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Numerical Solution of Mathieu's Equation

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A method is presented for the numerical solution of Mathieu's equation. The power of the method lies in the fact that it can be used equally for ordinary and extremely asymptotic problems, making possible the computation of Mathieu functions for large values of the parameter with an accuracy heretofore unattainable.

I. INTRODUCTION

Mathieu functions have been the subject of extensive investigations since they were introduced by Mathieu in 1868 in connection with the determination of the vibrational modes of an elliptical membrane. Their importance in mathematical physics and applied mathematics is well known [1–3].

In this paper, we describe briefly a numerical method for the solution of Mathieu's equation

$$d^2y/dx^2 + (\lambda - 2q\cos 2x)\, y = 0, \tag{1}$$

which gives accurate results in the range of values of the real parameter q

$$0 < q < \infty. \tag{2}$$

As is well known [1, 2], Eq. (1) has periodic solutions of period π or 2π when λ takes a countably infinite set of characteristic values. Here we follow the standard notation of [2]. Equation (1) with the associated boundary conditions

$$y'(0) = y'(\pi) = 0 \tag{3}$$

is a regular Sturm–Liouville system [4] whose eigenfunctions are the even periodic Mathieu functions

$$ce_r(x, q), \qquad r = 0, 1, 2, \ldots . \tag{4}$$

The eigenfunctions of Eq. (1) with the boundary conditions

$$y(0) = y(\pi) = 0 \tag{5}$$

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are the odd periodic Mathieu functions designated

$$se_r(x, q), \qquad r = 1, 2, 3, \ldots . \tag{6}$$

The reason for the notation ce_r and se_r is that for $q = 0$ the eigenfunctions of systems (1) and (3) and (1) and (5) become, respectively, the trigonometric cosines and sines. Because of their importance in the scattering of waves by an elliptic cylinder, the solutions of (1) with boundary conditions (3) or (5) are also known as elliptic-cylinder functions.[5]

The main motivation for this work was the fact that although there are adequate methods for the numerical solution of (1) when q is not too large [6], say, $q < 100$, we are not aware of the existence of analytical or numerical methods that can solve Mathieu's equation satisfactorily for q very large, e.g., when $q = O(10^4)$. The reasons for these difficulties are as follows. It is known [1, p. 240] that for q large, systems (1), (3) or (1), (5) have eigenvalues

$$\lambda = O(q). \tag{7}$$

Thus, a simple division of Eq. (1) by the parameter q shows that in the limit $q \to \infty$, we have a singular perturbation problem [7]

$$\begin{aligned} &\epsilon d^2y/dx^2 + (\Lambda - 2\cos 2x)\, y = 0, \\ &\epsilon \equiv 1/q \to 0, \qquad \Lambda \equiv \lambda/q = O(1). \end{aligned} \tag{8}$$

It is well known that, in general, the solution of these problems cannot be obtained in the form of a single series that is uniformly valid in the whole domain. A qualitative knowledge of the solution of (8) might be obtained by using some basic concepts of singular perturbation theory [7]. A direct expansion of the solution of (8) in powers of the small parameter ϵ gives to first order

$$y(x, \epsilon) = 0,$$

which is certainly an approximation to the solution in most of the domain. A preliminary analysis of the boundary layer near $x = \pi/2$ by means of the stretching transformation

$$\tilde{x} = (\pi/2 - x)/\epsilon^{1/2}$$

indicates that the thickness of the boundary layer is $O(\epsilon^{1/2})$. This means that in the limit $\epsilon \to 0$ the thickness of the region about $\pi/2$, where the solution is not negligibly small, approaches zero as $\epsilon^{1/2}$.

In his fundamental paper, Goldstein [8] obtained an asymptotic series valid only for small values of x, which becomes infinite for $x = \pi/2$. Twenty two years later, Sips [9] obtained another asymptotic series which gives very accurate values in a certain neighborhood of $x = \pi/2$. Blanch showed [10] that Goldstein's and Sips's expansions have a rather narrow common region in which both are valid, and thus can be matched. The matching is rather delicate because the region where Goldstein's and Sips's expansions overlap is a function of the real parameter q and of the eigenfunction index r. Thus, the choice of a convenient matching point is not straightforward. To our knowledge, for very large values of q this matching has not been carried out to the point of achieving an accurate computation of the Mathieu functions uniformly in the range $0 \leqslant x \leqslant \pi/2$.

