A general transformation method to solve the Schroedinger equation.

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LA THÈSE A ÉTÉ MICROFILMÉE TELLE QUE NOUS L'AVONS REÇUE
A GENERAL TRANSFORMATION METHOD TO SOLVE
THE SCHROEDINGER EQUATION

by

Edward Neilson Brewer

A Thesis
submitted to the Faculty of Graduate Studies
through the Department of
Physics in partial fulfillment
of the requirements for the Degree
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ABSTRACT

Some numerical methods of solution of the radial Schroedinger equation approximate the potential as a simple polynomial in numerous small intervals. In each interval, the solution to the Schroedinger equation is simple to find analytically. These interval solutions are then linked together by the continuity condition on the wave function and its derivative to form the overall solution. The accuracy of this solution depends on small interval size.

In the method proposed in this work, the Schroedinger equation is transformed exactly to a directly solvable 'model' equation (often the Airy equation). Although a given transformation may not be valid for the whole range of $x$, it will be valid over a large interval. Only a few such intervals need be linked together to form the overall solution. Note that the solution is theoretically exact regardless of the size of the intervals.

Solution of the transformation equation gives the transformation function $z(x)$ which can be shown to be a monotonic function. A close relationship between the formulation of this method and the JWKB and uniform JWKB approximation methods comes from this result.

Since the solution of the model equation is known, effort is concentrated on the solution of the transformation equation. Three methods of solution of this equation are presented; the iteration method, the power series method, and the coupled differential equation method with the latter currently preferred.

Examples of results using this method of solution are given
for the harmonic oscillator potential, the Eckart potential, and the N-fold periodic ring potential. An explanation and a full listing of a FORTRAN computer program implementing this method follow.
Acknowledgements

I would like to thank Dr. R.K.B. Helbing for hooking me on this problem and for the enormous amount of patience, respect, and understanding he has given me in the course of work. I would also like to thank Mr. Tim Scholl for his frustrating work obtaining the Airy functions to high accuracy and Mr. Murray Darragh for his valiant attempt to do the same for the Parabolic cylinder functions.

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A General Transformation Method to Solve the Schroedinger Equation

Chapter 1

Introduction

A common method of solution of the radial Schroedinger equation involves approximating the potential in an interval by some polynomial. These polynomials are chosen so that the solution to their corresponding Schroedinger equation is analytically soluble. Solutions in each interval are then linked together using the continuity conditions to form the overall wave function. Any desired accuracy can be achieved by the choice of sufficiently small intervals.

The simplest choice of a polynomial is a constant. In this case, the potential is replaced by a series of constant steps, the height of which is the average of the potential over the interval. In each interval, the Schroedinger equation becomes

\[
\frac{\hbar^2}{2\mu} \frac{d^2 \psi_0(r)}{dr^2} + (E-V_0)\psi_0(r) = 0
\]  

(1.1.1)

where \(\psi_0(r)\) is the radial wave function, \(\mu\) is the reduced mass, and \(E\) is the energy. The quantity \(V_0\) is the potential \(V_{\text{effective}}(r)\) averaged over the interval. The solution is:

for \(E>V_0\),

\[
\psi_0(r) = \psi(r_1) \cos[k(r-r_1)] + \psi'(r_1) k^{-1} \sin[k(r-r_1)]
\]  

(1.1.2)

for \(E<V_0\),

\[
\psi_0(r) = \psi(r_1) \cosh[k(r-r_1)] + \psi'(r_1) k^{-1} \sinh[k(r-r_1)]
\]  

(1.1.3)

and for \(E=V_0\),

\[
\psi_0(r) = \psi(r_1) + (r-r_1) \psi'(r_1).
\]  

(1.1.4)
\[ k = (2\mu/\hbar^2)^{1/2} (E - V_0)^{1/2} \]  \hspace{1cm} (1.1.5)

and

\[ k = (2\mu/\hbar^2)^{1/2} (V_0 - E)^{1/2} \]  \hspace{1cm} (1.1.6)

The solution \( \Psi_0(r) \) has a value of \( \Psi(r_1) \) and a derivative value of \( \Psi'(r_1) \) at one endpoint of the interval. These quantities are obtained from the solution of the previous interval. Thus the overall solution of the wave function is obtained by solving the intervals sequentially, starting at some \( \Psi(r_B), \Psi'(r_B) \) determined by a boundary condition at \( r_B \).

Higher order polynomials can be used to better approximate the potential. Linear polynomials are a common choice \(^{(2),(3)}\). In this case, the functions involved in the interval solutions are the independent Airy functions \( Ai \) and \( Bi \). Once again, the overall wave function is found by solving the intervals outward from a boundary condition point.

