

Highly Accurate Pseudospectral Approximations of the Prolate Spheroidal Wave Equation for Any Bandwidth Parameter and Zonal Wavenumber

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Received: 4 September 2016 / Revised: 22 October 2016 / Accepted: 5 November 2016 /
Published online: 24 November 2016
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Abstract The prolate spheroidal wave equation (PSWE) is transformed, using suitable mappings, into three different canonical forms which resemble the Jacobi, Laguerre and the Hermite differential equations. The eigenpairs of the PSWE are approximated with the corresponding classical orthogonal polynomial as a basis set. It is observed that for any zonal wavenumber m the Jacobi type pseudospectral methods are well suited for small bandwidth parameters c whereas the Hermite and Laguerre pseudospectral methods are appropriate for very large c values. Moreover, Jacobi pseudospectral methods work well for any parameter values such that $m \geq c$. Our numerical results confirm that for any values of m , the Jacobi $[(\alpha, \beta) = (\pm 1/2, m)]$ and the Laguerre ($\gamma = \pm 1/2$) pseudospectral methods formulated in this article for the numerical solution of the PSWE with small and very large bandwidth parameters, respectively, are highly efficient both from the accuracy and fastness point of view.

Keywords Prolate spheroidal wave equation · Classical orthogonal polynomials · Pseudospectral methods

Mathematics Subject Classification 33E10 · 33C45 · 65L60 · 65L15

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1 Introduction

The PSWE

$$\left[-\frac{1}{\cos \theta} \frac{d}{d\theta} \left(\cos \theta \frac{d}{d\theta} \right) + \frac{m^2}{\cos^2 \theta} + c^2 \sin^2 \theta \right] y = \lambda(c, m)y, \quad \theta \in \left(-\frac{\pi}{2}, \frac{\pi}{2} \right) \quad (1)$$

arises in many areas of physics such as the nuclear shell model, atomic and molecular physics, the study of light scattering in optics and theoretical cosmological models [3]. In (1), $\lambda(c, m)$ stands for the eigenvalue parameter, m the zonal wavenumber and c the bandwidth parameter. More background on the PSWE can be found, for example, in [1, 14, 19, 20]. Here, we are looking for the square integrable solutions of the PSWE. Singularities of (1) as well as the unboundedness of the term, containing the zonal wavenumber, at $\eta = \pm\pi/2$ imply that the eigenfunction $y(\eta)$ must vanish at the boundaries. Clearly, such an eigenfunction will be in the space $L_2(-1, 1)$ of the square integrable functions which suggests the use of the Dirichlet conditions

$$y \left(\pm \frac{\pi}{2} \right) = 0 \quad (2)$$

at the boundaries. Then, the transformation

$$\eta = \sin \theta, \quad \eta \in (-1, 1) \quad (3)$$

takes the equation into the following equivalent form

$$(1 - \eta^2)y'' - 2\eta y' - \left(\frac{m^2}{1 - \eta^2} + c^2 \eta^2 \right) y = -\lambda(c, m)y, \quad y(\pm 1) = 0, \quad (4)$$

whose solutions are the prolate spheroidal wave functions (PSWFs), which are very useful for approximating solutions of some ODEs and PDEs. In particular, it is observed in [25] that for problems involving bandlimited functions, spectral methods based on the PSWFs require fewer points per wavelength to achieve the same accuracy when compared to methods based on orthogonal polynomials such as Chebyshev or Legendre polynomials. Based on this observation, there are numerous studies on the use of PSWFs as a basis set in spectral schemes as an alternative to the classical bases such as Chebyshev and Legendre polynomials. In [16], the authors introduced a new class of numerical differentiation schemes constructed via the PSWFs which requires fewer points per wavelength (compared to existing differentiation schemes based on orthogonal polynomials) to achieve the same accuracy when it is used to approximate derivatives of bandlimited functions. In [9], the authors have examined the merits of using PSWFs as basis functions when solving hyperbolic PDEs using pseudospectral methods and concluded that one might gain from using the PSWFs over the traditional Chebyshev or Legendre methods in terms of accuracy and efficiency for marginally resolved broadband solutions. The authors of [23] have proposed a new well-conditioned prolate-collocation scheme which significantly outperforms Jacobi polynomial-based methods in approximating highly oscillatory bandlimited functions. In [5], author used PSWFs as an alternative to Chebyshev and Legendre polynomials for spectral element and pseudospectral algorithms. He showed that when compared to Chebyshev or Legendre polynomials, prolate functions give more uniform spatial resolution and when used as the spatial discretization for time-dependent PDEs in combination with explicit time-stepping, PSWFs allow a longer stable timestep than Legendre polynomials.

On the other hand, in solving the Helmholtz equations in spheroidal domains, one needs to solve the eigenvalue problem (4) with a wide range of the zonal wavenumber m and the

bandwidth parameter $c = ka$. Indeed, applying the separation of variables process in prolate spheroidal coordinates,

$$x = a\sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos(\phi), \quad y = a\sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin(\phi), \quad z = a\xi\eta, \quad (5)$$

one obtains the PSWE in (4) as the angular part of the Helmholtz equation. Therefore, it is very important to be able to obtain accurate numerical solutions of (4) for a wide range of wavenumber k , particularly very large k . In particular, one can adopt the Fourier-like spectral method developed in [22] for which fast and accurate solution of the eigenvalue problem (4) is essential.

Algorithms to compute the eigenpairs of the PSWE are still an active research area [3, 7, 8, 15, 18, 21]. Nevertheless, the computation of the eigensolutions is a challenging task especially when the bandwidth parameter c is very large. More recently, Ogburn et al. [18] and Huang et al. [15] have approximated the eigenvalues of the PSWE with very large bandwidth parameter by a finite difference and pseudospectral type schemes, respectively. In [18] a grid of 20000 points has been applied with high order finite differences to approximate the eigenvalues when $c = 10^7$. However their method is very expensive since it has occupied a gigabyte of memory and spent five hours on a laptop. On the other hand, in [15] the authors used radial basis functions on a uniform grid taking into account the reflection symmetry of the problem. That is, they used two different basis functions to treat the even and odd states of the PSWE. The numerical results are quite satisfactory when compared to those of [18], however, the method includes a scaling parameter whose optimum value must be determined empirically. In order to overcome this issue they used the Hermite function basis scaled by \sqrt{c} in a pseudospectral picture which also takes care of the symmetry. Furthermore, authors applied periodized Hermite basis for small values of the bandwidth parameter $c \in [0, 100]$ since the Hermite functions are not suitable for this parameter range. But, in this case the fixed scaling factor \sqrt{c} is too large and should be chosen by trial-and-error. The numerical results obtained by applying the last two approaches are also quite satisfactory.

