18) amount to

$$\frac{1}{2}\sum_{i=2}^{M}\sum_{j=i+1}^{\infty}\alpha_{is}\Omega_{rs(j-i+1)}T_{j-1}(x) + \frac{1}{2}\sum_{i=2}^{M}\sum_{j=i+1}^{\infty}\alpha_{is}\Omega_{rs(i+j-1)}T_{j-1}(x)$$

and thus $Q_{ij} = \frac{1}{2}(\Omega_{rs(i+j-1)} + \Omega_{rs(j-i+1)})$, $j > i$. Likewise, whenever $i > j$, the contributing terms from (18) are

$$\frac{1}{2}\sum_{i=2}^{M}\sum_{j=2}^{i-1}\alpha_{is}\Omega_{rs(i+j-1)}T_{j-1}(x) + \frac{1}{2}\sum_{i=2}^{M}\sum_{j=2}^{i-1}\alpha_{is}\Omega_{rs(i-j+1)}T_{j-1}(x)$$

and thus $Q_{ij} = \frac{1}{2}(\Omega_{rs(i+j-1)} + \Omega_{rs(i-j+1)})$, $i > j$. Of course, these three results can be unified into the form

$$Q_{ii} = \Omega_{rs1} + \tfrac{1}{2}\Omega_{rs(2i-1)}, \qquad Q_{ij} = \tfrac{1}{2}(\Omega_{rs(i+j-1)} + \Omega_{rs(|i-j|+1)}), \quad i, j \geq 2, \tag{19}$$

and hence the matrix Q is symmetric except for the first row and column and has the form described by expressions (17) and (19). In fact, this symmetry feature of the block matrix Q is true whatever the choice of basis polynomials.

The upshot of this analysis is that equation (10) is reduced to a generalized eigenvalue problem of type $EV = \lambda FV$, where E and F are complex square matrices of type $MN \times MN$. Boundary conditions must be added to the problem and these are included in a natural manner by overwriting the Nth, $2N$th, . . . , MNth rows of $EV = \lambda FV$. Theoretically their order is immaterial, but in practice it is beneficial to insert them in a manner which recognizes that any subsequent algebraic procedures will seek to upper triangularize F and reduce E to upper Hessenberg form. Thus any linear boundary eigenvalue problem is converted into a problem in numerical linear algebra and the spectrum can be computed using the 'Q' type transformations of numerical linear algebra.[14] Our examples handle the eigenvalue problem $EV = \lambda FV$ with the NAG routine F02BJF when E and F are real and the NAG routine F02GJF for complex E and F.

For a general polynomial basis of the type introduced in (3) and (4), the treatment of derivatives and constant matrix entries follows the same pattern as for Chebyshev polynomials. The major differences occur when A or B has non-constant terms and in this case the equivalent form for expression (3.7) is

$$\sum_{i=1}^{M}\left(\sum_{k=1}^{i}\Omega_{rsk}\sum_{j=i-k+1}^{i+k-1}\beta_{ik(k+i-j)}\pi_{j-1}(x) + \sum_{k=i+1}^{\infty}\Omega_{rsk}\sum_{j=k-i+1}^{k+i-1}\beta_{ki(k+i-j)}\pi_{j-1}(x)\right)\alpha_{is}.$$

The first row and column of Q are extracted from the terms

$$\alpha_{1s}\sum_{k=1}^{\infty}\Omega_{rsk}\pi_{k-1}(x)+\sum_{i=2}^{M}\Omega_{rsi}\beta_{ii(2i-1)}\alpha_{is}$$

and lead to the conclusion that

$$Q_{i1}=\Omega_{rsi},\qquad Q_{1j}=\Omega_{rsj}\beta_{jj(2j-1)}.$$

Without further justification it can be shown that the remaining entries of Q are represented by the form

$$Q_{ij}=\begin{cases}\sum_{k=i-j+1}^{i+j-1}\Omega_{rsk}c_{ik(k+i-j)}, & 2\leqslant j<i,\\ \sum_{k=1}^{2i-1}\Omega_{rsk}c_{ikk}, & j=i,\\ \sum_{k=j-i+1}^{i+j-1}\Omega_{rsk}c_{ik(k+i-j)}, & j>i\geqslant 2,\end{cases}\tag{20}$$

where the coefficient c_{ikr} are defined in terms of the β-coefficients of (5) by

$$c_{ikr}=\begin{cases}\beta_{ikr}, & k\leqslant i,\\ \beta_{kir}, & k>i.\end{cases}$$

It is clear from these results that the Chebyshev polynomial basis is substantially easier to use than any other polynomial basis, simply because the formula for $T_n(x)T_m(x)$ contains only two terms rather than the multitude of terms arising from other families of polynomials.

