A NEW COMPUTER METHOD OF CALCULATION OF EIGENVALUES AND EIGENFUNCTIONS FOR THE SCHRODINGER'S EQUATION

George Morales
Army Missle Test and Evaluation Directorate (TE-PC)
White Sands Missle Range, New Mexico 88002

and

Robert G. McIntyre
The University of Texas at El Paso, El Paso, Texas 79968
and Instituto de Ciencias Biomedicas, Universidad
Autonoma de Ciudad Juarez, Juarez, Chihuahua, Mexico

ABSTRACT

The potential function is approximated in the one dimensional Schrödinger equation by a step function with an arbitrary, finite number of steps. In each step the resulting differential equation has constant coefficients and is integrated exactly in terms of the trigonometric or hyperbolic functions. The solutions are then matched at the interface of each layer. The eigenfunction is then constructed over the entire domain. This numerical method has certain unique features: (a) the potential function does not have to be known analytically, (b) for a given fixed number of steps in the potential approximation, all the eigenfunctions and eigenvalues have the same absolute accuracy, (c) any number of eigenvalues and eigenfunctions can be obtained in a single computer run without any need to guess initial eigenvalues, (d) for a given fixed number of steps in the potential approximation we could obtain the whole infinite spectrum of eigenvalues and eigenfunctions, (e) very low computation time on the computer.

INTRODUCTION

This work represents the implementation and testing of a numerical algorithm which solves the Schrödinger equation for a step potential function with an arbitrary but finite number of steps.

In each step the resulting differential equation has constant coefficients and is integrated exactly in terms of trigonometric or hyperbolic functions. The solutions are then matched at the interface of each layer, and the eigenfunction is then constructed over the entire domain.

The only input into the computer program is a numerical table of the potential. No initial estimates of the eigenvalues are necessary. The computer program in a single pass will output any desired number of eigenvalues and the corresponding eigenfunctions and their nodes. Computation time is roughly equal for the eigenvalues as for the eigenfunctions.

In this numerical method the potential is approximated by a step function, but once the approximate Schrödinger equation is set up, it is solved exactly. What this implies is that all eigenvalues and eigenfunctions are all of the same accuracy. The reason for this is that all the eigenfunctions are exact solutions to a given Schrödinger equation (i.e., they are written down explicitly in terms of trigonometric and hyperbolic functions). The numerical results obtained substantiate this expectation. In more conventional methods such as Rayleigh-Ritz [1], the higher eigenvalues and eigenfunctions are not as accurate as the fundamental eigenvalue and eigenfunction, making it necessary to progressively increase the number of mesh points in order to compute higher eigenvalues and eigenfunctions.

STATEMENT OF THE PROBLEM

We restrict the problem to the one dimensional Schrödinger equation written in dimensionless form as

$$\frac{d^2}{dx^2} y - V(x)y + Ey = 0 , \tag{1}$$

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

where V(x) is the potential function and E is the energy eigenvalue. For central field problems and for bound states

(a) V(x) is infinite at the origin x = 0,
(b) V(x) has a negative minimum value for some x = a,
(c) V(x) approaches zero asymptotically as $x \to \infty$.

The boundary conditions (2) are rigorous for a potential well problem with infinitely high walls; for a central field problem it is necessary to approximate the right boundary condition such that the eigenfunctions remain finite for x by taking suitably large L in (2) [2]. This is a good approximation since for large enough L, the eigenfunctions approach infinitely small values.

ANALYTICAL ASPECTS

We begin by approximating an analytical potential V(x) such as the above, if available, by a step function in a well defined way which need not be specified now, in the following way:

$$V(x) \doteq \begin{cases} V_1 & 0 < x < x_1 \\ \cdot & \\ \cdot & \\ \cdot & \\ V_n & x_{n-1} < x < x_n = L \end{cases} . \tag{3}$$

Our approximate problem (3) can approach the exact problem as closely as we desire, solely by picking the desired step widths h [3]. The analytical form of the potential need not be known in order to apply the approximation (3). Once a given number of steps is chosen, the approximate problem is solved exactly in terms of elementary trigonometric and hyperbolic functions.