In a later paper, Sips [11] tried to find a single asymptotic expansion which would be uniformly valid in the whole domain $0 \leqslant x \leqslant \pi/2$. He only succeeded in again obtaining Goldstein's expansion valid in a neighborhood of $x = 0$ and also his own previous expansion valid near $x = \pi/2$. We now understand that because Mathieu's equation becomes a singular perturbation problem for large q, such uniformly valid expansion does not probably exist.

In this paper, we discuss briefly the numerical computation of Mathieu functions using a general method developed for the solution of Sturm–Liouville systems [12]. Of special interest is the fact that the method has been tested extensively and it has showed remarkable numerical stability and accuracy in the range of the real variables

$$0 < q \leqslant 10^4, \qquad 0 \leqslant x \leqslant \pi/2. \tag{9}$$

Thus, we have found a single numerical method with which we can compute Mathieu functions with any desired accuracy in the whole (q, x)-plane. The numerical algorithm gives in one pass the complete solution to the problem, i.e., any desired number of eigenvalues λ, the corresponding normalized eigenfunctions and their nontrivial zeros. Detailed numerical results are presented for a few selected cases and compared with some asymptotic results valid for large q. For completeness, we have also compared the results obtained with our method for low q with the values shown in Ince's Tables [5].

II. The Numerical Method

A detailed description of the numerical method has been given in a previous paper [12], and so here we give, for the sake of completeness, only a brief description of its salient features.

The coefficient $2q \cos 2x$ in (1) is approximated by the following step function:

$$V(x) \equiv 2q \cos 2x \approx V_s(x)$$
$$= \begin{cases} V_1 = V(0) = 2q, & 0 < x < x_1 ; \\ V_2 = [V(x_1) + V(x_2)]/2, & x_1 < x < x_2 ; \\ \cdots & \\ V_m = -2q, & x_{m-1} < x < x_m = \pi/2; \\ V_{m+1} = -2q, & x_m < x < x_{m+1} ; \\ V_{m+2} = [V(x_{m+1}) + V(x_{m+2})]/2, & x_{m+1} < x < x_{m+2} ; \\ \cdots & \\ V_n = V(x_n) = 2q, & x_{n-1} < x < x_n = \pi; \\ m \equiv n/2. \end{cases} \tag{10}$$

Here, n is the total number of steps of equal width used in the approximation. In each step, the resulting differential equation has constant coefficients and is integrated exactly in terms of circular or hyperbolic functions. Specifically, in each layer i, the solution of (1) with the approximation (10) is

$$y = A_i F(\beta_i x) + B_i G(\beta_i x), \qquad \alpha_i \equiv \lambda - V_i , \qquad \beta_i^2 \equiv | \alpha_i |, \qquad i = 2, 3 \cdots n - 1, \tag{11}$$

where F and G are the circular or hyperbolic cosine and sine, respectively, when α_i is positive or negative, and A_i and B_i are integration constants. If the boundary conditions are given by (3), the solutions at the boundary regions $i = 1$ and $i = n$, respectively, are

$$y = A_1 F(\beta_1 x), \qquad y = A_n F[\beta_n (x - \pi)], \tag{12}$$

and, similarly, for the boundary conditions (5). The solution and its derivative are now matched at the interfaces. In this way, we obtain a homogeneous system of equations for the integration constants ($A_i , i = 1, 2 \cdots n$; $B_i , i = 2, 3 \cdots n - 1$). The condition for the existence of a nontrivial solution is that the determinant of the coefficients be equal to zero. In this way, we obtain a *transcendental* equation with an *infinite* number of real roots which are the eigenvalues of our approximate problem (1), (3) and (10). For each eigenvalue there is a nontrivial solution for A_i, B_i that defines the corresponding eigenfunction. The matrix algebra analysis of the homogeneous system of equations is given in detail in [12]. Here we summarize the essential features of the method. These are as follows:

(1) The approximation of $2q \cos 2x$ by a step function is essential to the method. This is because certain numerical scaling problems that arise for very high values of q are solved analytically by using the elementary addition formulas for the hyperbolic functions.

(2) For any number of steps used in the approximation, we obtain in principle the whole infinite spectrum of eigenvalues and eigenfunctions, because the homogeneous system obtained is *transcendental* and has an infinite number of roots.

(3) As the approximate problem (1) and (10) is solved analytically, the absolute accuracy obtained for the eigenvalues and eigenfunctions is approximately independent of their index.

