Grid method for computation of generalized spheroidal wave functions based on discrete variable representation

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We present an efficient and accurate grid method for computations of eigenvalues and eigenfunctions of the generalized spheroidal wave equation. Different from previous studies, our method is based on the expansion of the spheroidal wave function by discrete-variable-representation basis functions constructed from the associated Legendre polynomials. The differential operator can be expressed analytically on the grid points, which are the zeros of the associated Legendre polynomials. The resultant potential matrix is simply diagonal and evaluated directly on the same grid. The corresponding differential equation is thus converted to an eigenvalue problem of a small matrix, whose eigenvalues and eigenvectors are converged very fast. The wave functions can then be evaluated accurately at any desired point from the expansion formula with the computed eigenvectors. Compared to previous methods, our method is direct and efficient for any parameter c, either small or large.

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I. INTRODUCTION

There have been many efforts to compute the eigenvalues and eigenfunctions of the ordinary and generalized spheroidal wave equations [1–12]. The spheroidal wave equations arise in many research areas such as atomic and molecular physics, quantum scattering theory, electromagnetic theory, astrophysics, and cosmology [5,6]. The calculations for large and complex size parameters remain a challenging problem [13].

It is well known that the solutions of generalized spheroidal wave equations are separable in prolate spheroidal coordinates (η,ξ,ϕ). Various computational methods, generally based on infinite expansions of the wave function in terms of some basis functions, have been developed. The angular part of the generalized spheroidal wave function is represented by a series expansion of associated Legendre polynomials, and the radial part can be expanded by Jaffe's method, spherical Bessel functions, or Coulomb wave functions. The first step to solve the generalized spheroidal wave equations is to calculate the eigenvalues. There have been several methods such as infinite continued fractions [1,3], matrix techniques [2,4,6], or direct use of recurrence relations [7]. Also, for large values of c, asymptotic expansion method can be used (see [13] and references therein). Given the eigenvalues, the expansion coefficients can be found by recursion relation [2,4,7,9] or matrix eigenvector [6]. If the eigenvalues are known, the solution can also be obtained by a direct integration as well [3].

In the present work, we propose a grid method for solving the angular generalized spheroidal wave equation. Our grid method is based on the discrete-variable-representation (DVR) method. In this method, the wave function is expanded by DVR basis functions constructed from the associated Legendre polynomials.

In Sec. II, we will first present the DVR grid method, followed by presentation of another method called five-term matrix method. Then we will present some numerical results with these two methods, compared with some previous results when available. In Sec. III, we will discuss and conclude.

II. NUMERICAL METHODS

The angular and radial parts of the generalized spheroidal wave functions satisfy respectively the following differential equations [7]:

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{d}{d\eta}S_{mn}(c,R_1,\eta)\right] + \left(R_1\eta - c^2\eta^2 - \frac{m^2}{1-\eta^2} + A_{mn}\right)S_{mn}(c,R_1,\eta) = 0, \quad (1)$$

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{d}{d\xi}R_{mn}(c,R_2,\xi)\right] + \left(R_2\xi + c^2\xi^2 - \frac{m^2}{\xi^2-1} - A_{mn}\right)R_{mn}(c,R_2,\xi) = 0, \quad (2)$$

where $-1 \leq \eta \leq 1$, $1 \leq \xi \leq \infty$, and A_{mn} is the eigenvalue (the separation constant). When the parameter $R_1 = R_2 = 0$, the above equations reduce to the wave equations for the usual spheroidal wave functions [14]. In this section, we will first present our simple DVR grid method for angular wave equation (1). For the purpose of comparison, we will then give a brief description of a five-term matrix method.

A. DVR grid method

The DVR method (or Lagrange mesh method) is a widely used grid method in many research fields, such as atomic and molecular physics [15–27]. It is especially very efficient and accurate for many kinds of eigenvalues problems. In this kind of method, one constructs a set of basis functions de-

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TABLE I. Convergence of eigenvalues A_{00} of ordinary spheroidal wave equation (i.e., $R_1=0$) against the number of the DVR bases, N, at various values of c. (N is indicated in the parentheses after each eigenvalue.) The exact results from Ref. [9] are also shown at the bottom line of the table when available.