Numerical solution of the PSWE for small bandwidth parameters is also discussed in [2]. Therein, we have tabulated several eigenvalues of the PSWE when the zonal wavenumber $m = 0$ and bandwidth parameter $c = \sqrt{10}$. Besides, we have reported the smallest truncation sizes necessary to obtain the ground state eigenvalue $\lambda_0(c, m)$ accurate within the machine epsilon as functions of c and m in a separate table which confirms that the truncation size N considerably increases as the bandwidth parameter c gets larger. Although, the method of [2] yields highly accurate results for small bandwidth parameters, it becomes useless when $c > 1000$.

Therefore, in this article, we construct several pseudospectral formulations of PSWE based on the classical orthogonal polynomials so that the lowest twenty eigenvalues with any bandwidth parameter c and zonal wavenumber m can be computed within the machine accuracy of quadruple precision arithmetic with a truncation size not exceeding 15 in a split second. Moreover, not only the lower eigenvalues but also the higher modes, as high as a thousand, can be computed within the machine accuracy just in a minute.

In Sect. 2, we give a general pseudospectral formulation of a hypergeometric like equation since in the forthcoming Sects. 3 and 4 we transform the PSWE into the equations of this kind. Then, in Sect. 3, we transform the PSWE into two separate equations resembling the Jacobi differential equation and hence, we construct two different Jacobi pseudospectral methods for small values of the bandwidth parameter. The first one approximates the full spectrum at once while the second one takes care of the symmetry of the problem and thus computes the even and odd eigenvalue sets separately. In Sect. 4, we transform the PSWE into another

two equations which appear much similar to the Hermite and Laguerre differential equations. Therefore, we construct the Hermite and Laguerre pseudospectral formulations of the PSWE for very large bandwidth parameters. The latter of the methods can separate the even and odd states which halves the truncation size and reduce the cost by a factor of four. Section 5, demonstrates and discusses the numerical results obtained by the methods constructed in Sects. 3 and 4 where the comparison with each other as well as the literature results are done. The last section concludes the paper with some remarks.

2 A General Pseudospectral Formulation for Hypergeometric Like Equation

Consider the equation

$$\sigma(x)y'' + \tau(x)y' + q(x)y = \lambda r(x)y, \quad x \in (a, b) \subseteq \mathbb{R} \tag{6}$$

where $q(x)$ and $r(x) > 0$ continuous functions, λ is an eigenvalue parameter and σ and τ are polynomials of degree at most two and one, respectively. The last equation reduces to the equation of hypergeometric type (EHT)

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0 \tag{7}$$

when $q(x) = 0$ and $r(x) = -1$. It is known that the n -th degree classical orthogonal polynomials $y(x) = p_n(x)$ denoted by the names Jacobi, Laguerre and Hermite are the solutions of the EHT for the specific values of the parameter

$$\lambda := \lambda_n = -n \left[\tau' + \frac{1}{2}(n - 1)\sigma'' \right]. \tag{8}$$

They are orthogonal in the sense that

$$\int_a^b p_m(x)p_n(x)\rho(x)dx = \delta_{mn}h_n^2 \tag{9}$$

where δ_{mn} is the Kronecker’s delta, h_n is the normalization constant and the weight function $\rho(x) > 0$ is the solution of the Pearson equation $[\sigma(x)\rho(x)]' = \tau(x)\rho(x)$. These polynomial solutions have exactly n real and distinct roots in (a, b) which are interlaced, i.e. sorting all the roots in ascending order, the roots of $p_{n+1}(x)$ alternate with those of $p_n(x)$. Now, for equation (6) we propose an approximate solution of the form

$$y(x) = \sum_{n=0}^N \ell_n(x)y_n \tag{10}$$

where

$$\ell_n(x) = \frac{p_{N+1}(x)}{(x - x_n)p'_{N+1}(x_n)}, \quad n = 0, 1, \dots, N \tag{11}$$

are the set of N th degree Lagrange interpolating polynomials in which $p_{N+1}(x)$ is the $(N + 1)$ -st degree polynomial solution of (7) and $y_n = y(x_n)$ are the exact values of the function $y(x)$ at the roots $\{x_n\}_{n=0}^N$ of $p_{N+1}(x)$. The zeros of the classical orthogonal polynomials may be determined as the eigenvalues of the tridiagonal matrix

Table 1 The coefficients of the recursion formula for the normalized classical orthogonal polynomials

Polyn.	A_n	B_n
Jacobi	$\frac{2}{2n + \alpha + \beta} \sqrt{\frac{n(n + \alpha)(n + \beta)(n + \alpha + \beta)}{(2n + \alpha + \beta - 1)(2n + \alpha + \beta + 1)}}$	$\frac{\beta^2 - \alpha^2}{(2n + \alpha + \beta)(2n + \alpha + \beta + 2)}$
Laguerre	$-\sqrt{n(n + \gamma)}$	$2n + \gamma + 1$
Hermite	$\sqrt{n/2}$	0

$$R = \begin{bmatrix} B_0 & A_1 & & 0 \\ A_1 & B_1 & A_2 & \\ & A_2 & B_2 & \ddots \\ & & \ddots & \ddots & A_N \\ 0 & & & A_N & B_N \end{bmatrix} \tag{12}$$

where the A_n and B_n are the coefficients in the three term recurrence relation

$$A_{n+1}\phi_{n+1}(\xi) + (B_n - \xi)\phi_n(\xi) + A_n\phi_{n-1}(\xi) = 0, \quad n = 0, 1, \dots \tag{13}$$

of the normalized classical orthogonal polynomials $\phi_n(x) = p_n(x)/h_n$. The procedure is known as the Golub-Welsch algorithm [13]. In Table 1, we present the coefficients A_n and B_n for the normalized Jacobi, Laguerre and the Hermite polynomials.