4. EXAMPLE 1

Gardner *et al.*[12] display the deficiencies of the Chebyshev spectral representation for the fourth-order boundary value problem

$$u''''+Ru'''-\sigma u''=0,\quad -1<x<1,\quad u(-1)=u(1)=u'(-1)=u'(1)=0,\tag{21}$$

where σ is the eigenvalue and R is a real parameter. They point out that even in such a straightforward equation the traditional spectral approach generates the spurious eigenvalue $\sigma=0$ when $R=0$. It is easily verified that

$$u(x)=A[\cosh(mx)-\cosh m]+B[\sinh(mx)-x\sinh m],\qquad m=\sqrt{(R^2+4\sigma)},$$

satisfies the boundary conditions $u(1)=u(-1)=0$. The eigencondition

$$f(\sigma)=(R^2+4\sigma)^{1/2}\left(1-\frac{\cosh[(R^2+4\sigma)^{1/2}]}{\cosh R}\right)+2\sigma\frac{\sinh[(R^2+4\sigma)^{1/2}]}{\cosh R}=0\tag{22}$$

can be established from the requirement $u'(1)=u'(-1)=0$. Indeed, the spurious eigenvalue satisfies the eigencondition. Under the change of variables

$$y_1=u,\qquad y_2=u',\qquad y_3=u'',\qquad y_4=u''',\tag{23}$$

this problem can be rewritten as the fourth-order system $Y' = AY + \sigma BY$, where Y has its usual meaning and A and B are respectively the real matrices

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -R \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{24}$$

Without any further mathematical effort it is immediately obvious that the final eigenvalue problem reduces to $EV = \sigma FV$, where the appropriate Chebyshev block forms of the matrices E and F are

$$E = \begin{bmatrix} D & -I & 0 & 0 \\ 0 & D & -I & 0 \\ 0 & 0 & D & -I \\ 0 & 0 & 0 & D+RI \end{bmatrix}, \quad F = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 \end{bmatrix},$$

in which D is the $M \times M$ Chebyshev differentiation matrix (13) and where the Mth, $2M$th, $3M$th and $4M$th rows of F are cleared and the same rows of E are overwritten respectively by the $4M$-dimensional vectors

$$\begin{gathered} P, 0, 0, 0, \qquad Q, 0, 0, 0, \qquad 0, P, 0, 0, \qquad 0, Q, 0, 0, \\ P = (1, 1, 1, \ldots, M \text{ times}), \qquad Q = (1, -1, 1, -1, \ldots, M \text{ times}). \end{gathered} \tag{25}$$

The vectors P and Q arise from the well-known results that $T_n(1) = 1$ and $T_n(-1) = (-1)^n$. During the investigation of equation (21), no spurious solutions arose. Compared with the traditional formulation of the problem as described in Reference 12, this formulation is as close to trivial as could reasonably be expected. When $R = 0$, the solutions of the eigencondition (22) can be represented by $\sigma = -\alpha_k^2$, where α_k, $k \geqslant 0$, satisfies $\alpha_k = \tan \alpha_k$ and can be estimated to high accuracy as the fixed point of the iterative scheme $y_{n+1} - k\pi = \tan^{-1} y_n$, $y_0 = k\pi + 1$. Table I displays the top of the spectrum (ordered in decreasing real part) when $R = 0$ for various numbers of Chebyshev polynomials.