The main advantage of these types of methods over other numerical methods \(^{(4),(5)}\) is that fewer points and hence intervals need be evaluated to obtain the same accuracy in the wave function. This is a result of the oscillatory functions used in each interval which better approximate the frequently oscillatory wave function.

It seems then that the way to further improve the numerical solution is by reducing the number of intervals. Intuitively this would imply a "better" fit is needed for the potential in each interval.

In the method presented in this work, the potential in each interval is, in effect, fitted exactly. This is done by the
transformation of the Schroedinger equation into another equation with known oscillatory solutions. In this way, fewer intervals are needed to obtain the overall wave function. This drastic improvement is partly offset by the extra calculations needed to solve the transformation.
Chapter 2

Theory of the Method

2.1 The Transformation Equations

Since the radial equation after the transformation \( y = \Psi(r)/r \) and the one dimensional Schrödinger equation have the same form

\[ y''(r) = \psi(r) y(r) \]

the latter is used for simplicity. Calling the independent variable \( x \), the one dimensional equation is

\[ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} y(x) - (E - V(x)) y(x) = 0 \]  

(2.1.1)

with \( E \) the energy and \( V(x) \) the potential. This can be written as

\[ y'' = W(x) y \]

(2.1.2)

where \( W(x) = \frac{2m}{\hbar^2} (V(x) - E) \). This function \( W(x) \) has the same form as the potential \( V(x) \) but has been 'energy adjusted' (the zeros of \( W \) are the classical turning points at energy \( E \) of \( V \)).

Because of this relationship, \( W(x) \) will be referred to as the 'potential' from now on.

For a general potential \( W(x) \), equation (2.1.2) is transformed into a 'model' equation with known solutions

\[ y(z)'' = g(z) y(z) \]

(2.1.3)

where \( z \) is a function of \( x \) and \( ' \) refers to differentiation by \( z \).

The function \( g(z) \) is chosen so that the solutions \( \varphi(z) \) are well known. For example, \( g(z) = z \) has Airy functions as solutions.

To transform (2.1.2) to (2.1.3), first change the variable \( x \) to the variable \( z \) using

\[ y' = \frac{dy}{dx} = \frac{dz}{dx} \frac{dy}{dz} = z' y' \]

(2.1.4)

\[ y'' = z'' y' + (z')^2 y'' \]

(2.1.5)

so (2.1.2) becomes

\[ (z')^2 y'' + z' y' - W(x) y = 0 \]

(2.1.6)
or
\[ y'' + (z''/(z')^2) y' - (W(x)/(z')^2) y = 0 \quad (2.1.7) \]
if \( z' \neq 0 \).

A general equation of the form \( y'''(z) + P(z)y''(z) + Q(z)y = 0 \) can be transformed (6) to the 'normal equation' form of (2.1.3) by using the substitution
\[ y(z) = \psi(z)u(z) \quad (2.1.8) \]
where
\[ u(z) = \exp \left[ -\frac{1}{z'} \int P(z) \, dz \right] \quad (2.1.9) \]
In this case \( P(z) = (z''/(z')^2) \) so
\[ u(z) = \exp \left[ -\frac{1}{z'} \int (z''/(z')^2) \, dz \right] \quad (2.1.10) \]
and since \( dz = z' \, dx \)
\[ u(z) = \exp \left[ -\frac{1}{z'} \ln z' \right] \quad (2.1.11) \]
so
\[ u(z) = (z')^{-\frac{1}{z'}} \quad (2.1.12) \]
Thus using
\[ y(z) = \psi(z)(z')^{-\frac{1}{z'}} \quad (2.1.13) \]
and noting that
\[ d(z')/dz = z''/z' \quad (2.1.14) \]
the other derivatives of \( y \) are obtained
\[ y' = \psi' - \frac{1}{z'} \psi z'' - \frac{5}{2} \quad (2.1.15) \]
\[ y'' = \psi'' z' - \frac{1}{z'} z'' \psi z' - \frac{5}{2} - \psi'' z' + \frac{3}{2} \psi z'' z' - \frac{7}{2} \]
\[ + (5/4) \psi z'^2 (z')^{-3/2} \quad (2.1.16) \]
Substituting into (2.1.7) gives
\[ 0 = v'' + (z')^{-2} \left[ -\Psi((z')^{-1} / z') - \left(3/2\right)(z''/z')^2 \right] - W(x) \] \quad (2.1.17)

The quantity \( \Psi \) in the curly brackets is known as the Schwarzian (7) and denoted \( (z,x) \).