	$c=1$	$c=10$	$c=50$	$c=100$
A_{00} (N)	0.31839 (3)	9.23 (10)	49.32 (20)	99.31 (30)
	0.31899996 (5)	9.22830424 (15)	49.24498 (25)	99.24818 (40)
	0.31900005514691 (8)	9.22830429727 (18)	49.246159 (30)	99.24810112 (50)
	0.31900005514689 (10)	9.2283042972500 (20)	49.24615252712 (40)	99.24810110898 (60)
	0.31900005514688 (20)	9.2283042972498 (30)	49.24615252711 (100)	99.24810110898 (100)
Ref. [9]	0.319000055146893	9.228304297249945		99.2481011089832

rived from classical orthogonal polynomials, which are used to expand the wave function under investigation. Normally, the differential operator matrix in the equation satisfied by the wave function can be expressed analytically as a function of the zeros of some kind of classical orthogonal polynomials of a certain order. At the same time, the potential matrix in the differential equation is diagonal and can be evaluated directly on the grid points, i.e., the zeros of the classical orthogonal polynomials. The DVR method has shown extraordinary accuracy and efficiency in many different problems. It even finds applications in some time-dependent problems such as atomic and molecular dynamics in strong laser fields [28–31].

Baye and Heenen [16] prescribed a general method to construct DVR basis functions from any kinds of orthogonal polynomials. They derived analytically the matrix elements for kinetic operators for several kinds of orthogonal polynomials. For the purpose of the present work, we are interested in the Lagrange mesh corresponding to the associated Legendre polynomials. Following Baye and co-workers [16,17], one defines

$$\varphi_N(x) = h_N^{-1/2}(1-x^2)^{m/2}\frac{d^m}{dx^m}P_N(x), \tag{3}$$

where $P_N(x)$ is the Legendre polynomial of order N, h_N is a normalization constant, and m is a *positive* integer. The DVR basis functions (or Lagrange functions) are then given by

$$f_i(x) = \frac{1}{\varphi_N'(x_i)}\frac{\varphi_N(x)}{x-x_i} \tag{4}$$

$$= \frac{(-1)^{i+1}\sqrt{1-x_i^2}}{\sqrt{2N+2m+1}}\frac{\varphi_N(x)}{x-x_i}, \tag{5}$$

where x_i $(i=1,2,3,\ldots,N-m)$ are zeros of $d^mP_N(x)/dx^m$.

According to the prescription in Refs. [16] and [17], it is easy to show that for the differential operator

$$T = \frac{d}{dx}(1-x^2)\frac{d}{dx}, \tag{6}$$

the matrix elements are given analytically by [32]

$$T_{ij} = \begin{cases} -\dfrac{1}{3}(N+m)(N+m+1) + \dfrac{m^2+2}{3(1-x_i^2)}, & i=j \\ -\dfrac{2(-1)^{i-j}}{(x_i-x_j)^2}\sqrt{(1-x_i^2)(1-x_j^2)}, & i\neq j. \end{cases} \tag{7}$$

Note that the same DVR kinetic matrix for the special case $m=0$ and its regularized version for $m\neq 0$ were recently used by Vincke and Baye [33] to study energy spectra of the hydrogen molecular ion in an aligned strong magnetic field.

In Eq. (1), one can expand $S_{mn}(c,R_1,\eta)$ in terms of DVR basis set of Eq. (5) as

$$S_{mn}(c,R_1,\eta) = \sum_{j=1}^{N-m} B_j^{mn}f_j(\eta). \tag{8}$$

Substituting expansion (8) into Eq. (1) and multiplying both sides by $(\lambda_i\lambda_j)^{-1/2}f_i^*(\eta)$, we finally get after integrating η over $[-1,1]$

$$\left[\sum_j T_{ij} + V(\eta_i)\delta_{ij}\right]B_j^{mn} = A_{mn}B_i^{mn}, \tag{9}$$

where the kinetic operator matrices T_{ij} are given by Eq. (7) and the diagonal elements of potential matrix are calculated by

$$V(\eta_i) = R_1\eta_i - c^2\eta_i^2 - \frac{m^2}{1-\eta_i^2}. \tag{10}$$

The eigenvalues A_{mn} can be simply calculated by diagonalization of the matrix $H=T+V$. Moreover, the generalized angular spheroidal wave function can be analytically evaluated at any value of η by using Eqs. (5) and (8) with the computed eigenvectors B_j^{mn}. For given values of m and c, we get the eigenvalues and eigenvectors for $n=m,m+1,m+2,\ldots$ from a single calculation.