In each layer i, the approximate problem becomes

$$\frac{d^2}{dx} y + (E - V_i)y = 0 , \quad i = 1,2,\ldots,n . \tag{4}$$

We shall define

$$a_i \equiv E - V_i , \quad b_i^2 \equiv |a_i| \tag{5}$$

so that the solution to (4) is

$$y = A_i F(b_i x) + B_i G(b_i x) , \quad i = 2,3,\ldots,n-1 , \tag{6}$$

where F and G are given in Table I, and A_i and B_i are integration constants.

Table I

Solutions of Equation (4)

	$a_i < 0$ (Forbidden Region)	$a_i = 0$	$a_i > 0$ (Allowed Region)
$F(b_i x)$	$\cosh(b_i x)$	1	$\cos(b_i x)$
$G(b_i x)$	$b_i^{-1} \sinh(b_i x)$	x	$b_i^{-1} \sin(b_i x)$

These solutions exhibit the well-known fact that the Schrödinger equation solutions are oscillatory within the region defined by the two classical turning points $a_i = E - V_i = 0$ and exponential elsewhere. It is interesting to note here that other approximations, namely the W.K.B.J. approximation, fail in the neighborhood of turning points and require special consideration [4].

Now applying boundary conditions (2) to the solutions, for regions 1 and n, we obtain

$$y = B_1 G(b_1 x) \ , \quad y = B_n G[b_n(x - L)] \tag{7}$$

since in neither region 1 or n is the function F equal to zero, which in turn implies that $A_1 = A_n = 0$. The function G is defined in Table I, and B_1 and B_n are integration constants.

We are now left with the straightforward task of determining the integration constants A_i and B_i. This is done by matching the solutions (6) and its derivatives at the interfaces, namely

$$y_i = y_{i+1} \ , \quad y_i' = y_{i+1}' \ . \tag{8}$$

The general equations for matching the solutions and its derivatives at the ith interface are

$$\begin{aligned} &A_i F(b_i x_i) + B_i G(b_i x_i) = A_{i+1} F(B_{i+1} x_i) + B_{i+1} G(b_{i+1} x_i) \ , \\ &A_i F'(b_i x_i) + B_i G'(b_i x_i) = A_{i+1} F'(b_{i+1} x_i) + B_{i+1} G'(b_{i+1} x_i) \ . \end{aligned} \tag{9}$$

The matching process is performed at all interfaces giving a homogeneous system involving 2n - 2 equations and 2n - 2 unknowns (A_i, i = 2,3,...,n - 1; B_i, i = 1,2,3,..., n). In order to solve for non-trivial solution of the unknowns we must require that the determinant of the coefficients be identically zero. That is,

$$|A| = \begin{vmatrix} G(b_1x_1) - F(b_2x_1) - G(b_2x_1) & & \\ G'(b_1x_1) - F'(b_2x_1) - G'(b_2x_1) & & \\ F(b_2x_2)\ G(b_2x_2) - F(b_3x_2) - G(b_3x_2) & & \\ F'(b_2x_2)\ G'(b_2x_2) - F'(b_3x_2) - G'(b_3x_2) & & \\ \ddots & & \\ F(b_{n-1}x_{n-1})\ G(b_{n-1}x_{n-1}) - G[b_n(x_{n-1} - L)] & & \\ F'(b_{n-1}x_{n-1})\ G'(b_{n-1}x_{n-1}) - G'[b_n(x_{n-1} - L)] & & \end{vmatrix} = 0 \tag{10}$$

where the primes indicate differentiation.

The zeros of this determinant equation are the eigenvalues of the approximate problem, (1), (2) and (3). For each eigenvalue, there is a non-trivial solution for A_i and B_i which in turn defines its corresponding eigenfunction. From this point on, $|A|$ will be looked upon as a function of a real variable E, namely $f(E) = |A|$.