A comparison of equation (2.1.3) with equation (2.1.17) yields the 'transformation' equation

\[ W(x) + \Psi(z,x) - g(z)(z')^2 = 0 \] \quad (2.1.18)

Using the function \( u(z) \) defined in (2.1.12) the Schwarzian becomes

\[ (z,x) = -2u''/u \] \quad (2.1.19)

so equation (2.1.18) can be expressed as

\[ W(x) - u''/u - g(z)u^{-4} = 0 \] \quad (2.1.20)

The transformation function \( z(x) \) is a solution of eqs. (2.1.12) and (2.1.20) simultaneously. The transformation will be valid as long as \( z'(x) \neq 0 \). Within this region, the two independent solutions of (2.1.2) from (2.1.8) become

\[ y_1(x) = u(x)\Psi_1(z) \]
\[ y_2(x) = u(x)\Psi_2(z) \] \quad (2.1.21)

if \( \Psi_1, \Psi_2 \) are the two independent solutions of (2.1.3). These solutions are selected so that, asymptotically, \( y_1 \) decreases while \( y_2 \) increases 'exponentially' in the classically forbidden region. Thus within the region the general solution can be expressed as

\[ y(x) = a_1y_1(x) + a_2y_2(x) \] \quad (2.1.22)

Changing the starting conditions yields solutions of \( y(x) \) valid over different ranges of \( x \). In this way, the entire \( x \)-axis can be covered by an overlapping set of solutions of \( y(x) \) each valid only in a finite region and having different solutions of
$z(x), u(x), u'(x)$, and $\nabla(z)$. To obtain the overall unique wave function, the conditions of continuity of the wave function and its derivative are applied to $y(x)$ and $y'(x)$ at a 'match' point located between each pair of overlapping regions. To aid in this process, some new terminology is introduced in the next section.

2.2 Connection Matrices

In each region, the solution $y(x)$ from (2.1.21) and (2.1.22) can be expressed as

$$y(x) = a_1 u(x) \nabla_1(z) + a_2 u(x) \nabla_2(z) \quad (2.2.22)$$

Now introduce a 'basis function' vector

$$b(x) = (u(x) \nabla_1(z), u(x) \nabla_2(z)) \quad (2.2.23)$$

and a 'coefficient' vector

$$a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad (2.2.24)$$

Then equation (2.2.22) can be written as a dot product

$$y(x) = b(x) \cdot a \quad (2.2.25)$$

Similarly, the derivative of $y(x)$ can be written

$$y'(x) = b'(x) \cdot a \quad (2.2.26)$$

Now a vector $y(x)$ can be constructed with the components $y(x)$ and $y'(x)$ to yield

$$\begin{bmatrix} y \\ y' \end{bmatrix} = \begin{bmatrix} y_1 & y_2 \\ y_1' & y_2' \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad (2.2.27)$$

or

$$y = B a \quad (2.2.28)$$

Note that the $x$ dependence is all in the matrix $B$. The coefficient vector $a$ is made up of constants.
A needed quantity will be $B^{-1} = (\det B)^{-1}$ (adjoint $B$).

The determinant of $B$ is

$$\det B = y_1y_2' - y_1'y_2 = \text{Wr}_x (y_1, y_2)$$

where $\text{Wr}_x (y_1, y_2)$ is the Wronskian of the basis functions $y_1, y_2$ with respect to their argument $x$. The inverse matrix $B^{-1}$ is now calculated as

$$B^{-1} = \frac{1}{\text{Wr}_x (y_1, y_2)} \begin{bmatrix} y'_1 & -y_2 \\ -y'_1 & y_2 \end{bmatrix}$$

(2.2.30)

It is clear from matrix algebra that

$$\det B^{-1} = (\text{Wr}_x (y_1, y_2))^{-1}$$

(2.2.31)

The relationship between the Wronskian of $y_1(x)$ and $y_2(x)$ with respect to $x$ and the Wronskian of $\psi_1(z)$ and $\psi_2(z)$ with respect to $z$ can be derived from (2.1.21)

$$\text{Wr}_x (y_1, y_2) = u(x)\psi_1 \frac{d}{dx} (u(x)\psi_2(z)) - \frac{d}{dx} (u(x)\psi_1(z)) u(x)\psi_2(z)$$

$$= u\psi_1 (u'\psi_2' + uz' \psi_2'') - (u'\psi_1' + uz' \psi_1'') u\psi_2$$

$$= z'u^2 (\psi_1' \psi_2'' - \psi_1'' \psi_2')$$

where $'$ refers to differentiation by $x$ and $''$ refers to differentiation by $z$. Thus

$$\text{Wr}_x (y_1, y_2) = z'u^2 \text{Wr}_z (\psi_1, \psi_2)$$

(2.2.32)