(4) In the implementation of the method, no initial guesses are required for the eigenvalues. We only give roughly the range where the eigenvalues lie

$$-2q < \lambda < \lambda_{\text{right}}, \tag{13}$$

where λ_{right} is arbitrary and is to be taken sufficiently larger than $-2q$ depending on the number of eigenvalues sought.

(5) As the linear system solution gives the coefficients A_i, B_i (Eqs. (11) and (12)), the Mathieu functions can be generated *continuously* in x. This is an essential property of the method because it allows us to obtain the zeros of the functions in a simple and efficient way.[1]

III. Perturbation Theory Analysis

When the coefficient $2q \cos 2x$ in the differential Eq. (1) is approximated by a step function (10), it undergoes a perturbation $O(h)$, where h is the step width [13]. A straightforward perturbation theory analysis then shows that we have a first-order method, i.e., absolute error both in the eigenvalues and eigenfunctions is $O(h)$ [14]. However, although no proof of this fact has yet been found, the numerical results below show quite clearly that the method is a second-order method, where the eigenvalue absolute errors are $O(h^2)$.

IV. Numerical Results

As the Mathieu functions are periodic with periods π or 2π, it is only necessary to compute them in the interval $0 \leqslant x \leqslant \pi/2$. The method has been extensively

[1] It has recently come to our attention that Gordon (*J. Chem. Phys.*, *51* (1969), 14) has used essentially the same idea as ours to solve Schrodinger's equation. Instead of approximating the potential (in Mathieu's equation $2q \cos 2x$) by a step function, he used a piecewise linear approximation to it. This results obviously in a higher order method, where the solutions in each linear step are expressed in terms of Airy functions. The qualitative features of both methods are, of course, identical. However, a very important advantage results from the simple choice of a constant step approximation. This is that we can solve extremely asymptotic problems, using the addition formulas for the hyperbolic functions to solve analytically the numerical scaling difficulties. We do not think that this can be achieved with the Airy function solutions.

tested, and we found that the Mathieu functions can be computed with high accuracy everywhere in the range

$$0 \leqslant x \leqslant \pi/2, \qquad 0 < q \leqslant 10^4, \tag{14}$$

provided that the number of steps n used in the approximation (see Eq. (10)) is sufficiently high. No motivation was found to solve the equation for $q > 10^4$, and the limit of application of the method with regards to these higher values of q has not yet been encountered.

1. *Ordinary Problems*

To illustrate the application of the method for low values of q, we have computed the first five even periodic Mathieu functions

$$ce_r(x), \qquad r = 0, 1, \ldots, 4, \tag{15}$$

for $q = 10$, by solving the Sturm–Liouville System (1), (3) with the approximation (10) where $n = 500$ steps. Only five-figure accuracy was sought as this is the accuracy given in Ince's Tables [5]. The results are shown in Tables I, II and III. In all the calculations performed in this work, we have used Ince's normalization:

$$\int_0^{\pi} [ce_r(x, q)]^2 \, dx = \int_0^{\pi} [se_r(x, q)]^2 \, dx = \pi/2 \tag{16}$$

2. *Asymptotic Problems*

As discussed in the Introduction, for large values of q the problem is of the singular perturbation type. The power of the numerical method is that it can be

TABLE I

Eigenvalues for First Five Even Periodic Mathieu Functions, $q = 10$

	λr	
r	Ince[a]	This work (500 steps)
0	−13.9370	−13.9369
1	−2.39914	−2.39907
2	7.71737	7.71739
3	15.5028	15.5028
4	21.1046	21.1046

[a] Ref. [5].