We have first checked the convergence of the eigenvalues A_{00} in Table I for different values of c. As one can see from Table I, A_{00} is fully converged for $N=10$, 20, 40, and 60 when $c=1$, 10, 50, and 100, respectively. We notice that a surprisingly small number N is able to give reasonable accuracy of the eigenvalues, especially when c is not large. This fast convergence property of the DVR method was discussed by Baye *et al.* [20]; they called it "unexplained accuracy." In the present study, similar fast convergence is also observed in Table II for the wave function S_{00} at different values of η

TABLE II. Convergence of the angular wave function S_{00} against the number of the DVR bases, N, for $c=1$ and 100 at different values of η. The wave function is normalized according to Eq. (11).

c	N	$\eta=0.0$	$\eta=0.2$	$\eta=0.5$	$\eta=0.8$
$c=1$	8	0.74399910	0.739261702	0.714693795	0.670400151
	10	0.743999111239	0.73926170027	0.71469379259	0.6704001506
	20	0.74399911126272	0.73926170026223	0.71469379261046	0.67040015058335
	50	0.74399911126274	0.73926170026223	0.71469379261046	0.67040015058331
$c=100$	40	2.3727	0.31957	8.666×10^{-5}	7.38×10^{-5}
	60	2.37302196	0.319523376	4.00368×10^{-6}	5.08×10^{-9}
	100	2.37302197686894	0.31952338590532	4.011201678×10^{-6}	1.96×10^{-15}
	150	2.37302197686894	0.31952338590533	4.011201679×10^{-6}	2.11×10^{-15}

for $c=1$ and 100. For the wave function, one typically needs a slightly larger number of DVR basis functions N than that needed for a converged eigenvalue A_{00}, especially for large c. Please note that we have adopted the following simple normalization for S_{mn} in the present work:

$$\int_{-1}^{1} S_{mn}^2(c,R_1,\eta)d\eta=1. \tag{11}$$

B. Five-term matrix method

For the purpose of comparison with the current DVR grid method, we provide here a different method for calculating eigenvalues and eigenfunctions of the angular generalized spheroidal wave equation. We call this method "five-term matrix method," which is similar to the matrix method proposed by Liu [6] but with the use of a five-term recursion relations given in Ref. [7] instead of a three-term recursion relation adopted in Ref. [6].

We first give a brief summary of the expansion used by Liu [6]. The solution of Eq. (1) is written in the form of series [3,6]

$$S_{mn}(c,R_1,\eta)=e^{-ic(1-\eta)}\sum_{k=0} d_k P_{m+k}^m(\eta). \tag{12}$$

Inserting expansion (12) into Eq. (1) leads to three-term recursion relation for the coefficients d_k,

$$\alpha_k d_{k+1}+(\beta_k-A_{mn})d_k+\gamma_k d_{k-1}=0, \tag{13}$$

where

$$\alpha_k=-(k+2m+1)[R_1+2ic(k+m+1)]/[2(k+m)+3],$$

$$\beta_k=(k+m)(k+m+1)+c^2,$$

$$\gamma_k=-k[R_1-2ic(k+m)]/[2(k+m)-1], \tag{14}$$

with the initial condition $d_{-1}=0$. Recursion (13) can be alternatively written as an infinite tridiagonal matrix equation as follows:

$$\begin{pmatrix} \beta_0-A_{mn} & \alpha_0 & 0 & 0 & 0 & \cdots \\ \gamma_1 & \beta_1-A_{mn} & \alpha_1 & 0 & 0 & \cdots \\ 0 & \gamma_2 & \beta_2-A_{mn} & \alpha_2 & 0 & \cdots \\ 0 & 0 & \gamma_3 & \beta_3-A_{mn} & \alpha_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \times \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}. \tag{15}$$

The eigenvalues A_{mn} and coefficients d_k can be obtained by calculating the eigenvalues and eigenvectors for the above matrix equation truncated to the dimension of N. However, in practice, we find that the convergence of eigenvalues for expansion (12) is very poor when c is large. Moreover, the convergence of the eigenfunctions is even worse for large c, as pointed out by Rankin and Thorson [4], and later by Hadinger *et al.* [7]. As an example, we have compared in Table III the convergences of the eigenvalues A_{00} by two different methods, i.e., the present DVR grid method and the three-term matrix method. As we can see from this table, the latter converges much more slowly than our DVR grid method. Actually for $c=1000$, even when the dimension N of the three-term matrix goes to as large as several thousands, we are still not able to get any result that is close to the exact one.