Results for the first two eigenvalues of this problem, generated using traditional Chebyshev methods, are presented in Reference 12 and merit some comparison with Table I. Two comments are worth a mention. For a given number of Chebyshev polynomials the accuracy returned by the procedure of this paper is clearly superior and so there is partial compensation for the additional size of the spectral matrices. More interestingly, the results of Reference 12 suggest that increasing the number of Chebyshev polynomials is causing a deterioration in the accuracy of the leading eigenvalue and this deterioration does not seem to be remedied by the modified scheme

Table I. Eigenvalues at $R = 0$

Eigenvalue ($M = 10$)	Eigenvalue ($M = 15$)	Eigenvalue ($M = 25$)	Accurate value
−9·86961365	−9·86960440	−9·86960440	−9.86960440
−20·19417167	−20·19072851	−20·19072856	−20·19072856
−39·68733153	−39·47845704	−39·47841760	−39·47841760
−62·64744349	−59·67978632	−59·67951594	−59·67951594
−119·0979878	−88·84327363	−88·82643962	−88·82643961

Table II. Eigenvalues at $R=4$

Eigenvalue ($M=30$)	$f(\sigma)$
$-17{\cdot}91292180 \pm 9{\cdot}45840144i$	$(-7+5i)\times 10^{-13}$
$-52{\cdot}95474066 \pm 13{\cdot}77106493i$	$(1-i)\times 10^{-12}$
$-107{\cdot}44870494 \pm 16{\cdot}32352728i$	$(-1-7i)\times 10^{-13}$

advocated in Reference 12. Results generated for the fourth-order system do not appear to display this instability.

As a further illustration, eigenvalues of (21) were computed when $R=4$ and the results are displayed in Table II, together with the value of $f(\sigma)$. In this case the leading eigenvalues are complex (nature changes around $R=2$).

5. EXAMPLE 2

The linear stability analysis of an incompressible, viscous, convecting magnetohydrodynamic fluid contained between horizontal boundaries $z=0$ and 1 and subject to a constant gravitational acceleration in the negative z-direction involves the determination of the eigenvalues σ of the system of non-dimensionalized equations

$$\begin{gathered}\sigma(D^2-a^2)w-\sigma P_m Db=(D^2-a^2)^2 w-Ra^2\theta-QD^2 w,\\ \sigma P_m b=QDw+(D^2-a^2)b, \qquad \sigma P_r\theta=(D^2-a^2)\theta+Rw,\end{gathered} \tag{26}$$

where w is the axial velocity component, a is the wave number, R^2 is the Rayleigh number, θ is the temperature, b is the axial component of magnetic induction, Q is the Chandrasekhar number, P_r and P_m are the viscous and magnetic Prandtl numbers respectively and D is the differential operator d/dz. A detailed discussion of this system can be found in Reference 15. To make the problem more specific, consider both boundaries to be thermally conducting, magnetically insulating, stationary and stress-free so that

$$w=0, \qquad D^2w=0, \qquad \theta=0, \qquad Db=0 \qquad \text{on } z=0,1. \tag{27}$$

In terms of the system variables

$$\begin{gathered}y_1=w, \qquad y_2=Dw, \qquad y_3=D^2w, \qquad y_4=D^3w,\\ y_5=\theta, \qquad y_6=D\theta, \qquad y_7=b, \qquad y_8=Db,\end{gathered} \tag{28}$$

equations (26) can be reformulated in the form $Y'=AY+\sigma BY$, where A and B are the real 8×8 matrices

$$A=\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\ -a^4 & 0 & Q+2a^2 & 0 & Ra^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\ -R & 0 & 0 & 0 & a^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1\\ 0 & -Q & 0 & 0 & 0 & 0 & a^2 & 0 \end{bmatrix}, \tag{29}$$

$$B=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -a^2 & 0 & 1 & 0 & 0 & 0 & 0 & -P_m \\ 0 & 0 & 0 & 0 & 0 & 0 & P_r & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & P_m & 0 \end{bmatrix}.$$