TABLE II

First Five Even Periodic Mathieu Functions, $q = 10$

x (degrees)	$ce_0(x)$		$ce_1(x)$		$ce_2(x)$		$ce_3(x)$		$ce_4(x)$	
	Ince	This work (500 steps)	Ince	This work (500 steps)	Ince	This work (500 steps)	Ince	This work (500 steps)	Ince	This work (500 steps)
0	.00763	.00763	.05360	.05360	.24589	.24589	.70483	.70483	1.12711	1.12711
10	.01189	.01189	.07276	.07276	.29252	.29252	.75142	.75143	1.10475	1.10476
20	.02882	.02882	.14047	.14047	.43766	.43766	.86848	.86848	.99948	.99948
30	.07258	.07258	.28437	.28437	.67953	.67953	.97386	.97386	.72026	.72026
40	.17020	.17020	.53217	.53217	.95851	.95851	.91414	.91414	.21401	.21400
50	.35704	.35704	.86565	.86565	1.10578	1.10578	.53580	.53580	−.38266	−.38267
60	.65271	.65271	1.16029	1.16029	.88828	.88827	−.11887	−.11887	−.69382	−.69382
70	1.01915	1.01915	1.18919	1.18919	.22835	.22834	−.66792	−.66792	−.39896	−.39896
80	1.33945	1.33945	.77440	.77439	−.56460	−.56460	−.63351	−.63350	.28583	.28583
90	1.46866	1.46866	0	0	−.92676	−.92676	0	0	.65132	.65133

TABLE III

Nontrivial Zeros of Even Periodic Mathieu Functions (in radians), $q = 10$

ce_2		ce_3		ce_4			
Ince	This work (500 steps)	Ince	This work (500 steps)	Ince	This work (500 steps)	Ince	This work (500 steps)
1.26988	1.26988	1.01737	1.01737	.759272	.759270	1.32485	1.32485

equally applied to solve Mathieu's equation with high accuracy in this region, $q > 10^3$, where other methods do not seem to be available.

We have computed first the even and odd Mathieu functions for $q = 1600$. This problem was chosen especially because some partial results on it have been published before [10]. Finally, Mathieu's equation was solved for $q = 2500$ and $q = 10000$. The results in the previous section and those to be shown below indicate that the same method is uniformly valid in all the range

$$0 < q \leqslant 10^4.$$

The accuracy of the method and the control of round-off errors will be discussed below together with the numerical results.

The first five eigenvalues for the even or odd periodic Mathieu functions are given in Table IV for the case $q = 1600$, together with the values obtained from the asymptotic formula obtained independently by Goldstein [8] and Ince [15, 16]. The asymptotic formula holds only when the ratio $8(2r + 1)^2/q$ is not too large; for the fifth eigenvalue, $r = 4$ and this ratio is 0.4, so that if higher eigenvalues

TABLE IV

Eigenvalues For First Five Even and Odd Periodic Mathieu Functions, $q = 1{,}600$

	$-\lambda_r$	
r	Goldstein's and Ince's	This work, (8000 steps)
0	3120.2508	3120.2507
1	2961.2571	2961.2571
2	2803.2779	2803.2779
3	2646.3232	2646.3232
4	2490.4031	2490.4033

were needed in this case, they could not be obtained analytically with the same accuracy as those shown in Table IV. In Table V, the absolute errors obtained in the eigenvalues for different numbers of steps are shown. It is seen that each time the number of steps is doubled, the absolute error in all eigenvalues decreases by a factor of four. This Table seems to provide experimental proof of the fact that the method is a second-order method, with the absolute error of the eigenvalues $O(h^2)$, where h is the step width. The perturbation theory analysis referred to before then gives a conservative estimate of the errors.

TABLE V

Absolute Errors in the Eigenvalues for Different Number of Steps, $q = 1600$[a]

Steps	$\Delta\lambda_0$[b]	$\Delta\lambda_1$	$\Delta\lambda_2$	$\Delta\lambda_3$	$\Delta\lambda_4$
500	−167	−202	−177	−191	−171
1000	−46	−50	−46	−47	−44
2000	−11	−12	−11	−11	−11
4000	−2	−3	−2	−2	−2
8000[c]	0	0	0	0	0

[a] Units in Eighth Significant Figure.
[b] $\Delta\lambda_i = \lambda$ approx. $-\lambda$ exact.
[c] The eigenvalues for 8000 steps are considered exact.

Obviously, if only the eigenvalues are sought, then Goldstein's and Ince's formula should be used wherever applicable, as it is a simple analytic expression [8, Eq. (36)]. In this respect, the asymptotic formula already gives about five-(significant)-figure accuracy in the first three eigenvalues for $q = 50$. For very large values of q, say, $q > 500$, it should be used to great advantage.

As discussed above, the asymptotic formula loses its accuracy for the higher eigenvalues. In this case, the continued fraction method of Blanch and Rhodes [17] and Blanch [18] gives the eigenvalues accurately.