Now, inserting the approximate solution in (10) into the equation (6) and requiring its satisfaction at the grid points x_m and using the fact that $\ell_n(x_m) = \delta_{mn}$ we obtain the set of $N + 1$ equations

$$\sum_{n=0}^N [\sigma(x_m)\ell_n''(x_m) + \tau(x_m)\ell_n'(x_m) + q(x_m)\delta_{mn}] y_n = \lambda(c, m)r(x_m) \sum_{n=0}^N \delta_{mn} y_n \tag{14}$$

leading to the discrete representation

$$\widehat{\mathbf{B}}\mathbf{y} = \lambda(c, m)\mathbf{y} \tag{15}$$

of (6) where the general entry $\widehat{\mathcal{B}}_{mn}$ of the resulting matrix $\widehat{\mathbf{B}} = [\widehat{\mathcal{B}}_{mn}]$ may be written as

$$\widehat{\mathcal{B}}_{mn} = \frac{1}{r(x_m)} [\sigma(x_m)\ell_n''(x_m) + \tau(x_m)\ell_n'(x_m) + q(x_m)\delta_{mn}], \quad m, n = 0, 1, \dots, N. \tag{16}$$

Actually the matrices with entries

$$d_{mn}^{(1)} := \ell_n'(x_m) = \frac{1}{2} \begin{cases} \frac{2}{x_m - x_n} \frac{p'_{N+1,m}}{p'_{N+1,n}} & \text{if } m \neq n \\ -\frac{\tau_n}{\sigma_n} & \text{if } m = n \end{cases} \tag{17}$$

and

$$d_{mn}^{(2)} := \ell_n''(x_m) = \frac{1}{3} \begin{cases} -\frac{3}{x_m - x_n} \left[\frac{\tau_m}{\sigma_m} + \frac{2}{x_m - x_n} \right] \frac{p'_{N+1,m}}{p'_{N+1,n}} & \text{if } m \neq n \\ \frac{1}{\sigma_n} \left\{ \frac{\tau_n}{\sigma_n} [\sigma_n' + \tau_n] + N \left[\tau' + \frac{1}{2}(N + 1)\sigma'' \right] \right\} & \text{if } m = n \end{cases} \tag{18}$$

are known as the pseudospectral differentiation matrices of order one and two, respectively which can be derived by keeping in mind that $p_{N+1}(x)$ satisfies the EHT in (7) when $\lambda = \lambda_{N+1}$ and $p_{N+1}(x_m) = 0$ for $m = 0, 1, \dots, N$ [2]. In (17) and (18) we adopt the abbreviations $p'_{N+1,k} = p'_{N+1}(x_k)$, $\sigma_k = \sigma(x_k)$ and $\tau_k = \tau(x_k)$.

Thus, inserting (17) and (18) into (16) we obtain an explicit representation for the entries

$$\widehat{\mathcal{B}}_{mn} = -\frac{1}{6r_m} \begin{cases} \frac{12\sigma_m}{(x_m - x_n)^2} \frac{p'_{N+1,m}}{p'_{N+1,n}} & \text{if } m \neq n \\ \frac{\tau_n}{\sigma_n} [\tau_n - 2\sigma_n'] - 2N \left[\tau' + \frac{1}{2}(N + 1)\sigma'' \right] - 6q_n & \text{if } m = n \end{cases} \tag{19}$$

of the matrix $\widehat{\mathcal{B}}$ where $r_k = r(x_k)$ and $q_k = q(x_k)$. By means of the similarity transformation $\mathcal{B} = S^{-1}\widehat{\mathcal{B}}S$ where S is a diagonal matrix with entries

$$S_{mn} = \sqrt{\frac{\sigma_m}{r_m}} p'_{N+1,m} \delta_{mn}, \quad m = 0, 1, \dots, N \tag{20}$$

it is possible to avoid the computation of the terms $p'_{N+1}(x_m)$. Moreover, the new matrix \mathcal{B} is symmetric whose entries are given by

$$\mathcal{B}_{mn} = -\frac{1}{6} \begin{cases} \frac{12}{(x_m - x_n)^2} \sqrt{\frac{\sigma_m \sigma_n}{r_m r_n}} & \text{if } m \neq n \\ \frac{1}{r_n} \left\{ \frac{\tau_n}{\sigma_n} [\tau_n - 2\sigma_n'] - 2N \left[\tau' + \frac{1}{2}(N + 1)\sigma'' \right] - 6q_n \right\} & \text{if } m = n. \end{cases} \tag{21}$$

Therefore, the eigenvalues of (15) and hence, the approximate eigenvalues of (6), may be determined by the symmetric matrix-eigenvalue problem

$$\mathcal{B}v = \lambda(c, m)v \tag{22}$$

since the similar matrices share the same spectrum. Clearly an eigenvector y of (15) is given by

$$y = Sv \tag{23}$$

in terms of an eigenvector v of the symmetric matrix \mathcal{B} .

3 The Jacobi Pseudospectral Methods for the PSWE

In (4), to get rid of the singular term proportional to $1/(1 - \eta^2)$ we transform the dependent variable by the mapping

$$y(\eta) = (1 - \eta^2)^{m/2} u(\eta) \tag{24}$$

leading to the equation

$$(1 - \eta^2)u'' - 2(m + 1)\eta u' + q(\eta)u = \mu u, \quad \mu = m(m + 1) - \lambda(c, m) \tag{25}$$

with

$$q(\eta) = -(c\eta)^2. \tag{26}$$

Note that the solution $u(\eta)$ does not have to satisfy any boundary conditions since the transformation in (24) takes care of the boundary conditions in (2).

Notice that, the system (1) is reflection symmetric, i.e., it is invariant under the replacement of the independent variable by its negative. Thus, the spectrum $\lambda_n(c, m)$ of PSWE can be decomposed into two subsets containing merely the symmetric $\lambda_{2n}(c, m)$ and anti-symmetric $\lambda_{2n+1}(c, m)$ states so that the corresponding eigenfunctions $y_{2n}(\eta)$ and $y_{2n+1}(\eta)$ are even and odd functions of η , respectively. By separating the even and odd states, one deals with two matrices of size $N \times N$ instead of a matrix of size $2N \times 2N$ to get the eigenvalues which reduces the cost by a factor of four. Now, starting with the even transformation

$$\eta = \cos 2\theta \tag{27}$$

the system in (1) may be written as

$$(1 - \eta^2)y'' + \frac{1}{2}(1 - 3\eta)y' - \left[\frac{m^2}{2(1 + \eta)} + \frac{c^2(1 - \eta)}{8} \right]y = -\frac{1}{4}\lambda(c, m)y, \quad y(-1) = 0. \tag{28}$$