The continuity condition of the wave function and its derivative at some match point between regions $n$ and $n+1$ located at $x = \xi^{(n+1,n)}$ can now be expressed as

$$\psi_{n+1}^{(n+1,n)}(x) = \psi_n^{(n+1,n)}(x)$$

(2.2.33)

In terms of the coefficient vectors $a$

$$\tilde{a}_{n+1} = M_{n+1,n} \tilde{a}_n$$

(2.2.34)

where

$$M_{n+1,n} = B_{n+1}^{-1}(\xi^{(n+1,n)}) B_n(\xi^{(n+1,n)})$$

(2.2.35)
is the 'match matrix' evaluated at the match point \( x = \xi^{(n+1,n)} \). In explicit terms, the match matrix is

\[
M_{n+1,n} = \langle 1/W \rangle \begin{pmatrix}
 y_1 \bar{y}_2 - y_1' \bar{y}_2' & y_2' y_2 - \bar{y}_2 y_2' \\
 \bar{y}_1 y_1' - \bar{y}_1 y_1' & \bar{y}_1 y_2' - y_1 y_1'
\end{pmatrix} \tag{2.2.36}
\]

The bar on top of a symbol signifies that it refers to region \( n+1 \) while unbarred symbols refer to region \( n \).

The determinant of the match matrix \( M_{n+1,n} \) is

\[
\det M_{n+1,n} = \det B_{n+1} \det B_n^{-1}
\]

\[
= \frac{z'u^2 \text{Wr}_z(\varphi_1(z), \varphi_2(z))}{z'^u^2 \text{Wr}_z(\overline{\varphi}_1(z), \overline{\varphi}_2(z))} \tag{2.2.37}
\]

Since \( z'u^2 = 1 \) from (2.1.12) then \( \det M_{n+1,n} \) reduces to a ratio of the Wronskians of the neighbouring regions. If the two regions have the same model equation, as they are assumed to have in most of this work, the Wronskians are equal so

\[
\det M_{n+1,n} = 1 \tag{2.2.38}
\]

In this work regional and global coordinates are used. While there is only one global coordinate \( x \), each individual region \( n \) has its own regional coordinates \( x_n \) and \( z_n \). Hence the match point is represented by the global coordinate \( x = \xi^{(n+1,n)} \) and simultaneously by the two regional coordinates \( x_n = \xi^{(n+1,n)} \) and \( x_{n+1} = \xi^{(n+1,n)} \).

2.3 Eigenvalue Condition

Suppose \( N \) regions cover the \( x \)-axis. Then the relation between the coefficients of the end regions is

\[
\hat{a}_N = M_{N,1} \hat{a}_1 \tag{2.3.39}
\]

where
\[ M_{N,1} = M_{N,N-1} M_{N-1,N-2} \cdots M_{3,2} M_{2,1} \]  \hspace{1cm} (2.3.40)

In order to obtain a bound state energy eigenvalue, the wave function must vanish as \( x \to \pm \infty \). At these extreme values of \( x \), the wave function is in a classically forbidden region. Recall from section 2.1 that the solution \( y_1(x) \) is chosen so that it exponentially decreases in classically forbidden regions. Thus the wave function in the limit as \( x \to \pm \infty \) must be proportional to \( y_1(x) \).

Without loss of generality, \( y(x) \) can be chosen in region 1 as

\[ y(x) = y_1(x) \]  \hspace{1cm} (2.3.41)

so

\[ a_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \]  \hspace{1cm} (2.3.42)

In region \( N \), the wave function \( y(x) \) must be chosen proportional to \( y_1(x) \). If \( R \) is the constant of proportionality then \( y(x) \) in this region becomes

\[ y(x) = Ry_1(x) \]  \hspace{1cm} (2.3.43)

so

\[ a_N = \begin{bmatrix} R \\ 0 \end{bmatrix} \]  \hspace{1cm} (2.3.44)

Thus from equation (2.3.39)

\[ \begin{bmatrix} R \\ 0 \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \]  \hspace{1cm} (2.3.45)

where the \( m_{ij} \) are the elements of the matrix \( M_{N,1} \). Expanding (2.3.45) gives
\[ m_{11} = R \]
\[ m_{21} = 0 \]

Since nothing is known about \( R \) except \( R \neq 0 \), the energy eigenvalue condition becomes

\[ m_{21} = 0 \]
Chapter 3

The Choice of the Model Equation

Although the form of the model equation has been specified in (2.1.3), exactly what equation it is depends on the choice of the function \( g(z) \). With this choice, the solutions \( \varphi_1, \varphi_2 \) of the model equation will be determined as well as the transformation equation (2.1.18). Even though simplicity in the solutions \( \varphi_1, \varphi_2 \) is desirable, this constraint is not as important as how the choice of \( g(z) \) will affect the solution \( z(x) \) of the transformation equation.