For the purpose of effective comparison with our DVR grid method, we thus adopt the expansion proposed by Rankin and Thorson [4]:

$$S_{mn}(c,R_1,\eta)=\sum_{t=0} a_t P_{m+t}^m(\eta). \tag{16}$$

Substitution of Eq. (16) into Eq. (1) yields a five-term recursion relation for coefficients a_t [7]:

$$g_5(t)a_{t-2}+g_4(t)a_{t-1}+[g_3(t)-A_{mn}]a_t+g_2(t)a_{t+1}+g_1(t)a_{t+2} =0, \tag{17}$$

where

$$g_5(t)=c^2t(t-1)/[(2t+2m-1)(2t+2m-3)],$$

TABLE III. Comparisons of the convergence of eigenvalues A_{00} at large values of c for the ordinary spheroidal wave equation (i.e., $R_1=0$) against the number of the DVR bases, N (or the dimension of the three-term matrix), by (a) the present DVR grid method and (b) the three-term matrix method from Eq. (15). The exact results from Ref. [9] are also shown at the bottom line of the table when available.

	$c=100$		$c=1000$	
N	(a) DVR grid	(b) Three-term	(a) DVR grid	(b) Three-term
50	99.24810112	3322.0	1281.5	914514.4
80	99.248101108982	990.3	1007.3	860407.4
120	99.248101108977	102.8	999.25395898	790173.8
200	99.248101108972	99.24810110882	999.249812265584	657806.7
300	99.248101108965	99.24810110901	999.249812265379	508847.4
Ref. [9]	99.2481011089832		999.2498122651815	

$$g_4(t) = -R_1 t/(2t+2m-1),$$

$$g_3(t) = c^2[2(t+m)(t+m+1) - 2m^2 - 1]/[(2t+2m-1)(2t+2m-3)] + (t+m)(t+m+1),$$

$$g_2(t) = -R_1(t+2m+1)/(2t+2m+3),$$

$$g_1(t) = c^2(t+2m+1)(t+2m+2)/[(2t+2m+3)(2t+2m+5)], \qquad (18)$$

with the initial condition $a_{-2}=a_{-1}=0$. The above recursion relation (17) can also be recast into the following matrix form:

$$\begin{pmatrix} g_3(0)-A_{mn} & g_2(0) & g_1(0) & 0 & 0 & 0 & \cdots \\ g_4(1) & g_3(1)-A_{mn} & g_2(1) & g_1(1) & 0 & 0 & \cdots \\ g_5(2) & g_4(2) & g_3(2)-A_{mn} & g_2(2) & g_1(2) & 0 & \cdots \\ 0 & g_5(3) & g_4(3) & g_3(3)-A_{mn} & g_2(3) & g_1(3) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}. \qquad (19)$$

Actually, one can arrive the same Eqs. (18) and (19) by an application of the direct variational method using associated Legendre polynomials as the basis set.

Our numerical tests indicate that for the same value of c, five-term recurrence (17) converges much faster than three-term recurrence (13). For large values of c, the inefficiency and insufficiency of the latter is especially apparent. According to normalization (11) of the wave function, the coefficients a_t should be recalculated by using the relation