It is a well-known fact that the eigenvalues of the even and odd periodic Mathieu functions defined by systems (1) and (3), and (1) and (5), approach each other asymptotically as q grows [8]. This is already detectable for $q = 40$, while, e.g., for $q = 100$, there is no difference whatever to five figures in the first sixteen eigenvalues of the two systems. Actually both the even and odd Mathieu functions also approach each other asymptotically in the whole domain $0 \leqslant x \leqslant \pi/2$. Sips argued in favor of this point stating that although $ce_r'(0, q) = se_{r+1}(0, q) = 0$, as both functions also approach zero near $x = 0$, it is true asymptotically that both functions and their derivatives are zero for $x = 0$, and thus both must have the same asymptotic expansion. In a later paper, Blanch proved this fact rigorously [19].

Tables VI and VII provide a striking experimental confirmation of the result. Table VI shows that except in a small neighborhood $x \to 0$, the even and odd functions are identical numerically. To nine figures, Table VII shows that they also have the same zeros.

It is our experience that whenever a given number of eigenvalues for the even and odd functions are the same to a certain accuracy, then the corresponding eigenfunctions are also approximately equal to the same accuracy.

TABLE VI

First Five Even and Odd Periodic Mathieu Functions, $q = 1600$[a]
(Notation: $1.5 - 20 = 1.5 \times 10^{-20}$)

x (degrees)	$ce_0(x)$ $se_1(x)$	$ce_1(x)$ $se_2(x)$	$ce_2(x)$ $se_3(x)$	$ce_3(x)$ $se_4(x)$	$ce_4(x)$ $se_5(x)$
0	1.437829 − 34	3.631844 − 33	6.456225 − 32	9.326067 − 31	1.160991 − 29
	0	0	0	0	0
5	7.353967 − 32	1.701256 − 30	2.768224 − 29	3.658015 − 28	4.163293 − 27
	7.353953 − 32	1.701252 − 30	2.768216 − 29	3.658004 − 28	4.163277 − 26
10	7.159121 − 29	1.515930 − 27	2.256453 − 26	2.725978 − 25	2.834611 − 24
20	4.736343 − 23	8.363306 − 22	1.036717 − 20	1.041577 − 19	8.994520 − 19
30	1.380230 − 17	2.008541 − 16	2.048252 − 15	1.689781 − 14	1.195895 − 13
40	1.205248 − 12	1.416048 − 11	1.162701 − 10	7.701102 − 10	4.362488 − 9
50	2.226840 − 8	2.041578 − 7	1.301759 − 6	6.660784 − 6	2.898455 − 5
60	6.447388 − 5	4.350742 − 4	2.020884 − 3	7.445416 − 3	2.302085 − 2
70	2.293028 − 2	0.1018120	0.3019907	0.6839989	1.236274
80	0.8372609	1.844382	2.269957	1.360523	0.4794243
90	2.812111	0	−1.978909	0	1.705239

[a] Only for the 0° and 5° entries do the even and odd functions differ, the values corresponding to ce_r and se_{r+1} are at the top and the bottom of these entries, respectively.

TABLE VII

Nontrivial Zeros of First Five Even
and Odd Periodic Mathieu Functions (in radians), $q = 1{,}600$

ce_2 se_3	ce_3 se_4	ce_4 se_5	
1.49140500	1.43299094	1.38463889	1.51170705

Tables VIII, IX, and X show the results for the even and odd periodic Mathieu functions for $q = 2500$. Only system (1) and (3) was solved in this case. Obviously, the entries for all even and odd functions are the same except for $x = 0$. Tables XI, XII, and XIII give the results for $q = 10\,000$.

TABLE VIII

Eigenvalues For First Five Even and Odd Periodic Mathieu Functions, $q = 2{,}500$

	$-\lambda_r$	
r	Goldstein's and Ince's	This work (10 000 steps)
0	4900.3506	4900.2505
1	4701.2557	4701.2556
2	4503.2723	4503.2722
3	4306.3082	4306.3082
4	4110.3716	4110.3717