As in Example 1, equations (26) have no variable coefficients and can be instantly converted into the spectral representation $EV=\sigma FV$, where E and F have the block forms

$$E=\begin{bmatrix} D & -I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & D & -I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & D & -I & 0 & 0 & 0 & 0 \\ a^4 I & 0 & -(Q+2a^2)I & D & -Ra^2 I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & D & -I & 0 & 0 \\ RI & 0 & 0 & 0 & -a^2 I & D & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & D & -I \\ 0 & QI & 0 & 0 & 0 & 0 & -a^2 I & D \end{bmatrix}, \tag{30}$$

$$F=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -a^2 I & 0 & 1 & 0 & 0 & 0 & 0 & -P_m I \\ 0 & 0 & 0 & 0 & 0 & 0 & P_r I & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & P_m I & 0 \end{bmatrix}$$

and where the Mth, $2M$th, . . . , $8M$th rows of F are cleared and then corresponding rows of E are filled respectively with the $8M$-dimensional vectors

$$P,0,0,0,0,0,0,0, \quad Q,0,0,0,0,0,0,0, \quad 0,0,P,0,0,0,0,0, \quad 0,0,Q,0,0,0,0,0,$$
$$0,0,0,0,P,0,0,0, \quad 0,0,0,0,Q,0,0,0, \quad 0,0,0,0,0,0,0,P, \quad 0,0,0,0,0,0,0,Q,$$

with P and Q as defined in (25).

For computational purposes let $P_r=1$, $P_m=3$, $Q=100$ and $a=3{\cdot}702$. It is well known that overstability is possible in this problem whenever $P_m>P_r$ and for the chosen parameters it is strongly preferred. Table III presents the two most competitive eigenvalues (in the sense of largest real part) for a range of R^2-values above R^2_{crit}.

These results display some well-known features of eigenvalue problems and nicely illustrate the true value of spectral methods. It would be wrong to analyse the stability of equations (26) using compound matrices or inverse iteration, since unless you know exactly where to look at each step (generally you do not), the only critical value of R^2 that could sensibly be computed by these methods is $R^2 \approx 2653{\cdot}7$, i.e. $\sigma=0$, and this is not correct. In effect, a spectral method is essential for problems of this type. Even if you think you know where to look, the very unstable behaviour of the critical eigenvalue around $R^2=2600$ ought to persuade you to reconsider your strategy. Of

Table III. Eigenvalues for selected R^2-values

R^2	Top of spectrum
2550	$1.9935 \pm 2.0141i$
2590	$2.1525 \pm 0.5229i$
2591	$2.1565 \pm 0.4228i$
2592	$2.1605 \pm 0.2898i$
2593	2.2680 and 2.0608
2652	4.7654 and 0.0274
2653	4.7893 and 0.0113
2654	4.8131 and −0.0046
2655	4.8367 and −0.0204

course, compound matrices or inverse iteration can be very effectively employed to check eigenvalues computed by spectral methods.

6. EXAMPLE 3

The Orr–Sommerfeld equation occurs in the linear stability analysis of the pressure-driven laminar flow of a Navier–Stokes fluid between two stationary parallel plates and has the non-dimensional form

$$(D^2-a^2)^2 v = \mathrm{i}aR[(1-x^2-\sigma)(D^2-a^2)+2]v, \quad x\in(-1,1), \tag{31}$$

where $D=\mathrm{d}/\mathrm{d}x$, $v(x)$ is the perturbed velocity component normal to the horizontal boundaries $x=-1$ and 1, R is the Reynolds number and a is the wave number. Equation (31) is to be solved with boundary conditions

$$v(x)=\frac{\mathrm{d}v}{\mathrm{d}x}=0 \quad \text{on } x=-1, 1. \tag{32}$$

In terms of the system variables

$$y_1(x)=v(x), \qquad y_2(x)=Dv, \qquad y_3(x)=D^2v, \qquad y_4(x)=D^3v, \tag{33}$$

equation (31) has the standard form $Y'=AY+\sigma BY$, in which A and B are the matrices

$$A=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \beta_2 T_2(x)-\beta_3 & 0 & \beta_4-\beta_1 T_2(x) & 0 \end{bmatrix}, \qquad B=\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2\beta_2 & 0 & -2\beta_1 & 0 \end{bmatrix}, \tag{34}$$

where the coefficients β_1, β_2, β_3 and β_4 are defined by

$$\beta_1=\frac{\mathrm{i}aR}{2}, \qquad \beta_2=\frac{\mathrm{i}a^3R}{2}, \qquad \beta_3=a^4-2\mathrm{i}aR+\frac{\mathrm{i}a^3R}{2}, \qquad \beta_4=2a^2+\frac{\mathrm{i}aR}{2}.$$