$$\sum_{t=0} \frac{2}{2t+2m+1} \frac{(t+2m)!}{t!} |a_t|^2 = 1. \qquad (20)$$

C. Numerical results

Now, we present some numerical results for the eigenvalues and eigenfunctions for the generalized angular spheroidal wave function. In Table IV, we list the eigenvalues A_{mn} for various values of m, n, c, and R_1. In the calculations, we only use the number of DVR basis functions $N \leq 120$ to get all the converged eigenvalues for all the cases listed in the tables. It is also nice to observe that the five-term matrix method discussed above shows almost as good convergence performance as the DVR grid method does. In other words, in the calculations presented in Table IV by the five-term matrix method, the converged eigenvalues are achieved when the dimension of the matrix is taken to be comparable to those for the number of DVR basis functions used. The comparable accuracies of both methods may not be so surprising if one compares their expansions (8) and (16) of $S_{mn}(c, R_1, \eta)$, respectively. In Eq. (8), S_{mn} is expanded by $(N-m)$ DVR functions [polynomials of order $(N-m-1)$], while in Eq. (16), if t is truncated to $(N-m-1)$, S_{mn} is expanded by $(N-m)$ polynomials of different orders ranging from m to $(N-m-1)$. In other words, both expansions are mathematically equivalent. Indeed, it is somehow a little surprising that, despite the Gaussian quadrature approximation in the DVR grid method, it can still give results of high accuracy. It is mainly due to the almost exact representation of the differential operator and excellent approximation of the quadratic potential. [The term $m^2/(1-\eta^2)$ in Eq. (10) can actually be exactly included in the kinetic matrix [16].] For both the DVR grid method and five-term matrix method, it is fairly

TABLE IV. Comparisons of eigenvalues A_{mn} for various values of m, n, c, and R_1, calculated by different methods: (a) Liu's method in Sec. III B 3 of Ref. [6]; (b) DVR grid method in the present work; (c) five-term matrix method in the present work; and (d) exact results from Ref. [9] when available.

(m,n)	c	Method	$R_1=0$	$R_1=1$	$R_1=2$
(0,0)	1.0	(a)	0.3190000552	0.1896847197	−0.1543049703
		(b)	0.3190000551451	0.1896847196751	−0.154304970278
		(c)	0.3190000551469	0.1896847196676	−0.154304970280
		(d)	0.319000055146893		
	25	(a)	24.242093541	24.241685016	24.240459438
		(b)	24.242093541233	24.241685015471	24.240459438184
		(c)	24.242093541228	24.241685015472	24.240459438188
	50	(a)	49.246152523		
		(b)	49.246152527106	49.246051495767	49.245748401711
		(c)	49.246152527108	49.246051495758	49.245748401712
	100	(a)	99.248101119		
		(b)	99.248101108945	99.248075982093	99.248000601309
		(c)	99.248101108991	99.248075982074	99.248000601307
		(d)	99.2481011089832		
(1,9)	1.0	(a)	90.496130233	90.497489135	90.501565970
		(b)	90.496130233172	90.497489135053	90.501565969773
		(c)	90.496130233165	90.497489135058	90.501565969765
	25	(a)	385.72349350	385.72282121	385.72080432
		(b)	385.72349350415	385.72282120902	385.72080432062
		(c)	385.72349350415	385.72282120901	385.72080432062
(4,8)	1.0	(a)	72.389418915	72.389987373	72.391691694
		(b)	72.389418914697	72.389987372799	72.391691694233
		(c)	72.389418914698	72.389987372795	72.391691694219
	25	(a)	233.57957221	233.57911294	233.57773512
		(b)	233.57957220972	233.57911293651	233.57773511743
		(c)	233.57957220971	233.57911293651	233.57773511743

easy for us to get fully converged eigenvalues for significantly large values of c. For example, when $c=10\,000$, we get the fully converged result of $A_{00}=9\,999.249\,981\,22$ when $N\sim 800$. By using the three-term matrix method, we are unable to get any reasonable result close to this value even when $N\sim 10\,000$.

As examples, we present in Fig. 1 the lowest four ordinary spheroidal wave functions S_{mn} for different values of parameters calculated by the DVR grid method. These fully converged results are calculated under the condition that $N \leq 120$. The corresponding results calculated by the five-term matrix method in these cases are completely numerically identical to those from the DVR grid method. For the purpose of clarity we thus choose not to show them. However, we have to emphasize that for the five-term matrix method, we find much worse convergence of the wave functions than our DVR grid method in the case where m and c are simultaneously large. One example is that when $m=20$ and $c=1000$, our DVR grid method achieves fully converged wave function $S_{20,20}$ when $N\sim 200$ but five-term matrix method needs the dimension of the matrix N go larger than 800 to get a similar accuracy. We also notice that higher eigenvalues converge much more slowly as well for the five-term matrix method.