Then proposing a solution of type

$$y(\eta) = (1 + \eta)^{m/2}u(\eta) \tag{29}$$

satisfying the boundary condition at $\eta = -1$, we get the equation

$$(1 - \eta^2)u'' + \left[m + \frac{1}{2} - \left(m + \frac{3}{2} \right) \eta \right] u' + q(\eta)u = \mu u, \tag{30}$$

where $\mu_n = \frac{1}{4}[m(m + 1) - \lambda_{2n}(c, m)]$ and

$$q(\eta) = \frac{c^2}{8}(\eta - 1) \tag{31}$$

for the even states of the PSWE. On the other hand, for the treatment of the odd states first letting

$$y(\theta) = \sin \theta \phi(\theta) \tag{32}$$

where ϕ is necessarily an even function of θ , we transform the Eq. (1) into

$$-\phi'' + (\tan \theta - 2 \cot \theta)\phi' + \left(\frac{m^2}{\cos^2 \theta} + c^2 \sin^2 \theta \right) \phi = [\lambda(c, m) - 2]\phi \tag{33}$$

with the transformed boundary conditions $\phi(\pm 1) = 0$. The evenness of the function ϕ suggests the application of the same maps $\eta = \cos 2\theta$ and $\phi(\eta) = (1 + \eta)^{m/2}u(\eta)$ to reach at the equation

$$(1 - \eta^2)u'' + \left[m - \frac{1}{2} - \left(m + \frac{5}{2} \right) \eta \right] u' + q(\eta)u = \mu u \tag{34}$$

where $\mu_n = \frac{1}{4}[(m + 1)(m + 2) - \lambda_{2n+1}(c, m)]$ and $q(\eta)$ has already given in (31). Notice that when $c = 0$, Eq. (25) resembles the Jacobi differential equation

$$(1 - \eta^2)y'' + [\beta - \alpha - (\alpha + \beta + 2)\eta]y' + n(n + \alpha + \beta + 1)y = 0 \tag{35}$$

with $(\alpha, \beta) = (m, m)$ whereas (30) and (34) are much akin to the Jacobi differential equation with $(\alpha, \beta) = (-\frac{1}{2}, m)$ and $(\alpha, \beta) = (\frac{1}{2}, m)$, respectively. Actually, the equations in (30) and (34) can be put together to give the equation

$$(1 - \eta^2)u'' + [\beta - \alpha - (\alpha + \beta + 2)\eta]u' + q(\eta)u = \mu u, \tag{36}$$

where

$$\mu = \frac{1}{4} [(\alpha + \beta + \frac{1}{2})(\alpha + \beta + \frac{3}{2}) - \lambda(c, m)]. \tag{37}$$

Here $(\alpha, \beta) = (-\frac{1}{2}, m)$ and $(\alpha, \beta) = (\frac{1}{2}, m)$ yield the even and odd states, respectively, which can be seen on returning back to the original variable θ by (27), (29) and (32). In fact, the interrelations

$$P_{2n}^{(m,m)}(\eta) = (-1)^n \frac{n!(2n+m)!}{(2n)!(n+m)!} P_n^{(-\frac{1}{2},m)}(1-2\eta^2) \tag{38}$$

and

$$P_{2n+1}^{(m,m)}(\eta) = (-1)^n \frac{n!(2n+m+1)!}{(2n+1)!(n+m)!} P_n^{(\frac{1}{2},m)}(1-2\eta^2) \tag{39}$$

between the Jacobi polynomials with integer parameters m and n , supports that separation of the even and odd states halves the truncation size since one only needs to use $P_n^{(\pm\frac{1}{2},m)}(1-2\eta^2)$ instead of $P_{2n}^{(m,m)}(\eta)$ or $P_{2n+1}^{(m,m)}(\eta)$ in the construction of the Lagrange polynomials in (11).

Note that, equation (36) is of the form (6) with $r(\eta) = 1$, $\sigma(\eta) = 1 - \eta^2$ and $\tau(\eta) = \beta - \alpha - (\alpha + \beta + 2)\eta$. Hence, in this case, the matrix in (21) reads as

$$\mathcal{B}_{mn} = \begin{cases} \frac{-2\sqrt{(1-\eta_m^2)(1-\eta_n^2)}}{(\eta_m - \eta_n)^2} & \text{if } m \neq n \\ \frac{[\beta - \alpha - (\alpha + \beta + 2)\eta_n][\beta - \alpha - (\alpha + \beta - 2)\eta_n]}{-6(1-\eta_n^2)} - \frac{1}{3}N(N + \alpha + \beta + 3) + q(\eta_n) & \text{if } m = n. \end{cases} \tag{40}$$

The eigenvalues μ_n of the matrix in (40) leads to the approximate eigenvalues

$$\lambda_n(c, m) = m(m + 1) - \mu_n \tag{41}$$

of PSWE when $q(\eta_n) = -(c\eta_n)^2$ where η_n are the roots of the Jacobi polynomial $P_{N+1}^{(m,m)}(\eta)$ while it yields the even

$$\lambda_{2n}(c, m) = m(m + 1) - 4\mu_n \tag{42}$$

and odd

$$\lambda_{2n+1}(c, m) = (m + 1)(m + 2) - 4\mu_n \tag{43}$$

states when $q(\eta_n) = c^2(\eta_n - 1)/8$ where η_n are the roots of the Jacobi polynomial $P_{N+1}^{(-\frac{1}{2},m)}(\eta)$ and $P_{N+1}^{(\frac{1}{2},m)}(\eta)$, respectively.

4 The Hermite and Laguerre Pseudospectral Methods for the PSWE

Eigenfunctions of the PSWE are confined to a small interval around the origin for very large values of the bandwidth parameter c . On the other hand, the zeros of the Jacobi polynomials are denser at the boundaries and coarser in the middle of the interval $(-1, 1)$. Thus, if the Jacobi pseudospectral methods described in the last section are used, most of the grid

points are wasted in the interval where the eigenfunctions are too close to zero. Although the Jacobi pseudospectral methods are very efficient for small bandwidth parameters $c < 1000$, they are not feasible for very large c values. However, the prolate functions can accurately be approximated by the Hermite or the Laguerre functions with $\gamma = \pm 1/2$ when c tends to infinity [4, 10, 12, 15, 19]. Therefore, in this section, we construct the Hermite and the Laguerre pseudospectral formulations of the PSWE for very large values of $c > 1000$ where the former computes the full spectrum at once and the latter separates it as the even and odd in order to halve the truncation size N .

Since the Hermite polynomials are defined over the real line, we apply the transformation

$$x = \alpha \operatorname{arctanh} \eta, \quad x \in (-\infty, \infty) \tag{44}$$

to the equation in (4), where α is an optimization parameter. It is important to note that the optimum value α_{opt} of the scaling parameter α will not be chosen empirically which will be explained later. This leads to the equation

$$-y'' + \frac{1}{\alpha^2} V(x/\alpha) y = \frac{1}{\alpha^2} \lambda(c, m) W(x/\alpha) y, \quad y(\pm\infty) = 0 \tag{45}$$

over the real line with

$$V(t) = c^2 \operatorname{sech}^2 t \tanh^2 t + m^2 \quad \text{and} \quad W(t) = \operatorname{sech}^2 t. \tag{46}$$