TABLE IX

First Five Even and Odd Periodic Mathien Functions, $q = 2500$
(Notation: $1.5 - 20 = 1.5 \times 10^{-20}$)

x (degrees)	$ce_0(x)$ $se_1(x)$	$ce_1(x)$ $se_2(x)$	$ce_2(x)$ $se_3(x)$	$ce_3(x)$ $se_4(x)$	$ce_4(x)$ $se_5(x)$
0	3.133350 − 43	8.851492 − 41	1.761445 − 40	2.851118 − 39	3.981161 − 38
	0	0	0	0	0
10	5.029117 − 36	1.191197 − 34	1.985731 − 33	2.689930 − 32	3.140436 − 31
20	9.650844 − 29	1.906485 − 27	2.647796 − 26	2.985009 − 25	2.896999 − 24
30	6.626605 − 22	1.078942 − 20	1.233308 − 19	1.142665 − 18	9.100183 − 18
40	1.006166 − 14	1.322761 − 14	1.218192 − 13	9.072734 − 13	5.794502 − 12
50	2.187203 − 10	2.243885 − 9	1.606424 − 8	9.262558 − 8	4.560010 − 7
60	4.677522 − 6	3.532214 − 5	1.846097 − 4	7.700923 − 4	2.715460 − 3
70	7.259596 − 3	3.607157 − 2	0.1211428	0.3155416	0.6704233
80	0.6534798	1.610986	2.337216	1.990763	0.4092900
90	2.974151	0	−2.094999	0	1.807176

[a] Only for the 0° entry do the even and odd functions differ.

TABLE X

Nontrivial Zeros of First Five Even and Odd Periodic Mathieu Functions (in radians), $q = 2{,}500$

ce_2 / se_3	ce_3 / se_4	ce_4 / se_5	
1.49984711	1.44769870	1.40458616	1.51802416

TABLE XI

Eigenvalues for First Five Even and Odd Periodic Mathieu Functions, $q = 10{,}000$

	$-\lambda_r$	
r	Goldstein's and Ince's	This work (10 000 steps)
0	19800.2503	19800.2501
1	19401.2528	19401.2525
2	19003.2610	19003.2607
3	18606.2788	18606.2785
4	18210.3099	18210.3096

TABLE XII

First Five Even and Odd Periodic Mathieu Functions, $q = 10\,000$[a]
(Notation: $1.5 - 20 = 1.5 \times 10^{-20}$)

x (degrees)	$ce_0(x)$ / $se_1(x)$	$ce_1(x)$ / $se_2(x)$	$ce_2(x)$ / $se_3(x)$	$ce_3(x)$ / $se_4(x)$	$ce_4(x)$ / $se_5(x)$
0	1.385951 − 86	5.540359 − 85	1.563132 − 83	3.594063 − 82	7.142961 − 81
	0	0	0	0	0
10	7.740289 − 72	2.595363 − 70	6.139168 − 69	1.182916 − 67	1.969241 − 66
20	3.049238 − 57	8.529588 − 56	1.682314 − 54	2.701391 − 53	3.745709 − 52
30	1.520331 − 43	3.505917 − 42	5.696413 − 41	7.529950 − 40	8.588816 − 39
40	3.668898 − 31	6.832328 − 30	8.955079 − 29	9.538546 − 28	8.757022 − 27
50	1.797856 − 20	2.612971 − 19	2.667791 − 18	2.209153 − 17	1.573546 − 16
60	8.453103 − 12	9.043767 − 11	6.769447 − 10	4.092237 − 9	2.118370 − 8
70	2.076111 − 5	1.461597 − 4	7.115789 − 4	2.762292 − 3	9.053322 − 3
80	0.1701774	0.5944281	1.345308	2.218352	2.689422
90	3.538554	0	−2.497398	0	2.158656

[a] Only for the 0^0 entry do the even and odd functions differ.

TABLE XIII

Nontrivial Zeros of the First Five
Even and Odd Periodic Mathieu Functions (in radians), $q = 10\,000$

ce_2	ce_3	ce_4	
se_3	se_4	se_5	
1.52071250	1.48397540	1.45367652	1.53359058

The well-known phenomenon of condensation of the zeros toward $x = \pi/2$ when $q \to \infty$ is shown very strikingly in Tables VII, X, and XIII.

The ease with which the eigenvalues are obtained should be noted here. For example, for the calculation of the eigenvalues given in Table XI, the search range (13) was $-19800.4 \leqslant \lambda \leqslant 16400$; the transcendental function whose zeros are the eigenvalues was evaluated at 25 points in it. Whenever a change of sign is detected, the zero is found by Muller's method [20]; the search then continues to the right until the next zero is detected. The search is terminated when the range (13) is completely scanned or when a predetermined number of eigenvalues has been found. As Muller's method converges quadratically, even in this extreme calculation, convergence to any of the five eigenvalues required a maximum of seven iterations, and each of these only requires in turn the evaluation of the function at two points.