III. DISCUSSIONS

In summary, we have presented in this paper a simple, efficient, and accurate method for computing the eigenvalues and eigenfunctions of the angular generalized spheroidal wave equation. Our method is to directly solve this differential equation on a DVR grid, and the wave function is expanded in terms of DVR basis functions constructed from the associated Legendre polynomials. Our method is efficient for any value of c, small or large, and the wave function can be analytically evaluated at any spatial point from our expansion formula. The efficiency and accuracy are demonstrated by comparative studies with other methods.

Of course, our method can be naturally applied to the case when the number c is purely imaginary. Numerical results have not been shown in the present paper. When the number c is not purely imaginary, we have also tested our DVR grid method and five-term matrix method. Both methods actually work in this case, but the numbering and ordering of the eigenvalues is quite difficult and messy, as pointed out recently by Barakat *et al.* [12].

Finally, we have only investigated the DVR grid method to the angular equation. However, it should be noted that, in principle, it is also possible to solve the radial equation using

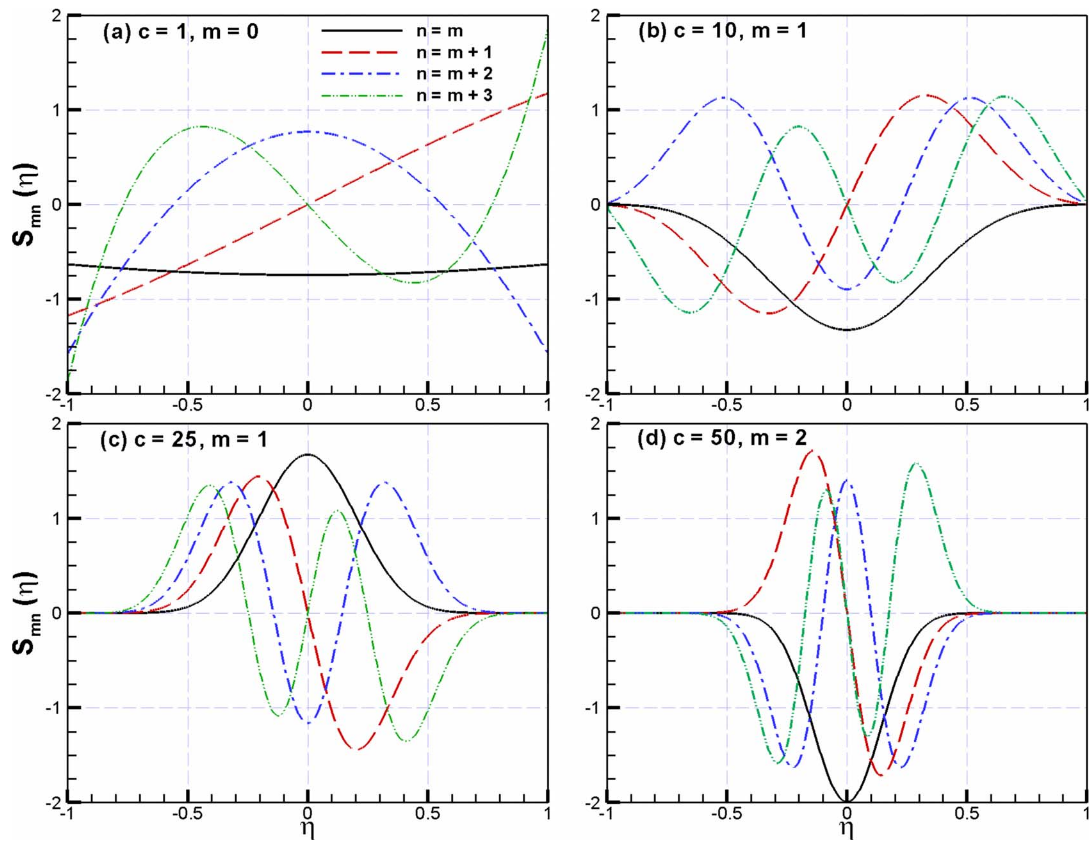

FIG. 1. (Color online) The lowest four ordinary spheroidal wave functions S_{mn} (i.e., $R_1=0$) for various values of c and m: (a) $c=1,m=0$; (b) $c=10,m=1$; (c) $c=25,m=1$; and (d) $c=50,m=2$.

similar DVR grid method with careful choice of the right DVR basis functions. For instance, the DVR grid method based on the generalized Laguerre polynomials [16,18] will be a natural choice for the radial equation. The relevant work is still under progress.

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