Finally, letting

$$y(x) = e^{-x^2/2} u(x) \tag{47}$$

satisfying the boundary conditions at infinity, we get an equation of type (6)

$$u'' - 2xu' + q(x)u = \mu r(x)u, \quad \mu = \frac{1}{\alpha^2} \lambda(c, m) \tag{48}$$

with $\sigma(x) = 1, \tau(x) = -2x, \lambda = \mu,$

$$q(x) = x^2 - 1 - \frac{1}{\alpha^2} V(x/\alpha) \tag{49}$$

and

$$r(x) = W(x/\alpha). \tag{50}$$

Notice that (48) resembles the Hermite differential equation $u'' - 2xu' + 2nu = 0$ and in this case (21) reads as

$$\mathcal{B}_{mn} = \begin{cases} \frac{-2 \cosh(x_m/\alpha) \cosh(x_n/\alpha)}{(x_m - x_n)^2} & \text{if } m \neq n \\ \cosh^2(x_n/\alpha) \left[-\frac{2}{3} (x_n^2 + N) + q(x_n) \right] & \text{if } m = n \end{cases} \tag{51}$$

where $q(x_n)$ are the values of (49) at the roots of $H_{N+1}(x)$. Then the eigenvalues μ_n of (51) leads to the approximate eigenvalues

$$\lambda_n(c, m) = \alpha^2 \mu_n \tag{52}$$

of the PSWE for very large values of the bandwidth parameter c . On the other hand, reflection symmetric character of (4) suggests the use of even transformation

$$x = (\alpha \operatorname{arctanh} \eta)^2, \quad x \in (0, \infty) \tag{53}$$

in order to separate the symmetric and anti-symmetric states. This leads to the equation

$$xy'' + \frac{1}{2}y' - \frac{1}{4\alpha^2}V(\sqrt{x}/\alpha)y = -\frac{1}{4\alpha^2}\lambda(c, m)W(\sqrt{x}/\alpha)y, \quad y(\infty) = 0 \tag{54}$$

where V and W are defined in (46). Lastly, proposing a solution of type

$$y(x) = x^a e^{-x/2} \Phi(x) \tag{55}$$

satisfying the boundary condition at infinity where the polynomial term has been introduced to cope with the artificial singularity at $x = 0$, we obtain the equation

$$\begin{aligned} &x\Phi'' + \left(2a + \frac{1}{2} - x\right)\Phi' + \frac{1}{4}\left[\frac{2a(2a-1)}{x} - (4a+1) + x - \frac{1}{c}V(\sqrt{x}/\alpha)\right]\Phi \\ &= -\frac{1}{4\alpha^2}\lambda(c, m)W(\sqrt{x}/\alpha)\Phi. \end{aligned} \tag{56}$$

Then for simplicity letting $2a + \frac{1}{2} = \gamma + 1$ and choosing $\gamma = \pm\frac{1}{2}$ (or $a = 0, a = \frac{1}{2}$) we eliminate the term proportional to $1/x$ in order to end up with the equation

$$x\Phi'' + (\gamma + 1 - x)\Phi' + q(x)\Phi = \mu r(x)\Phi, \quad \mu = -\frac{1}{4\alpha^2}\lambda(c, m) \tag{57}$$

which is also an equation of type (6) with

$$q(x) = \frac{1}{4}\left[x - 2(\gamma + 1) - \frac{1}{c}V(\sqrt{x}/\alpha)\right] \quad \text{and} \quad r(x) = W(\sqrt{x}/\alpha). \tag{58}$$

Clearly the solutions in (55) with $\gamma = -\frac{1}{2}$ and $\gamma = \frac{1}{2}$ yield even and odd states of the PSWE, respectively, which can be seen on returning back to the original variable η via (53). To approximate the even

$$\lambda_{2n}(c, m) = -4\alpha^2\mu_n \tag{59}$$

and odd

$$\lambda_{2n+1}(c, m) = -4\alpha^2\mu_n \tag{60}$$

state eigenvalues of the PSWE we only need to diagonalize the matrix

$$\mathcal{B}_{mn} = \begin{cases} \frac{-2\sqrt{x_m x_n} \cosh(\sqrt{x_m}/\alpha) \cosh(\sqrt{x_n}/\alpha)}{(x_m - x_n)^2} & \text{if } m \neq n \\ \cosh^2(\sqrt{x_n}/\alpha) \left\{ \frac{1}{6x_n} [1 - (\gamma - x_n)^2] - \frac{1}{3}N + q(x_n) \right\} & \text{if } m = n. \end{cases} \tag{61}$$

when $\gamma = -\frac{1}{2}$ and $\gamma = \frac{1}{2}$, respectively where $q(x_n)$ are the values of the function $q(x)$ in (58) at the zeros of $L_{N+1}^{(\gamma)}(x)$.

In [15] the authors used the even and odd indexed Hermite functions to approximate the symmetric and anti-symmetric state eigenvalues of the PSWE, respectively. On the other hand, our Hermite pseudospectral formulation yields the full spectrum at once. Nevertheless, the Laguerre pseudospectral formulation of the present study can separate the even ($\gamma = -\frac{1}{2}$) and odd ($\gamma = \frac{1}{2}$) states. Actually, the approach of [15], i.e. the use of even and odd indexed Hermite functions in a pseudospectral picture and the present Laguerre pseudospectral methods with $\gamma = \pm\frac{1}{2}$ can be regarded as equivalent methods if we remember the interrelations

$$H_{2n}(x) = (-1)^n 2^{2n} n! L_n^{(-1/2)}(x^2) \tag{62}$$

and

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{(1/2)}(x^2) \tag{63}$$

between the Hermite and Laguerre polynomials. Notice that in [15] the Hermite pseudospectral method with even and odd indexed Hermite functions is directly applied to the PSWE whereas the present Laguerre pseudospectral method with $\gamma = \pm \frac{1}{2}$ is applied to the transformed equation. For this reason, there may be some differences between these two approaches from the numerical point of view which will be clear in the numerical tables of the next section.

5 Numerical Results and Discussion

In this section, we present extended numerical results obtained by applying the methods described in Sects. 3 and 4 and compare them with each other as well as the results from literature. In all tables, n stands for the eigenvalue index, $\lambda_n(c, m)$ the n -th eigenvalue of the PSWE with the specified c and m and N the truncation order for which the desired accuracy for the corresponding eigenvalue is obtained. The accuracy of the results reported in this study has been checked by inspecting the number of stable digits between two consecutive truncation orders.

Computer programs are executed in quadruple precision arithmetic in *gfortran-4.8* on a laptop having 4GB of memory and intel i5 processor. In all cases we are able to obtain the results within the machine accuracy at most in a minute when approximating $\lambda_{1000}(c, m)$ even in the case where $c = 10^{11}$ and the lower eigenvalues are obtained in a split second. The figures are plotted in Matlab in which the computer programs have also been implemented.