At this point we shall point out differences between this method and those obtained by the variational methods, in particular the Rayleigh-Ritz method [1]. In the latter variational method one obtains a homogeneous system in which E is a dependent variable, that is, an algebraic system. If the algebraic system is of order n, one can only obtain n eigenvalues and eigenfunctions. Moreover, there is no definite guarantee that the values of E obtained in this method will be the exact values, as there is no rigorous establishment of convergence in the Rayleigh-Ritz method. On the other hand, the homogeneous system that we derived is a transcendental system. The merits of this system are obvious. The determinant Eq. (10) is a transcendental equation and will always have an infinite number of real roots (zeros). As will be seen later, one can easily define an iterative process whereby we can span a definite energy range, thereby driving the determinant equation to zero at the real eigenvalues encountered in that range. As with any trancendental system, the accuracy desired is only limited by a practical consideration, namely, computational time. The fact that all the roots are real is guaranteed by the fact that (1), (2) and approximation (3) form a Sturm-Liouville system [5].

THE NUMERICAL METHOD

In this section we shall deal primarily with the algebraic manipulations necessary to implement a numerical solution of Eq. (10). We will first cover the matrix algebra analysis and then discuss the computation of the eigenfunctions.

The Eigenvalue Equation

Equation (10), from now on, will be referred to as the eigenvalue equation. We have already stated that the determinant equation will have an infinite number of real roots that are the bound state eigenvalues for the approximate problem (1), (2) and (3). At this point we will shift the elements in the last column to the second column and group the elements in 2 x 2 sub-matrices as follows

$$|A| = \begin{vmatrix} A_{11} & -A_{12} & 0 & & 0 \\ 0 & A_{22} & -A_{23} & & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & A_{n-2,n-2} & -A_{n-2,n-1} \\ A_{n-1,1} & 0 & 0 & 0 & A_{n-1,n-1} \end{vmatrix} = 0 \ . \tag{11}$$

where

$$\begin{aligned} A_{11} &= \begin{pmatrix} G(b_1x_1) & 0 \\ G'(b_1x_1) & 0 \end{pmatrix} \\ A_{n-1,1} &= \begin{pmatrix} 0 & -G[b_n(x_{n-1} - L)] \\ 0 & -G'[b_n(x_{n-1} - L)] \end{pmatrix} \\ A_{ij} &= \begin{pmatrix} F(b_jx_i) & G(b_jx_i) \\ F'(b_jx_i) & G'(b_jx_i) \end{pmatrix} \ . \end{aligned} \tag{11a}$$

The sub-matrices in the first and last row of first column of determinant correspond to the first and last regions specified by b_1 and b_n and the first and last interfaces specified by x_1 and $x_{n-1} - L$. All other sub-matrices of determinant are of the same form and refer to a single region specified by b_i, i = 2,3,...,n - 1 and a single interface specified by x_i, i = 1,2,...,n - 1.

Post multiplying the last column by $-A_{n-1,n-1}^{-1}A_{n-1,1}$ and adding the result to the first column we obtain a determinant with the last row containing all zeros except the last element. Expanding about the last row we have this element times a new determinant similar in form to (11) but smaller. This procedure is repeated, each time expanding about the last row until (11) finally reduces to

$$|A| = |A_{n-1,n-1}|X|A_{n-2,n-2}|X|A_{n-3,n-3}|X \cdots X|A_{22}|$$
$$\times \ |A_{11} + A_{12}A_{22}^{-1} \cdots A_{n-1,n-1}^{-1}A_{n-1,1}| = 0 \ . \tag{12}$$

From Eq. (11a) and Table I it is evident that $|A_{ii}| = 1$, i = 2,3,...,n - 1.

Therefore, Eq. (12) reduces to

$$|A| = |A_{11} + A_{12}A_{22}^{-1} \cdots A_{n-1,n-1}^{-1}A_{n-1,1}| = 0 \ . \qquad (13)$$

We have, thus, reduced the evaluation of the determinant of a (2n - 2) x (2n - 2) matrix to that of a 2 x 2 matrix.

Consider a bound state eigenvalue corresponding to an eigenfunction with two turning points. In the classically forbidden regions, the eigenfunction behaves exponentially, that is $a_i \equiv E - V_i < 0$.