This problem thus has the Chebyshev spectral representation $EV=\sigma FV$, where

$$E=\begin{bmatrix} D & -I & 0 & 0 \\ 0 & D & -I & 0 \\ 0 & 0 & D & -I \\ \beta_3 I-\beta_2 Q & 0 & \beta_1 Q-\beta_4 I & D \end{bmatrix}, \qquad F=\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2\beta_2 I & 0 & -2\beta_1 I & 0 \end{bmatrix}, \tag{35}$$

Table IV. Eigenvalues of Orr–Sommerfeld equation with $a=1$

$R=10^4$, $M=40$	$R=10^5$, $M=60$	$R=10^6$, $M=80$	$R=10^7$, $M=150$
0·23752649+0·00373967i	0·98881959−0·01116361i	0·99646446−0·00353387i	0·99888197−0·00111787i
0·96464251−0·03518658i	0·14592479−0·01504204i	0·99363603−0·00636015i	0·99798754−0·00201208i
0·93635178−0·06325157i	0·97987513−0·02008635i	0·99080759−0·00918649i	0·99709311−0·00290629i
0·90805630−0·09131288i	0·97093050−0·02900898i	0·98797947−0·12012779i	0·99619868−0·00380051i
0·87975567−0·11937098i	0·19820039−0·03731080i	0·06592528−0·01398326i	0·99530425−0·00469472i

in which the auxiliary matrix Q is defined by

$$Q_{i(i+1)}=\tfrac{1}{2}, \quad 1\leqslant i\leqslant M-1, \qquad Q_{(i+1)i}=\tfrac{1}{2}, \quad 3\leqslant i\leqslant M, \quad Q_{21}=1, \qquad \text{rest zero}$$

and where the Mth, $2M$th, $3M$th and $4M$th rows of F are cleared and the same rows of E are overwritten respectively by the $4M$-dimensional vectors

$$P,0,0,0, \qquad Q,0,0,0, \qquad 0,P,0,0, \qquad 0,Q,0,0.$$

The Orr–Sommerfeld equation differs slightly from the previous examples in the respect that the eigenvalues are ordered by decreasing imaginary part. The results presented in Table IV show the five top members of the eigenlist and have been generated with $a=1$ and R in the range 10^4–10^7. This is a severe test of any numerical eigenvalue method and it is significant that no spurious eigenvalues were ever detected. The number of polynomials used is in excess of the minimum required for sensible convergence and is included for rough guidance.

7. EXAMPLE 4

The linear stability analysis of convection in a porous medium has been discussed by Straughan[16] and involves the investigation of the eigenvalue problem

$$\left.\begin{aligned}(D^2-a^2)w&=-Ra^2H(z)\theta\\ \sigma P_r\theta&=RN(z)w+(D^2-a^2)\theta\end{aligned}\right\}\quad 0<z<1, \tag{36}$$

$$\theta(0)=w(0)=\theta(1)=w(1)=0, \tag{37}$$

where P_r is the Prandtl number, R^2 is the Rayleigh number, θ and w are perturbations in temperature and the axial component of velocity respectively and the functions $H(z)$ and $N(z)$ are defined in terms of two constants ε and δ and two constitutive functions $h(z)$ and $q(z)$ by the formulae

$$H(z)=1+\varepsilon h(z), \qquad N(z)=1+\delta q(z).$$

When ε and δ are small, an analysis due to Davis[17] leads to the conclusion that the eigenvalues of (36), (37) are real. However, if $H(z)=N(z)$, it is a straightforward matter to verify that

$$\sigma a^2P_r\int_0^1|\theta|^2\,dz=\int_0^1(|Dw|+a^2|w|)\,dz-a^2\int_0^1(|D\theta|^2+a^2|\theta|^2)\,dz \tag{38}$$

and hence σ is real for any function $H(z)$, and this raises the conjecture that σ is real for a large class of functions $N(z)$ and $H(z)$, i.e. a principle of exchange of stabilities holds in this case, although traditional analytic methods, to our knowledge, have been unable to establish the validity of this conjecture. In terms of the system variables

$$y_1=w, \qquad y_2=Dw, \qquad y_3=\theta, \qquad y_4=D\theta,$$

equations (36) can be rewritten in the form $Y' = AY + \sigma BY$, where A and B are given by