Finally, in Table XIV, we show a comparison of the numerical results with those obtained from the asymptotic results of Sips [9, 11]. These results were checked by Blanch and put in a convenient form for computation [19]; the analytical results provide us with an invaluable check of our numerical calculations.

It is worth mentioning here that if we use a given number of steps which result in eigenvalues of lower accuracy than those obtained from the asymptotic formula, the accuracy of the eigenfunctions is *not* improved if we use instead the more accurate asymptotic eigenvalues; to the contrary, the accuracy of the eigenfunctions decreases considerably. This is due to the fact that the more accurate asymptotic eigenvalues are not those that give the solution to the homogeneous system for the given number of steps. In other words, the homogeneous system has to be solved in a self-consistent way.

3. *Error Analysis*

The accuracy of the calculations presented is now discussed. One possible way to give error bounds for a given calculation would be to approximate $2q \cos 2x$ in (1) by two different step functions with the same number of steps, one that would give an upper bound to the eigenvalues and the other a lower bound. We have not

TABLE XIV

Comparison of Asymptotic With Numerical Results

	$ce_0(0, q)$		$ce_0(\pi/2, q)$		$ce_2(0, q)$		$ce_2(\pi/2, q)$	
q	Asymptotic value[a]	This work	Asymptotic value[a]	This Work	Asymptotic value[a]	This Work	Asymptotic value[a]	This Work
1,600	1.437827 − 34	1.437829 − 34	2.812112	2.812111	6.456216 − 32	6.456225 − 32	−1.978924	−1.978909
2,500	3.133347 − 43	3.133350 − 43	2.974152	2.974151	1.761443 − 40	1.761445 − 40	−2.095008	−2.094999
10,000	1.385949 − 86	1.385951 − 86	3.538554	3.538554	1.563129 − 83	1.563132 − 83	−2.497399	−2.497398

[a] From Eqs. (50) and (51) of Ref. [9], and Eqs. (3.14) and (3.15) of Ref. [19].

chosen to do so for the following reasons. Analytically, if we approximated $2q \cos 2x$ by a step function with an arbitrarily large number of steps, we could also get arbitrary accuracy in the solutions, provided that the computations could be performed without round-off errors. Of course, this is impossible.

The solutions of Sturm–Liouville systems such as (1) and (3) are defined except for an arbitrary factor. Thus, the arbitrary value we assign $ce_r(0, q)$ in order to start the calculation is by definition exact or round-off free. As we proceed in the computation marching from $x = 0$ to $x = \pi/2$, the round-off effects will increase and propagate. However, the solutions of (1) and (3) are symmetric or antisymmetric about $x = \pi/2$. Therefore, *if the computation can be performed until* $x = \pi/2$ with round-off errors of higher order that the number of significant figures desired, then the results are not affected by round-off. There is a very simple way to obtain an upper bound for the round-off error at $x = \pi/2$. Figure 1 illustrates the point for $ce_0(x, q)$. If we carry the computation from $x = 0$ to a point to the right of $x = \pi/2$, then the difference

$$\epsilon = \| ce_0(\pi/2 + \Delta, q)| - | ce_0(\pi/2 - \Delta, q)\| \tag{17}$$

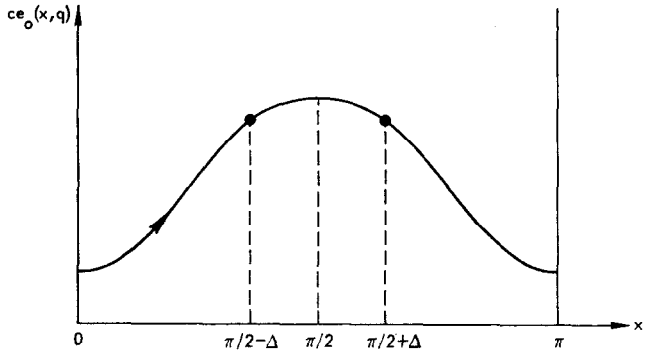

FIG. 1. Illustration showing that the difference between the computed values $ce_0(\pi/2 + \Delta, q)$ and $ce_0(\pi/2 - \Delta, q)$ is an upper bound to the round-off error at $x = \pi/2$.