By Table I, the eigenfunctions in these forbidden regions are expressed in terms of hyperbolic functions, reflecting their exponential behaviour. At this point it is necessary to point out that we would run into formidable numerical problems if we were to evaluate Eq. (13) directly because in the classically forbidden region the eigenfunction might be several orders of magnitude smaller than in the allowed region. In numerical methods these problems are known as scaling problems [6] or as asymptotic problems. The reasons can be understood by further examination of Eq. (13). Consider the nonsingular matrix in (13) furthest to the right of the turning point.

$$A_{n-2,n-1} = \begin{pmatrix} \cosh b_{n-1}x_{n-2} & \sinh(b_{n-1}x_{n-2})/b_{n-1} \\ b_{n-1}\sinh b_{n-1}x_{n-2} & \cosh b_{n-1}x_{n-2} \end{pmatrix} . \qquad (14)$$

In quantum mechanics problems, the arguments of the hyperbolic functions in (14) can grow quite big, say in the neighborhood of 100. We would be in trouble because $\sinh 100 = \cosh 100 = e^{100}/2$.

When numerically multiplying the 2 x 2 matrices in (13), while evaluating the determinant $A \equiv f(E)$, differences such as sinh 100 - cosh 100 must be evaluated numerically and the computer returns them as zero. That is, the direct evaluation of $A \equiv f(E)$ gives the result $A \equiv f(E) \equiv 0$, for E in the range of interest. We can remedy this problem by grouping the matrices in (41) except the two singular A_{11} and $A_{n-1,1}$ whose arguments are b_1x_1 and $b_n(x_{n-1} - L)$, respectively.

For the classically forbidden region outside the turning points we find from Eq. (11a) and Table I

$$A_{i-1,i}A_{ii}^{-1} = \begin{pmatrix} \cosh(b_i(x_i - x_{i-1})) & -b_i^{-1}\sinh(b_i(x_i - x_{i-1})) \\ -b_i\sinh(b_i(x_i - x_{i-1})) & \cosh(b_i(x_i - x_{i-1})) \end{pmatrix} . \qquad (15)$$

And for the allowed region inside the turning points

$$A_{i-1,i}A_{ii}^{-1} = \begin{pmatrix} \cos(b_i(x_i - x_{i-1})) & -b_i^{-1}\sin(b_i(x_i - x_{i-1})) \\ b_i\sin(b_i(x_i - x_{i-1})) & \cos(b_i(x_i - x_{i-1})) \end{pmatrix} . \qquad (15a)$$

This simple manipulation has, thus, eliminated in one stroke all the scaling difficulties connected with the eigenvalue equation, because the arguments of the hyperbolic functions have been reduced by at least two orders of magnitude.

This section is concluded with a description of the numerical method used to find the roots of the determinant Eq. (13), whose matrices have been grouped as shown in (15) and (15a). These roots are approximations to the eigenvalues for the bound states. It will be useful to think of A in (13) as a function of real variable, $f(E) = |A|$, whose zeros will be determined numerically. The eigenvalue search is facilitated by the fact that all eigenvalues are bounded from below by the minimum of the potential [7] $E_n \geq V_{min}$.

In (asymptotic) quantum mechanics problems with deep potential wells, the fundamental energy eigenvalue, E_o, approaches asymptotically the potential minimum [8] $E_o \to V_{min}$.

A computer subroutine EIGEN was written that computes the function f(E) in a predetermined number of integral points in a range

$$V_{min} \leq E \leq V_{right} \ , \qquad (16)$$

where V_{right} is chosen arbitrarily and is to be sufficiently to the right of V_{min} depending on how many eigenvalues are desired. Integral values for V_{min} and V_{right} are chosen. EIGEN computes f(E) for all integral values of E in the range (16). Whenever a change in sign of the function f(E) at two successive (integral) values of E, it will store those two values, and proceeds until it encounters another sign change, whereupon, it will store the two successive (integral) values of E at which the sign change occurs, and so on. This process is continued until the entire range (16) of E is scanned.

Having stored all integral intervals of E for which a sign change for f(E) occurred, the subroutine EIGEN will then subdivide these intervals into ten increments of 0.1 and re-scan each of the intervals for a change in sign of the function f(E) at two successive points. Each one of these integral intervals will contain two successive points for which the function f(E) will change in sign. This latter set of pairs of successive points is stored by EIGEN. Again this last set of intervals is subdivided into ten parts of 0.01 and the process is repeated.