Table 2 demonstrates the eigenvalues of the PSWE when $(c, m) = (1, 0)$ and $(c, m) = (10^4, 10^5)$ by using the Jacobi pseudospectral methods with $(\alpha, \beta) = (m, m)$ leading to the full spectrum $\lambda_n(c, m)$ at once and $(\alpha, \beta) = (-\frac{1}{2}, m)$ which yields only even states $\lambda_{2n}(c, m)$. Clearly, we observed doubling in the truncation size of the former which can be

Table 2 First ten even indexed eigenvalues of the PSWE by using the Jacobi pseudospectral methods when $c = 1, m = 0$ and $c = 10^4, m = 10^5$

n	$\lambda_n(1, 0)$	$\lambda_n(10^4, 10^5)$
	$N = 30, (\alpha, \beta) = (m, m) = (0, 0)$ $N = 15, (\alpha, \beta) = (-\frac{1}{2}, m) = (-\frac{1}{2}, 0)$	$N = 36, (\alpha, \beta) = (m, m) = (10^5, 10^5)$ $N = 18, (\alpha, \beta) = (-\frac{1}{2}, m) = (-\frac{1}{2}, 10^5)$
0	0.31900005514689273978398198587	10003718790.89441837932164694879414
2	6.53347180052379648149253793608	10003316726.90881862885526988403506
4	20.50827436257093855722413803743	10002914670.80448417197006796181199
6	42.50381812695760418937576753119	10002512622.58140565743349373881942
8	72.50220271616845965220476590024	10002110582.23957373310332149558751
10	110.50143426911587261839976720230	10001708549.77897904592754281189537
12	156.50100843283168454389569748128	10001306525.19961224194426212851822
14	210.50074780399421213520590446291	10000904508.50146396628159229530631
16	272.50057668263170278361763094472	10000502499.68452486315755010559373
18	342.50045828232841844781777619114	10000100498.74878557587995181693492

Table 3 Smallest eigenvalue $\lambda_0(10^4, m)$ of the PSWE while m varies by using the Jacobi pseudospectral method with $(\alpha, \beta) = (-\frac{1}{2}, m)$ and the Laguerre pseudospectral method with $\gamma = -\frac{1}{2}$

m	N_J	$N_L (\alpha_{opt} = \sqrt{c})$	$N_L (\alpha_{opt} = \sqrt{m})$	$\lambda_0(10^4, m)$
0	380	7		9999.24998124765580750912
1	380	7		10000.250003125515727660609
10	380	7		10099.25498199656447497212
10^2	330	7		19999.75004375671960453056
10^3	130	7		1010049.13302966955376799298
10^4	17	17		100014141.76064030461520225821
10^5	10	150	6	10000100498.74878557587995181693
10^6	3	1500	5	1000001000049.998675070107813935151

Table 4 Several high indexed eigenvalues of the PSWE by using the Jacobi pseudospectral method with the specified (α, β) when $c = 1$ and $m = 0$

n	$N (\alpha, \beta) = (0, 0)$	$N (\alpha, \beta) = (-\frac{1}{2}, 0)$	$\lambda_n(1, 0)$
100	110	55	10100.500015471905647093185536399
200	210	105	40200.500003886917446770035728532
500	510	255	250500.50000062375510956230988949
1000	1010	505	1001000.5000001560940698291003783

avoided either by the use of symmetric Jacobi basis $\{P_{2n}^{(m,m)}(\eta)\}_{n=0}^N$ or the present Jacobi basis $\{P_n^{(-1/2,m)}(\eta)\}_{n=0}^N$ [see Eqs. (38) and (39)].

It is clear that for small values of c Jacobi pseudospectral methods are suitable. However, it can be seen from Table 3 that they are not appropriate for very large values of bandwidth parameter such that $m \leq c$ since in this case the eigenfunctions are localized around a small interval about the origin where the zeros of the Jacobi polynomials are coarser when compared to the end points of the interval $(-1, 1)$ (see Fig. 1). This can also be observed from Table 3. In fact, when $c = 10^4$ and $m \leq 10^3$, truncation orders for the Jacobi pseudospectral methods are considerably high which dramatically increase as c gets larger.

Surprisingly, for very large c values with $m \geq c$, Jacobi pseudospectral methods yield highly accurate results at small truncation orders N , too. To be specific, $N = 18$ is enough to produce the first ten states to the accuracy quoted in Table 2 when $c = 10^4$ and $m = 10^5$ and $N = 10$ is enough to obtain the ground state eigenvalue (see the seventh row of Table 3).

It is known that as $c \rightarrow \infty$ for fixed eigenvalue index n , the prolate functions are more accurately approximated by the n -th Hermite (or Laguerre function with $\gamma = 1/2$) function whose argument is scaled by the square root of the bandwidth parameter c [4, 12, 15]. Therefore, for $c \geq m$, $\alpha = \sqrt{c}$ is optimum in the sense that the desired accuracy is obtained with the smallest possible truncation order N . However, for $m \geq c$, the optimization parameter should be rechosen as $\alpha = \sqrt{m}$ in order not to take truncation orders as high as 1500 to get the tabulated accuracy. Thus, the optimum value of the scaling parameter α might be taken as

Table 5 Accuracy improvement for $\lambda_0(1, 0)$ and $\lambda_{1000}(1, 0)$ when the Jacobi pseudospectral method with $(\alpha, \beta) = (-\frac{1}{2}, m)$ is used

N	$\lambda_0(1, 0)$	N	$\lambda_{1000}(1, 0)$
4	0.3190000551469	501	1001000.50001
5	0.3190000551468927398	502	1001000.5000001560941
6	0.319000055146892739783982	503	1001000.50000015609406982910038
7	0.31900005514689273978398198587	504	1001000.5000001560940698291003783
8	0.31900005514689273978398198587	505	1001000.5000001560940698291003783

$$\alpha_{opt} = \sqrt{\max(c, m)} \tag{64}$$

for any m and very large values of c . However, by looking at the truncation orders in Table 3 we may say that for very large values of the bandwidth parameter $c \geq m$, the Hermite or Laguerre pseudospectral methods scaled by (64) are more suitable than their Jacobi counterparts.

On the other hand, Table 4 shows that the methods described here not only give satisfactory results for lower eigenvalues but also higher states.

Another remarkable issue for Tables 4 and 5 is the fast accuracy improvement of the methods. For example, when the even and odd states are separated, the smallest truncation size necessary to print the eigenvalue $\lambda_{1000}(c, m)$ on the screen is $N = 501$ regardless of its accuracy. However, when 32 digits of accuracy is required, we only need to increase the truncation size by three. That is, when $N = 504$ the error is less than or equal to 10^{-32} which is the machine zero of quadruple precision arithmetic. Actually, we expect an error much less than this since increasing N by one results in an accuracy gain of 8 – 10 digits (See Table 5). This is typical for all parameter ranges considered in this study. It is known that the numerical eigenvalue problems suffer from the problem of computing the full set of eigenvalues with a uniform accuracy. Only the portion of the eigenvalues can be obtained with a desired accuracy and rarely more than $2N/\pi$ are accurate enough, moreover often the fraction is $N/2$ or considerably smaller for a fixed truncation order N [6,24]. However, with the present formulation, all but the last few eigenvalues (three or four) of the PSWE, are obtained to the machine accuracy for a fixed truncation order N .