is an upper bound to the round-off error at $x = \pi/2$. This is because for the exact solutions we know that

$$\epsilon = 0, \tag{18}$$

and as we started with the exact value $ce_0(0, q)$, the computed ϵ must be an upper bound to the round-off error at $\pi/2$. This seems reasonable because $V_s(x)$ in (10) is symmetric and the truncation error must also be symmetric, thus, the asymmetry in the numerical solutions revealed by the value of ϵ can only be due to the essen-

tially nonsymmetric round-off error. Strictly, the fact that ϵ is of higher order than the value obtained for $ce_r(\pi/2, q)$ proves only that there is no loss of significance in the computation of $ce_r(\pi/2, q)$, although this argument does not apply to the computation of $ce_r(x, q)$ in $0 < x < \pi/2$. However, we feel that, as we start with a round-off free value for $ce_r(0, q)$, if $ce_r(\pi/2, q)$ is not affected by round-off then this will also be true in the whole range $0 < x \leqslant \pi/2$. The results shown in Table XIV make us confident that this conclusion is justified.

For each eigenfunction of (1), we print ϵ and thus we have an a posteriori check of whether in any calculation we have lost significance or not. The number of steps with which $2q \cos 2x$ in (1) approximated can now be increased until convergence to any desired number of figures is obtained, provided that the significance as checked by the value of ϵ is not lost.

The results given in the tables for $q = 1{,}600$ were obtained with 8,000 steps. The maximum difference relative to the results obtained with 7,000 steps was of three units in the seventh significant figure for any of the five functions computed. The value of ϵ was five orders of magnitude smaller than the seventh significant figure kept in $ce_r(\pi/2, q)$. The zeros were identical to nine figures in the 7,000 and 8,000 step calculations.

For $q = 2{,}500$ and $q = 10\,000$, it was necessary to go up to 10 000 steps to obtain convergence to within three units in the seventh significant figure. Again, no difference was detected to nine figures in the zeros when using 9000 or 10 000 steps. Here ϵ was four orders of magnitude smaller than the seventh significant figure kept in $ce_r(\pi/2, q)$. Apart from having obtained convergence with the number of steps used, we feel confident that the values given for the Mathieu functions in Tables VI, IX and XII are accurate to within three units in the seventh significant figure; this is because the agreement with the asymptotic results shown in Table XIV is best for $q = 10\,000$, when the asymptotic formulas are known to have their greatest accuracy. The values for the zeros given in Tables VII, X and XIII are believed accurate to nine significant figures.

Finally, it must be noted that for very large q, the problem of normalization of the eigenfunctions could not have been solved if we did not have the zeros or if it were not possible to compute the functions continuously in x. In a numerical procedure, normalization requires the evaluation of the integral

$$\int_0^{\pi/2} [ce_r(x, q)]^2 \, dx. \tag{19}$$

As the zeros of the higher eigenfunctions are so close together and as they lie precisely in the boundary-layer region where the eigenfunctions are not negligibly small, it is not possible to obtain convergence in the numerical integration (19), except for $r = 0$ and 1, no matter how many integration steps are taken, if the

integration is done simply between $x = 0$ and $x = \pi/2$. For convergence, it is essential to divide the integration interval in subintervals bounded by the zeros of $ce_r(x, q)$. In this way, the integrand varies smoothly between the integration limits. The number of steps required to obtain convergence in the integrals (19) was found to be $(r + 1) \times 360$.

The calculations were performed with an IBM 360/91 computer. Typically, the computer time for a 10 000 step calculation that gives in one pass the results summarized in Tables XI, XII, and XIII was eight minutes.

V. Conclusion

We have discussed a numerical method for the computation of the Mathieu functions which gives the complete solution to the problem with any desired accuracy in the range of any conceivable practical application $0 < q \leqslant 10^4$, $0 \leqslant x \leqslant \pi/2$. Its use is very simple, because no initial guesses for the eigenvalues are required. Although higher order methods for Sturm–Liouville systems exist, it is doubtful that they can be used for the asymptotic problems discussed here, because of the enormous numerical scaling problems. In the present semianalytic method, these scaling problems are solved analytically.

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Note added in proof. It has now come to our attention that Dr. Ixaru (Institute of Atomic Physics, Bucharest) has independently discovered the same method as ours for solving Schrödinger equation. In an unpublished paper, he has proved in an elegant and simple way that the method is a second order method. He further proved that the approximation of the potential by a series of chords as was done by Gordon results also in a second order method. This seems to indicate that there is not much to be gained by using the chord approximation instead of the present method.

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