It should now be obvious that this process can be continued indefinitely until the desired accuracy of the eigenvalues is reached. For example, if four iterations are performed, the location of the eigenvalues is ascertained with three decimal accuracy (see the computer output for further examples). The search is terminated when the range (16) is scanned completely or when a predetermined number of eigenvalues has been found.

Computation of the Eigenfunctions

It has been found convenient to rewrite our system as

$$\begin{aligned} A_{11}\vec{c}_1 - A_{12}\vec{c}_2 &= 0 \\ A_{22}\vec{c}_2 - A_{23}\vec{c}_3 &= 0 \\ &\vdots \\ A_{n-2,n-2}\vec{c}_{n-2} - A_{n-2,n-1}\vec{c}_{n-1} &= 0 \\ A_{n-1,1}\vec{c}_1 + A_{n-1,n-1}\vec{c}_{n-1} &= 0 \end{aligned} \qquad (17)$$

where A_{ij} are the 2 x 2 matrices given by (11a) and $\vec{c}_i$ are the following 2 x 1 vectors:

$$\vec{c}_1 = \begin{pmatrix} B_1 \\ B_n \end{pmatrix}, \ \vec{c}_i = \begin{pmatrix} A_i \\ B_i \end{pmatrix}, \ i = 2,3,\ldots,n-1 \ . \qquad (18)$$

The components of the vectors $\vec{c}_1$ are the coefficients of the eigenfunctions in the boundary regions 1 and n. The first equation in (17) represents the first two equations in our system, which on performing the matrix multiplication, reduce to

$$\begin{pmatrix} B_1G(b_1x_1) & -A_2F(b_1x_1) - B_2G(b_2x_1) \\ B_1G(b_1x_1) & -A_2F(b_1x_1) - B_2G(b_2x_1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \qquad (19)$$

The components of the vectors $\vec{c}_i$, $i \neq 1$, are the coefficients of the eigenfunctions in the inner regions. Once the eigenvalues have been determined, the matrices A_{ij} are explicitly determined. A direct numerical solution of (17) would fail because we would encounter scaling problems of a

nature mentioned before in the computation of the eigenvalue equation.

It is obvious that we can now write system (17) in terms of the vector $\vec{c}_1$ as follows:

$$\begin{aligned}
\vec{c}_2 &= A_{12}^{-1}A_{11}\vec{c}_1 \ , \\
\vec{c}_3 &= A_{23}^{-1}A_{22}A_{12}^{-1}A_{11}\vec{c}_1 \ , \\
&\vdots \\
\vec{c}_m &= A_{m-1,m}^{-1}A_{m-1,m-1}\cdots A_{12}^{-1}A_{11}\vec{c}_1 \ .
\end{aligned} \tag{20}$$

The last equation in (20), for m = n - 1, determine $\vec{c}_{n-1}$ in terms of $\vec{c}_1$, and the last equation of (17) also express $\vec{c}_{n-1}$ in terms of $\vec{c}_1$.

This cannot be readily done because of, again, scaling (asymptotic) problems. That is, numerical errors would accumulate and propagate if (17) were solved from top to bottom; that is the same as starting with an arbitrary value of the eigenfunction at the left boundary and integrating all the way to the right boundary. To avoid this difficulty, the solution of (17) as given by (20) is stopped at m = n/2, i.e., the midpoint of the domain, which is always taken at the minimum (x = a) of the potential function. In symmetric potential problems this is all that is needed, since the eigenfunction is either symmetric or antisymmetric about this point (x = a). For central field problems with asymmetric potentials, after computing the eigenfunction from the left to the midpoint, (17) is solved via (20) from the bottom till the midpoint, i.e., the eigenfunction is now computed from the right inward to the midpoint, and then both pieces of the eigenfunction are matched at the center. The eigenfunctions so computed on either side of the point x = a are the same except that they differ by a constant factor, i.e., their derivatives match at the midpoint.

