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Matrix Solution of Periodic Mathieu Equations

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The application of matrix methods to periodic Mathieu equations is discussed, and it is shown that accurate solutions may be found for any real value of the parameter, including the asymptotic case.

I. INTRODUCTION

The Mathieu differential equation, which may be written

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

with boundary conditions,

$$y(0) = y(\pi) = 0, \tag{2a}$$

and

$$y'(0) = y'(\pi) = 0, \tag{2b}$$

is of importance in several fields of physics, especially in quantum mechanics where it is the prototype of the wave equation for any system with a periodic potential. However it has long been recognized that the numerical solution of Eq. (1) can become difficult for large values of q because the zeros of the eigenfunctions condense about $\pm\pi/2$ as $q \to \infty$. Previous attempts to find numerical solutions for large values of q (greater than about 200) have recently been reviewed by Canosa [1], who has suggested a new method that is capable of finding both accurate eigenvalues and eigenfunctions over the domain $0 - \pi$ for q up to 10^4.

In this paper we wish to point out that it is possible using conventional matrix methods to rapidly solve the Mathieu equation for $q = 0$ to $q = 10^4$ with accuracy which is sufficient for most problems of physical interest. Second, we will develop a practical matrix method for which no upper limit on q exists. These results are to be contrasted particularly with the method of Canosa and Oliveira [2] and with similar methods described in Ref. [1].

II. General Matrix Method

Matrix solutions of Sturm–Liouville problems have been discussed by several authors, such as in a recent review of Schwartz [3]. Briefly the method involves finding the matrix elements of the differential operator L of the form

$$\langle n \mid L \mid m \rangle = \int z_n L z_m \, dx,$$

where **z** is any complete orthonormal set of functions and the integration is carried out over the entire domain x of the operator. Then if a unitary transformation matrix T is found such that the matrix $T^{\dagger}LT$ is diagonal, these diagonal elements will be the eigenvalues of L and the columns of T will be the coefficients of an expansion of the eigenfunctions in terms of the set **z**.

The choice of basis functions is governed by three requirements. The first is that the set be complete. In those cases where it is necessary to truncate an infinite set, the convergence of the matrix solution is assured by the Ritz variational condition so long as all of the first n functions are included. The Ritz condition states that with increasing number of basis functions the calculated eigenvalues must monotonically approach the true eigenvalues from above. The eigenfunctions will then be a least-squares fit to the true eigenfunctions although they need not converge at a given point. The second requirement is that methods be available for the evaluation of the matrix elements. The practical considerations of computer time, storage, and round-off error establish the third requirement that the basis set be as close to the eigenfunctions as possible.

III. Application to the Mathieu Equation

The exact solutions of the Mathieu equation in the limits of very large and small q are well known. These form convenient basis sets for intermediate values of q. For $q = 0$ the eigenfunctions y_n are the circular functions $(2\pi)^{-1/2}\exp(inx)$ and $\lambda_n = n^2$ for all positive and negative integers n including zero. In the limit $q \to \infty$ the y_n occur in degenerate pairs given by

$$y_n(x) = 2^{-1/2}[f_n(x - \pi/2) \pm f_n(x + \pi/2)], \tag{3}$$

for all positive integers n including zero. Here $f_n(x)$ are the linear oscillator functions

$$f_n(x) = [(\gamma/\pi)^{1/2}(1/2^n n!)]^{1/2} H_n(\gamma^{1/2}x)\exp(-\gamma x^2/2),$$

where H_n is the nth Hermite polynomial and $\gamma = 2q^{1/2}$. The $+$ and $-$ in Eq. (3)

correspond to solutions satisfying boundary conditions (2b) and (2a), respectively, and $\lambda_n = -2q + (2n + 1)\gamma$. For intermediate values of q it may be shown that y_n must be small and monotonically decreasing for all x not within some value θ_n of $\pm\pi/2$, where θ_n is approximately $[(2n + 1)/\gamma]^{1/2}$. This is the reason for the difficulty encountered by previous methods in finding accurate eigenfunctions for large values of q.

The matrix elements of the Mathieu equation in the circular function basis are simply

$$\langle n \mid L \mid m \rangle = n^2\delta_{nm} - q\delta_{n,m\pm 2}\,, \tag{4}$$

where δ is the Kronecker delta function. This matrix may be factored by symmetry into four tridiagonal blocks and each block diagonalized separately. The matrix elements in the linear oscillator basis may be found by the method of Harris et al. [4] using the relations

$$\langle n \mid x^2 \mid m \rangle = (n + \tfrac{1}{2})\,\delta_{n,m}/\gamma + (2\gamma)^{-1} \times \{[(n + 1)(n + 2)]^{1/2}\,\delta_{n,m-2} + [n(n - 1)]^{1/2}\,\delta_{n,m+2}\}, \tag{5a}$$

and

$$\langle n \mid d^2/dx^2 \mid m \rangle = -(n + \tfrac{1}{2})\,\gamma\delta_{n,m} + (\gamma/2) \times \{[(n + 1)(n + 2)]^{1/2}\,\delta_{n,m-2} + [n(n - 1)]^{1/2}\,\delta_{n,m+2}\}. \tag{5b}$$

Both of these matrices may be factored by symmetry into two tridiagonal blocks.