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ a^2 & 0 & -Ra^2H(z) & 0 \\ 0 & 0 & 0 & 1 \\ -RN(z) & 0 & a^2 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & P_r \end{bmatrix}, \tag{39}$$

leading to a spectral representation of the problem in the form $EV = \sigma FV$, with

$$E = \begin{bmatrix} D & -I & 0 & 0 \\ -a^2I & D & Ra^2H & 0 \\ 0 & 0 & D & -I \\ RN & 0 & -a^2I & D \end{bmatrix}, \qquad E = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & P_rI \end{bmatrix}, \tag{40}$$

where H and N are spectral matrices appropriate to the functions $H(z)$ and $N(z)$ and in which the Mth, $2M$th, $3M$th and $4M$th rows of F are cleared and the same rows of E are overwritten respectively by the $4M$-dimensional vectors

$$P,0,0,0, \qquad Q,0,0,0, \qquad 0,0,P,0, \qquad 0,0,Q,0.$$

Results for a variety of function pairs of polynomial/non-polynomial type and with multiple signs in [0, 1] suggest that the conjecture is true, i.e. system (36), (37) has real eigenvalues for a large variety of function pairs.

8. EXAMPLE 5

Davis[17] investigated the buoyancy–surface tension instability in a horizontal layer of viscous fluid using energy methods. The heart of the analysis requires the determination of ρ, where

$$\frac{1}{\rho} = \mathrm{Max}\left(\frac{\mu+N}{\sqrt{\mu}}\int_0^1\int_{A(z)} w\theta\,\mathrm{d}A\,\mathrm{d}z - \frac{1}{\sqrt{\mu}}\int_{A(1)}\theta\frac{\partial w}{\partial z}\,\mathrm{d}A\right),$$
$$\int_0^1\int_{A(z)}(|\nabla \mathbf{v}|^2 + |\nabla\theta|^2)\,\mathrm{d}A\,\mathrm{d}z = 1, \tag{41}$$

where the horizontal layers are $z=0$ and 1, $A(z)$ is the cross-section of the convection cells on constant z-planes and N and μ (>0) are known parameter constants. Also, w is the axial component of the solenoidal vector $\mathbf{v}$ and has the property that $\mathbf{v}=\mathbf{0}$ on the boundary $z=0$ whereas $w=0$ on the boundary $z=1$. Similarly, θ is a scalar function with value zero on $z=0$. In addition, $\mathbf{v}$ and θ are assumed to satisfy whatever differentiability conditions are necessary for the construction of the Euler equations for functional (41).

The analytical details of the constrained variational problem are suppressed except to say that the presence of surface integrals in the functional leads to a set of transversality conditions. The Euler equations are ultimately reduced to the form

$$(D^2-a^2)^2w = \rho a^2\left(\frac{\mu+N}{2\sqrt{\mu}}\right)\theta, \qquad (D^2-a^2)\theta = -\rho\left(\frac{\mu+N}{2\sqrt{\mu}}\right)w, \tag{42}$$

in which a is essentially a wave number and w and θ satisfy the boundary conditions

$$\left.\begin{aligned} w&=0\\ Dw&=0\\ \theta&=0 \end{aligned}\right\} \text{ on } z=0, \qquad \left.\begin{aligned} w&=0\\ D^2w&=-\rho(a^2/2\sqrt{\mu})\theta\\ D\theta&=-\rho(1/2\sqrt{\mu})Dw \end{aligned}\right\} \text{ on } z=1. \tag{43}$$