The matching of the eigenvalues is done by multiplying each piece by its reciprocal value at x = a, so that both pieces also have the same midpoint value, that is

$$y(x) = \frac{1}{y_L(a)}\, y_L(x) \ , \quad 0 < x \leq a \ , \tag{21}$$

$$y(x) = \frac{1}{y_R(a)}\, y_R(x) \ , \quad a \leq x < \infty \ . \tag{22}$$

Equation (20) will now be written

$$\begin{aligned}
\vec{c}_2 &= A_{12}^{-1}\vec{v}_2 \ , & \vec{v}_2 &= A_{11}\vec{c}_1 \ , \\
\vec{c}_3 &= A_{23}^{-1}\vec{v}_3 \ , & \vec{v}_3 &= A_{22}A_{12}^{-1}A_{11}\vec{c}_1 \ , \\
\vec{c}_4 &= A_{34}^{-1}\vec{v}_4 \ , & \vec{v}_4 &= A_{33}A_{23}^{-1}A_{22}A_{12}^{-1}A_{11}\vec{c}_1 \ , \\
&\vdots & &\vdots \\
\vec{c}_m &= A_{m-1,m}^{-1}\vec{v}_m \ , & \vec{v}_m &= A_{m-1,m-1}A_{m-2,m-1}^{-1}\cdots A_{11}\vec{c}_1 \ ,
\end{aligned} \tag{23}$$

where from Eq. (14) and Table I we find for the classically forbidden region

$$A_{ii}A_{i-1,1}^{-1} = \begin{pmatrix} \cosh[b_i(x_i - x_{i-1})] & b_i^{-1}\sinh[b_i(x_i - x_{i-1})] \\ b_i\sinh[b_i(x_i - x_{i-1})] & \cosh[b_i(x_i - x_{i-1})] \end{pmatrix}, \tag{24}$$

and for the allowed region

$$A_{ii}A_{i-1,1}^{-1} = \begin{pmatrix} \cos\, b_i(x_i - x_{i-1}) & b_i^{-1}\sin\, b_i(x_i - x_{i-1}) \\ -b_i\, \sin\, b_i(x_i - x_{i-1}) & \cos\, b_i(x_i - x_{i-1}) \end{pmatrix}. \tag{25}$$

Notice that the arguments of the hyperbolic functions in (24) are two orders of magnitude smaller than if the matrices were computed individually.

The vectors $\vec{v}_i$ in (23) are evaluated by grouping the matrices in pairs as shown in (24) and (25) except the last matrix A_{11} where the arguments of the hyperbolic functions are $b_i x_i$. As indicated before, the vectors $\vec{v}_i$ involve only one arbitrary integration constant B_1. But we are still in numerical trouble since the inverse matrices A_{ij}^{-1} at the left in (23) still involve large arguments and therefore these inverse matrices are numerically unstable. The computation of the coefficients $\vec{c}_i$ still present numerical difficulties.

We can circumvent this problem since we do not need to compute the vectors of the coefficients $\vec{c}_i$ per se. After the 2 x 1 vectors $\vec{v}_i$ in (23) have been computed they will be of the form

$$\vec{v}_i = \begin{pmatrix} v_{i1} \\ v_{i2} \end{pmatrix}, \ i = 2,\ldots,m \ . \tag{26}$$

From Eqs. (6), (18) and (23) we have the following expression for the eigenfunctions in vector form or notation:

$$\begin{aligned}
y(x) &= \vec{c}_i \cdot \vec{f}(x) \ , \\
y(x) &= A_{i-1,i}^{-1}\vec{v}_i \cdot \vec{f}(x) \ , \quad i = 2,3,\ldots,n-1
\end{aligned} \tag{27}$$

where f(x) is the vector function

$$\vec{f}(x) = \begin{pmatrix} F(b_i x) \\ G(b_i x) \end{pmatrix}. \tag{28}$$

Now using Eqs. (7), (26) and (28) we obtain the following expression for the inner product in (27)

$$\begin{aligned}
y(x) = {} & v_{i1}G'(b_i x_{i-1})F(b_i x) - v_{i2}G(b_i x_{i-1})F(b_i x) \\
& - v_{i1}F'(b_i x_{i-1})G(b_i x) + v_{i2}F(b_i x_{i-1})G(b_i x) \ , \\
& \qquad i = 2,3,\ldots,n-1 \ ,
\end{aligned} \tag{29}$$

which reduces, in the classically forbidden region, to

$$y(x) = v_{i1}\cosh\, b_i(x_{i-1} - x) - b_i^{-1}v_{i2}\sinh\, b_i(x_{i-1} - x) \ , \quad i = 2,3,\ldots,n-1, \tag{30}$$

and in the allowed region, to

$$y(x) = v_{i1}\cos\, b_i(x_{i-1} - x) - b_i^{-1}v_{i2}\, \sin\, b_i(x_{i-1} - x) \ , \quad i = 2,3,\ldots,n-1 \ . \tag{31}$$

In Eqs. (30) and (31) v_{i1} and v_{i2} are components of the vector $\vec{v}_i$ as defined in (23) and (26).