Table 6 demonstrates the effect of increasing m for fixed c and vice versa on the truncation order that is necessary to obtain the eigenvalues to the machine accuracy. Interestingly, the increase in m results in a decrease in the truncation size N while c remains unchanged. However, the increase in c while m is fixed has an opposite effect on N as expected. Actually, in (1) the term containing the zonal wavenumber m is singular at the end points ± 1 which may be problematic from the numerical point of view. Fortunately, transformations get rid of this singularity so that the nonzero m values are not a disadvantage but an advantage for our formulation.

In Table 7 we present the first eleven even indexed eigenvalues of the PSWE when $c = 10^7$ and $m = 0$. Since the Laguerre pseudospectral methods with $\gamma = \pm \frac{1}{2}$ separates the even and odd states, the truncation size is halved when compared to the Hermite pseudospectral method. Clearly, our methods yield more accurate results with a smaller truncation sizes than the radial basis functions (RBF) or the Hermite functions methods [15] and eight order finite differences [18]. It is worth noting that although our Hermite pseudospectral formulation is not able to separate the even and odd states, the better results are obtained with relatively

Table 6 Smallest truncation sizes to obtain $\lambda_{11}(c, m)$ to the quoted accuracy by using the Jacobi pseudospectral method with $(\alpha, \beta) = (\frac{1}{2}, m)$ when c and m vary

$c = 10$		
m	N	$\lambda_{11}(c, m)$
0	26	184.54761858852457640833705901739
10^{-1}	20	186.80600167867847699593805333280
1	19	207.70676111785875039455851329530
10	17	501.10179565732031970129421278971
10^2	12	12441.764971364585860241721862947
10^3	9	1023133.1303999773054788754589760
$m = 10$		
c	N	$\lambda_{11}(c, m)$
0	6	462.0000000000000000000000000000000
10^{-1}	9	462.00391869871637233605123379790
1	12	462.39186517444384925685069161521
10	17	501.10179565732031970129421278971
10^2	51	2345.010135577631447774866243889
10^3	162	23034.2246949267005286970936261

Table 7 First eleven even indexed eigenvalues of the PSWE by using the Hermite and Laguerre pseudospectral methods when $c = 10^7$ and $m = 0$.

n	$\lambda_n(10^7, 0)$		
	Hermite ($N = 30$) Laguerre, $\gamma = -\frac{1}{2}$ ($N = 15$)	Ref [15] ($N = 80$) RBF/Hermite func.	Ref [18] High order fd.
0	9999999.24999998124999765625	9999999.249999993 /980	9999990.96371903
2	49999996.24999971874993671874	49999996.24999970 /970	49999514.6707898
4	89999989.24999870624957578106	89999989.24999884 /869	
6	129999978.24999634374838984279	129999978.2499964 /970	
8	169999963.24999203124555390291	169999963.2499923 /922	
10	209999944.24998516873994295962	209999944.2499855 /853	
12	249999921.24997515623013201006	249999921.2499755 /752	
14	289999894.24996139371439605005	289999894.2499620 /613	
16	329999863.24994328119071007391	329999863.2499434 /439	
18	369999828.24992021865674907413	369999828.2499201 /199	
20	409999789.24989160610988804118	409999789.2498933 /919	

small truncation orders when compared to the Hermite function pseudospectral method of [15] which treats the even and odd states separately.

Table 8 demonstrates highly accurate results for high indexed even and odd eigenvalues such as $\lambda_{1000}(10^8, 0)$ and $\lambda_{1001}(10^8, 0)$ with notably small truncation sizes $N = 509$ with separation (Laguerre pseudospectral method with $\gamma = -\frac{1}{2}$) and $N = 1018$ without separation (Hermite pseudospectral method), respectively. To the best of our knowledge since there is no numerical results in literature for $c > 10^7$, we compare our results with 5-term asymptotic formula [1]

Table 8 Several high indexed eigenvalues of the PSWE when $c = 10^8$ and $m = 0$ by using the Laguerre with $\gamma = \pm \frac{1}{2}$ and Hermite pseudospectral methods

n	$N_{Laguerre}$	$N_{Hermite}$	$\lambda_n(10^8, 0)$ Laguerre pseudospectral method/ 5-term asymptotic eigenvalues in (65)
100	56	112	20099994949.24873080982749384641/621
101	56	112	20299994848.24869255229528585981/953
250	132	264	50099968624.23035043610929771799/784
251	132	264	50299968373.23011417811510489187/170
500	257	514	100099874749.09327857037294827490/443
501	257	514	100299874248.09233730894313876727/735
1000	509	1018	200099499497.99811279487282947333/344
1001	509	1018	200299498496.99435525602855264486/499

Table 9 Several eigenvalues of the PSWE when $c = 10^{11}$ and $m = 0, 10^3$ by using the Laguerre pseudospectral methods with $\gamma = -\frac{1}{2}$

n	m	N	$\lambda_n(10^{11}, m)$ Laguerre pseudospectral method	Asymptotic eigenvalues in (65)
0	0	4	9999999999.249999999971	9999999999.24999999998125
10		8	209999999944.24999999851648	209999999944.249999998516875
100		55	2009999994949.24999873081032	2009999994949.249998730810624
1000		505	200099999499499.24874812061533	200099999499499.248748120615297
0	10^3	4	10000099999.250004999997	10000099999.25000499998125
10		8	210000099944.2501049985165	210000099944.250104998516892
100		55	20100000994949.2510037308123	20100000994949.251003730812139
1000		505	20010000499499.25875312076566	20010000499499.258753120765447

$$\begin{aligned}
 \lambda_n(c, m) = & ck + m^2 - \frac{1}{8}(k^2 + 5) - \frac{k}{64c}(k^2 + 11 - 32m^2) \\
 & - \frac{1}{1024c^2} [5(k^4 + 26k^2 + 21) - 384m^2(k^2 + 1)] \\
 & - \frac{1}{c^3} \left[\frac{1}{128^2}(33k^5 + 1594k^3 + 5621) - \frac{m^2}{128}(37k^3 + 167k) + \frac{m^4}{8}k \right] \\
 & + O(c^{-4}), \quad k = 2n + 1
 \end{aligned} \tag{65}$$

valid for large bandwidth parameters. For $c \geq 10^8$, 5-term asymptotic formula is sufficient to produce results at least accurate to thirty two decimal places.