In terms of the system variables

$$y_1=w, \quad y_2=Dw, \quad y_3=D^2w, \quad y_4=D^3w, \quad y_5=\theta, \quad y_6=D\theta, \tag{44}$$

the Euler equations (42) can be written in the form $Y'=AY+\rho BY$, in which A and B are given by

$$A=\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0\\ -a^4 & 0 & 2a^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0 & a^2 & 0 \end{bmatrix}, \qquad B=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & a^2G & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ -G & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{45}$$

where $G=(\mu+N)/2\sqrt{\mu}$. The boundary conditions (43) can now be expressed as

$$\left.\begin{aligned} y_1&=0\\ y_2&=0\\ y_5&=0 \end{aligned}\right\} \text{ on } z=0, \qquad \left.\begin{aligned} y_1&=0\\ y_3&=-\rho(a^2/2\sqrt{\mu})y_5\\ y_6&=-\rho(1/2\sqrt{\mu})y_2 \end{aligned}\right\} \text{ on } z=1. \tag{46}$$

As in the previous examples, it is immediately obvious that the system (42) can be expressed in the form $EV=\rho FV$, where the spectral matrices E and F are

$$E=\begin{bmatrix} D & -I & 0 & 0 & 0 & 0\\ 0 & D & -I & 0 & 0 & 0\\ 0 & 0 & D & -I & 0 & 0\\ a^4I & 0 & -2a^2I & D & 0 & 0\\ 0 & 0 & 0 & 0 & D & -I\\ 0 & 0 & 0 & 0 & -a^2I & D \end{bmatrix}, \qquad F=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & a^2GI & 0\\ 0 & 0 & 0 & 0 & 0 & 1\\ -GI & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{47}$$

Table V. Values of Marangoni number M_a

μ	a	N	M_a
16·78	2·223	0	56·773
22·43	2·091	10	33·636
35·22	2·063	25	19·732
59·12	2·065	50	11·460
108·4	2·072	100	6·191
257·7	2·079	250	2·594

in which the Mth, $2M$th, . . . , $6M$th rows of E and F are respectively overwritten by the $6M$-dimensional vectors

E-matrix	F-matrix	E-matrix	F-matrix
$P,0,0,0,0,0,$	$0,0,0,0,0,0,$	$Q,0,0,0,0,0,$	$0,0,0,0,0,0,$
$0,Q,0,0,0,0,$	$0,P,0,0,0,0,$	$0,P,P,0,0,0,$	$0,0,0,0,-(a^2/2\sqrt{\mu})P,0,$
$0,0,0,0,Q,0,$	$0,0,0,0,0,0,$	$0,0,0,0,0,P,$	$0,-(1/2\sqrt{\mu})P,0,0,0,0.$

This problem is different from the other examples to the extent that the eigenvalue appears in the boundary conditions. Calculated values of $M_a = \rho^2$, the Marangoni number, are presented in Table V for various values of μ, a and N.

9. CONCLUSIONS

We believe that the variant of the spectral tau method exemplified in this paper can be easily and effectively applied to an extensive range of linear eigenvalue problems arising in many areas of applied mathematics, theoretical physics, geophysics and engineering science. The critical components of this method are now reviewed.

(i) The equations describing the mathematical problem are reformulated as a system of first-order equations. This is frequently easy to do since their formulation is usually based on a series of conservation laws, each of which generates a low-order differential equation. Often the coefficients of these equations are non-constant and so, on practical grounds alone, in many cases it may well be unreasonable to assimilate the individual conservation equations into one high-order differential equation in keeping with the strategy of more traditional spectral methods.

(ii) Each variable in the first-order system is now assigned its own spectral expansion. In this way derivatives are treated as independent variables and therefore enjoy a more accurate numerical representation. Although this leads to larger spectral matrices, numerical calculations indicate that the spectral expansion of each variable requires lower polynomials to achieve a prescribed accuracy. The convergence characteristics of the spectral method are so good that expansions containing 15–20 polynomials are frequently adequate. Not only is this a practical way of analysing systems of substantial order, but the superior representation of high-order derivatives appears to render the technique less susceptible to the creation of spurious eigenvalues. None arose in any of the discussed examples.