Using the elementary addition formulas has allowed us to analytically perform the inner product in (27), thus eliminating the need to evaluate hyperbolic functions with very large arguments. It can readily be seen that in the computation of the eigenfunctions in (30) and (31), it is

only necessary to evaluate the vectors $\vec{v}_i$ in (23) and not the coefficients $\vec{c}_i$. The computation of the vectors $\vec{v}_i$ does not present any numerical problems.

NUMERICAL RESULTS

In this section we will describe some of the results obtained with the computer subroutine EIGEN. First we dealt with a central field quantum mechanics problem, the radial Schrödinger Eq. (1) with Morse's potential [9],

$$V(x) = D(1 - \exp(-a(x - x_e)))^2 - D \ , \tag{32}$$

where

$$a = 0.711248 \ , \ x_e = 1.9975 \ , \ D = 188.4355 \ . \tag{33}$$

The boundary conditions (2) used are

$$y(0) = y(10) = 0 \ . \tag{34}$$

The second problem covered was that of Mathieu's equation [10], where

$$V(x) = 2q \cos 2x \ . \tag{35}$$

The boundary conditions (2) used are in this case

$$y(0) = y(\pi) = 0 \ . \tag{36}$$

Although Mathieu's equation is not a true quantum mechanics problem, Eqs. (1), (34) and (35) can be thought of as the bound states of a particle in a box of length π and infinitely high walls with the potential inside the box given by (35).

The primary reasons why these two problems were chosen are that Morse's potential has well-known analytic solutions [11], and provides a good check for the numerical solutions of the eigenvalues; and Mathieu's equation has also been well documented [12] and is a good check for the numerical results obtained for the nodes of the eigenfunctions.

Schrödinger's Equation with Morse's Potential

Morse's potential was approximated by a step function with an equal number of steps m = n/2 in the ranges

$$0 \leq x \leq 1.9975 \ , \quad 1.9975 \leq x \leq 10 \ . \tag{37}$$

The interface was chosen at the abscissa of the minimum value of the potential

$$V(1.9975) = V_{min} = -188.4355 \ . \tag{38}$$

This potential varies rapidly in the neighborhood of its minimum than towards the right boundary, where it is relatively flat. The n/2 potential steps in the right range of (37) were taken as follows:

n/4 steps in $1.9975 \leq x \leq 4$, n/4 steps in $4 \leq x \leq 10$.

The step function approximation is

$$V(x) = \begin{cases} V_1 = (V(0) + V(x_1))/2 \ , \ 0 < x < x_1 \ ; \\ V_2 = (V(x_1) + V(x_2))/2, \ x_1 < x < x_2; \\ \vdots \qquad\qquad\qquad \vdots \\ V_m = -188.4355 \ , \ x_{m-1} < x < x_m = 1.9975; \\ V_{m+1} = -188.4355, \ x_m < x < x_{m+1}; \\ V_{m+2} = (V(x_{m+1}) + V(x_{m+2}))/2 \ , \ x_{m+1} < x < x_{m+2}; \\ \vdots \qquad\qquad\qquad \vdots \\ V_n = (V(x_{n-1}) + V(x_n))/2 \ , \ x_{n-1} < x < x_n = 10; \\ m = n/2 \ . \end{cases} \tag{39}$$

The three step widths used are

$$0 < x < 1.9975 \ , \quad h_1 = 1.9975/(n/2) \ ,$$

$$1.9975 < x < 4 \ , \quad h_2 = (4 - 1.9975)/(n/4) \ ,$$

$$4 < x < 10 \ , \quad h_3 = (10 - 4)/(n/4) \ .$$

The eigenvalues were obtained by searching for the roots of the eigenvalue Eq. (10) in the range

$$-188.0 \leq E \leq -108.0 \ . \tag{40}$$

The numerical results for the first five eigenvalues, when the potential is approximated by n = 200 steps, together with the exact, analytical results are given in Table II. Table III contains the nodes of these first five eigenfunctions.