Finally, Table 9 present highly accurate results for an extreme case $c = 10^{11}$ and $m = 0$ or $m = 10^3$ with quite reasonable truncation orders. Our results agree with those obtained by 5-term asymptotic formula to the accuracy quoted.

It is clear from Fig. 1 that when the bandwidth parameter c is large, most of the nodes are wasted in the interval where the eigenfunction is to close to zero if the Jacobi pseudospectral methods are used. On the other hand, by the use of Hermite/Laguerre polynomials scaled by

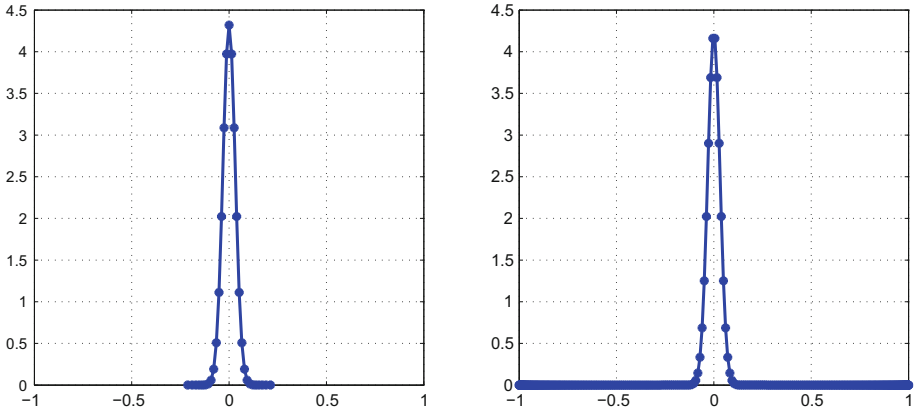


Fig. 1 Normalized (in L_2 sense) ground state eigenfunction $y_0(\eta)$ of the PSWE in (4) when $c = 1000$ and $m = 0$ by using the Hermite polynomial $H_{29}(\alpha x)$ (left) and the Jacobi polynomial $P_{143}^{(-1/2,0)}(\eta)$ in a pseudospectral formulation

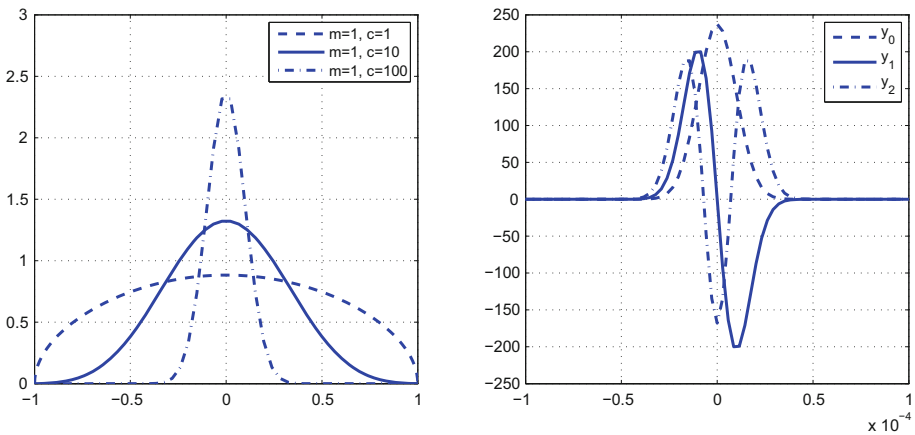


Fig. 2 Normalized (in L_2 sense) ground state eigenfunction $y_0(\eta)$ of the PSWE in (4) when $m = 1$ and c varies by using the Jacobi pseudospectral method with $(\alpha, \beta) = (-\frac{1}{2}, 0)$ (left). First three normalized eigenfunctions of the PSWE when $c = 10^{10}$ and $m = 0$ by using the Laguerre pseudospectral method with $\gamma = \pm \frac{1}{2}$

the square root of the bandwidth parameter c , all the nodes are collected to the interval where the wavefunction is nonzero. Therefore, $N = 30/15$ nodes are enough to resolve the ground state eigenfunction with the Hermite/Laguerre pseudospectral methods whereas we need $N = 144$ points when the Jacobi pseudospectral methods are used for the parameter values $c = 1000$ and $m = 0$. Moreover, as c gets larger the Jacobi methods becomes useless. The confinement of the eigenfunctions to a small interval as the bandwidth parameter increases may also be observed from the first part of Fig. 2. The second part of the same figure demonstrates the first three normalized eigenfunctions when $c = 10^{10}$ and $m = 0$.

6 Conclusion

In this article, we developed very accurate and efficient pseudospectral methods based on the Jacobi, Laguerre and Hermite polynomials to approximate the eigenvalues and eigenfunctions of the PSWE. To this end the PSWE is transformed into several equations resembling the hypergeometric type equation since the classical orthogonal polynomials are solutions to this equation. These particular transformations led us to use the most suitable classical orthogonal polynomial with specific parameter(s) as basis sets for the approximation of the eigenpairs.

Numerical results show that the Jacobi type pseudospectral methods are well suited for small c values as well as the large ones with $c \leq m$. On the other hand, the eigenfunctions with large bandwidth parameter c are confined to a small interval around the origin where the roots of Jacobi polynomials are coarser. Thus, most of the nodes are wasted in the interval where the eigenfunctions are close to zero making the Jacobi pseudospectral methods unsuitable for large c values with $c \geq m$. However, for large bandwidth parameters and any zonal wavenumber the Hermite and Laguerre pseudospectral methods scaled by $\sqrt{\max(c, m)}$ is more appropriate. Clearly, with this idea, we don't need to search for a suitable scaling parameter optimizing the accuracy of the Hermite or Laguerre pseudospectral method since it is a priori set to be the square root of the maximum of the bandwidth parameter and the zonal wavenumber. In contrast to the periodized Hermite basis of [15], we also do not have an optimization parameter in the Jacobi pseudospectral methods when approximating the eigenvalues for small values of the bandwidth parameter $c < 1000$.

The methods developed here will be useful in a variety of applications where accurate solutions of (1) are needed, in particular, in solving Helmholtz equations in spheroidal domains or more generally domains which can be considered as a perturbation of a spheroidal domain through the transformed field approach [11, 17].

Acknowledgements The first author would like to dedicate this research to the memory of his father who suddenly passed away just two days later than the author's arrival to USA. He feels a heartfelt sadness for being thousands of miles away at the moment he passed away. The first author's research was supported by a grant from TUBITAK, the Scientific and Technological Research Council of Turkey. The second author's research was partially supported by NSF DMS-1419053 and AFOSR FA9550-16-1-0102.

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