(iii) The spectral matrices are constructed in block form and boundary conditions are expressed as algebraic relations connecting spectral coefficients. Since the mathematical problem is expressed as a first-order system, boundary conditions, which traditionally involve derivatives of the dependent variable, are now straightforwardly expressed as linear combinations of the system variables. In particular, it is no longer necessary to evaluate derivatives of the spectral basis polynomials at boundary points. The boundary information overwrites the last row of each block.

(iv) The final eigenvalue problem is now treated with the 'QR' algorithm or the like. A variety of high-quality subroutines are available for this purpose (e.g. NAG or IMSL software libraries).

In addition to elucidating different aspects of the methodology, the examples presented in this paper have been chosen because they are of contemporary interest or have been judged by other authors to be interesting in their own right.

The Orr–Sommerfeld equation (Example 3) occupies a niche in the folklore of spectral analysis, partly for historical reasons, but also because its solution in the vicinity of $|x|=1$ exhibits boundary layer behaviour with typical scale thickness $(aR)^{-1/3}$. Thus it is an ideal vehicle for testing eigenvalue methods, since the procedure can be made arbitrarily severe by suitably increasing R. The pioneering paper of Orszag[5] investigated the case $a=1$, $R=10^4$ and these values have now become historically associated with the Orr–Sommerfeld equation. Increasing R makes the equation stiffer and therefore more susceptible to the generation of spurious eigenvalues. We encountered no numerical difficulties up to $R=10^9$, although we did experience a spot of bother from computing services. As an aside, the results of Table IV indicate that the competitive eigenvalue is a discontinuous function in parameter space. It is for this reason that spectral techniques are so important; critical eigenvalues cannot be found in this application using a tracking method. The critical eigenvalue at $R=10^4$ occupies the second slot at $R=10^5$, the fifth slot at $R=10^6$ and has completely faded at $R=10^7$.

Example 1 was selected on the basis that it gratuitously proffers spurious eigenvalues and has recently attracted research interest for this reason. Gardner *et al.*[12] develop a technique which they claim completely eradicates this difficulty, but, judging from the work involved in treating this low-order equation, we believe that the technicalities of their approach severely limit its applicability. Although we do not claim to have eradicated spurious eigenvalues, none appeared in this example and, moreover, the achieved accuracy seems more reliable than that attained by Gardner *et al.* This is easily checked by direct evaluation of the eigencondition. We speculate that this anomaly may well be due to the numerical degradation incurred during the extensive numerical preamble required by those authors before arriving at their eigenvalue problem.

Examples 2 and 4 pertain to Benard or buoyancy-driven convection. Problems of this ilk are fairly common in the literature of applied mathematics and geophysics and so it is appropriate that the related eigenvalue problems should be represented here. Example 2 characterizes the linear stability analysis of a horizontal layer of magnetic fluid, whereas Example 4 describes a comparable stability problem for the convection of a viscous fluid through a porous medium. Both examples are presented in their simplest possible form When rotation effects are incorporated into Example 2, as may be necessary in geophysical or astrophysical applications, the order of the differential system jumps to 12. Table III from Example 2 nicely illustrates the sensitivity of the spectral analysis to small changes in the Rayleigh number R^2.

Finally, Example 5 is included to remind readers that eigenvalue problems often stem from constrained variational problems, in this case something akin to a Rayleigh quotient. This particular application is unusual in that the eigenvalue appears in both the Euler equations and the related boundary conditions (Steklov problem). This frequently happens when the variational problem involves conditions of transversality.

Looking further afield, we believe the applications for this technique are many and varied. A large number of physical systems can be simplistically considered in terms of driving mechanisms such as buoyancy, surface tension, salting, etc. interacting with damping mechanisms such as viscosity, resistivity, imposed magnetic fields, etc. The stability analyses of such systems often lead directly to eigenvalue problems for linear theory or lead to constrained variational problems for energy theory. If the related eigenvalue problem can be sensibly expressed in terms of ordinary differential equations, e.g. via a normal modes analysis, then the methodology of this paper will be most appropriate, particularly if the nature of the spectrum is unknown or the principle of exchange of stabilities is inoperative.

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