Goldstein [5] has shown that for large but finite q the differences between the two eigenfunctions given in the limit of infinite q by Eq. (3), and also between the corresponding eigenvalues, decrease as $q^{(2n+3)/4}\exp(-2\gamma)$. This difference is too small to be calculated by matrix methods for any q greater than about 200, so for these problems the basis functions $f_n(x \pm \pi/2)$ may be used with no loss of accuracy.

The eigenvalues of the tridiagonal matrices may be found extremely efficiently by the variation of the method of Sturm sequences proposed by Ortega [6] and the eigenvectors if desired may be found by the method described by Wilkinson [7]. The final diagonalization in the linear oscillator basis was found to be performed most efficiently by the Givens method [8].

The rate of convergence of the eigenvalues found using both sets of basis functions is shown in Table I, which gives the minimum total number of basis functions needed for convergence of the first five even and odd eigenvalues to ten significant figures as a function of q. Additional eigenvalues to the same accuracy would require a correspondingly larger basis set. The first several eigenfunctions near $\pm\pi/2$ were found to converge at approximately the same rate. In Tables II and III are given explicitly the eigenvalues and eigenfunctions for $q = 10^4$ and compared to the corresponding results given in [2]. All computations were per-

TABLE I

Minimum Number of Circular and Linear Oscillator Basic Functions Required for Convergence of First 10 Eigenvalues of Mathieu's Equation to 10 Places as a Function of q

q	No. basis functions: Circular	No. basis functions: Linear oscillator
1	21	>100
10^2	57	24
10^4	165	12
10^6	>300	10

TABLE II

First 5 Even and Odd Eigenvalues of Mathieu's Equation, $q = 10^4$

n	Present work	Canosa[a]
1	−19800.25031	−19800.2501
2	−19401.25283	−19401.2525
3	−19003.26104	−19003.2607
4	−18606.27878	−18606.2785
5	−18210.30995	−18210.3096

[a] Reference [2].

TABLE III

First and Fifth Mathieu Functions, $q = 10^4$
The Notation is $1.5 - 5 = 1.5 \times 10^{-5}$

x in deg	$n = 1$: Present work	$n = 1$: Canosa[a]	$n = 5$: Present work	$n = 5$: Canosa[a]
90	2.8233577	2.823358	+1.7223490	1.722358
80	0.13578192	0.1357819	+2.1458405	2.145843
60	6.645919-12	6.744600-12	+1.5462453-8	1.690215-8
40	5.3355774-32	2.927357-31	+4.4429854-28	6.987092-27
20	1.3829003-62	2.432940-57	+1.5243986-58	2.988643-52
0	6.0-104	1.1058289-86	7.0-100	5.6992583-81

[a] Reference [2].

formed on the UCSB IBM 360/75 computer with double precision words (64 bits). The computation of the first five solutions to the accuracy shown in Tables II and III required 0.9 sec of computer time. This may be compared to Canosa's results, which required 8 min to execute on an IBM 360/91. However, as will be discussed in the next section, the matrix method does not yield accurate eigenfunctions in the region where they are negligibly small. None of the computations shown in Table I showed round-off error beyond the final digit.

V. Discussion

Tables I–III show that matrix solutions of Eq. (1) with both large and small q are at least as accurate as the results given in [2] except for the eigenfunctions between 60 and 0 degrees. As noted in [2] approximate formulas are known for the eigenfunctions in this region that improve in accuracy with increasing q. Moreover the solutions of most physical problems do not depend critically on the value of the eigenfunctions where they are negligibly small. In quantum mechanical applications, for example, it is clear that the matrix elements of even an operator that depends more strongly on the eigenfunctions near zero than near $\pi/2$ may still be well approximated by using a matrix solution.

The properties of matrix solutions discussed above can be directly generalized to the solution of any eigenproblem of the form

$$d^2y/dx^2 + [\lambda - V(x)]\, y = 0, \tag{6}$$

where $V(x)$ is a periodic function of x. In the circular function basis this requires expanding $V(x)$ in a Fourier series and using the matrix elements

$$\langle n \mid d^2/dx^2 \mid m \rangle = n^2 \delta_{n,m}\,, \tag{7a}$$

$$\langle n \mid \cos kx \mid m \rangle = \tfrac{1}{2}\delta_{n,m\pm k}\,, \tag{7b}$$

$$\langle n \mid \sin kx \mid m \rangle = (\pm i/2)\, \delta_{n,m\pm k}\,. \tag{7c}$$

The method of Harris et al. [4] may be used to find the matrix elements in the linear oscillator basis either from an analytic expression for $V(x)$ or by interpolation from discrete points such as from a table or graph. We conclude that matrix methods are suitable for the solution of eigenproblems of the form of Eq. (6) including problems that are asymptotic in the sense used in [1].

The matrix method described in this paper is similar in concept to one recently discussed by Canosa [9]. In this method $V(x)$ is expanded in a power series in x, the matrix elements of the series are evaluated in a linear oscillator basis and the eigenvalues and eigenvectors are obtained by the approximate diagonalization of

the matrix representation of Eq. (6) by second order perturbation theory. It should be noted, however, that although our method is subject to some of the limitations discussed in [9], the evaluation of $V(x)$ by the technique given in [4] is far more accurate than using a truncated power series approximation. In addition, the exact diagonalization of the resulting matrix is equivalent to employing infinite rather than second order perturbation theory. As a consequence, the matrix method is applicable over a wider range of values of q or for a wider variety of functional forms for $V(x)$. In fact, the method gives good results even in those cases where $V(x)$ is not a continuous function of x and hence not expressable as a power series in x [4].

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