Table II

First Five Eigenvalues of Schrödinger's Equation With Morse's Potential

N	E_0	E_1	E_2	E_3	E_4
200	-178.777	-160.264	-142.763	-126.275	-110.796
Exact	-178.799	-160.283	-142.760	-126.288	-110.809

Table III

Nodes of Morse's Eigenfunctions

I	N_{11}	N_{12}	N_{13}	N_{14}	N_{15}
1	0.000	0.000	0.000	0.000	0.000
2	1.888	0.000	0.000	0.000	0.000
3	1.768	0.000	0.000	0.000	0.000
4	1.688	0.000	0.000	0.000	0.000

$\overline{N_{ij}}$ means the jth node of the ith eigenfunction.

Mathieu's Equation

The Mathieu's "potential" is approximated as follows:

$$V(x) = \begin{cases} V_1 = V(0) = 2q , & 0 < x < x_1 ; \\ V_2 = (V(x_1) + V(x_2))/2 , & x_1 < x < x_2 ; \\ \vdots \qquad\qquad\qquad\qquad \vdots & \\ V_m = -2q , & x_{m-1} < x < x_m = \pi/2 ; \\ V_{m+1} = -2q , & x_m < x < x_{m+1} ; \\ \vdots \qquad\qquad\qquad\qquad \vdots & \\ V_n = V(x_n) = 2q , & x_{n-1} < x < x_n = \pi ; \end{cases} \tag{41}$$

$$m = n/2 .$$

The potential has the minimum at the center

$$V_{min} = V(\pi/2) = -2q . \tag{42}$$

The eigenvalues were obtained by searching for the roots of the eigenvalue Eq. (10) in the range

$$-70.0 \leq E \leq 30.0 . \tag{43}$$

The numerical results for q = 40 are given in Tables IV and V, for n = 200, together with the exact, analytical results taken from Ince's paper [12].

Table IV

First Five Eigenvalues of Schrödinger's Equation With Mathieu's Potential

N	E_0	E_1	E_2	E_3	E_4
200	-67.595	-43.342	-20.000	1.736	22.337
Exact	-67.606	-43.352	-20.208	1.730	22.332

Table V

Nodes of Mathieu's Eigenfunctions

I	N_{11}	N_{12}	N_{13}	N_{14}	N_{15}
1	1.563	2.757	3.118	0.000	0.000
2	1.359	1.767	2.882	0.000	0.000
3	1.202	1.563	1.924	3.071	3.118
4	1.060	1.406	1.720	2.066	3.087

N_{ij} means the jth node of the ith eigenfunction.

REFERENCES

[1] P. M. Morse and H. Feshbach, "Method of Theoretical Physics," Vol. II, McGraw-Hill Book Company, Inc., New York, 1953, p. 1117.

[2] J. W. Cooley, Math. Comp., 15, 363 (1961).

[3] B. Wendroff, "Theoretical Numerical Analysis," Academic Press, New York, 1966, p. 23.

[4] Reference 1, p. 1092.

[5] Reference 1, Vol. I, p. 719.

[6] J. M. Blatt, J. Comp. Phys., 1, 382 (1967).

[7] R. Courant and J. Hilbert, "Methods of Mathematical Physics," Vol. I, Wiley (Interscience), New York, 1962, p. 445.

[8] J. Canosa and J. D. Cole, J. Math. Phys., 9, 1915 (1968).

[9] Reference 5, p. 304.

[10] N. W. McLahlan, "Theory and Application of Mathieu Functions," Dover Publications, Inc., New York, 1964.

[11] P. M. Morse, Phys. Rev., 34, 57 (1929).

[12] E. L. Ince, Proc. Roy. Soc. (Edinburgh) Sec. A, 52, 355 (1931-32). Also ibid., 52, 424 (1931-32).