3.1 The Case of \( g(z) = 0 \)

The simplest choice is \( g(z) = 0 \). Now the model equation becomes

\[
\varphi''(z) = 0
\]

which has solutions

\[
\varphi_1 = 1
\]
\[
\varphi_2 = z
\]

which certainly qualify as simple solutions. The two independent solutions become

\[
\varphi_1 = u(x)
\]
\[
\varphi_2 = u(x) \int_{x_0}^{x} \frac{dx}{u^2(x)}
\]

since

\[
z(x) = \int_{x_0}^{x} \frac{dx}{u^2(x)}
\]

When the associated transformation equation is obtained from
(1.2.20) it becomes
\[ W(x) - u^*/u = 0 \]  \hspace{1cm} (3.1.5)
or
\[ u^* = W(x)u \]  \hspace{1cm} (3.1.6)

A comparison of this equation with (2.1.2) shows that it is identical to the Schrödinger equation. Since the aim of this method was the simplification of the solution of the Schrödinger equation by its transformation clearly nothing has been achieved.

3.2 Derivation of Approximation Methods

A non-zero \( g(z) \) means that the transformation equation (2.1.18)
\[ W(x) + \beta(z,x) - g(z)(z')^2 = 0 \]
contains three terms and is no longer identical to the Schrödinger equation.

To gain a better understanding of the effect of the choice of \( g(z) \) the transformation equation is examined when \( x \) is far from the turning point. Nothing can be said about the \( W(x) \) term since no initial assumptions about the potential were made. Nothing can yet be said about the \( g(z)z^2 \) term since nothing is yet known about \( g(z) \). However, the \( \beta(z,x) \) term does give some information.

A restriction on the transformation function \( z(x) \) that \( z'(x) \neq 0 \) was introduced in the derivation of (2.1.7). As a result within the region where the transformation is valid, \( z(x) \) must be a monotonically increasing or decreasing function of \( x \). This implies that \( z(x) \) is a 'univalent' function (7). The Schwarzian (7)
\( (z,x) \) goes as \( |x|^{-4} \) for large \( |x| \). Thus it will be small compared
with the other terms and a good approximation for the transformation equation will become

$$W(x) - g(z)z'z^2 = 0$$  \hspace{1cm} (3.2.7)

for x far from the turning point.

For the choice $g(z)=1$, the model equation is

$$\psi''(z) = \psi(z)$$  \hspace{1cm} (3.2.8)

which has independent solutions

$$\psi_1(z) = e^z$$
$$\psi_2(z) = e^{-z}$$  \hspace{1cm} (3.2.9)

From (3.2.7) the transformation equation for x far from the turning point is

$$W(x) = z'(x)^2$$  \hspace{1cm} (3.2.10)

Solving this equation yields

$$z(x) = \int_{x_0}^{x} W(x')^{1/2} dx$$  \hspace{1cm} (3.2.11)

where $x_0$ is the turning point. The other transformation function $u(x)$ is

$$u(x) = z'(x)^{-1/2} = W(x)^{-1/2}$$  \hspace{1cm} (3.2.12)

Thus the general solution $y(x)$ for x far from the turning point is

$$y(x) = a_1 W(x)^{-1/2} \exp \left\{ \int_{x_0}^{x} W(x)^{1/2} dx \right\} + a_2 W(x)^{-1/2} \exp \left\{ -\int_{x_0}^{x} W(x)^{1/2} dx \right\}$$  \hspace{1cm} (3.2.13)

This is the well known JWKB approximate solution to the Schroedinger equation in the forbidden region. Similar analysis with $g(z)=-1$ yields the sine and cosine solutions of the JWKB method in the classical region. It is clear that these solutions
\( y(x) \) have a singularity at the turning point since there \( W(x) \) has the value 0.

For the choice \( g(z) = z \), the model equation becomes
\[
\psi''(z) = z \psi(z)
\]  
(3.2.14)
which has the independent solutions
\[
\psi_1(z) = Ai(z) \\
\psi_2(z) = Bi(z)
\]  
(3.2.15)
where \( Ai, Bi \) are the linearly independent Airy functions. The transformation equation for \( x \) far from the turning point from (3.2.7) is
\[
W(x) = z(x) z'(x)^2
\]  
(3.2.16)
so
\[
z'(x) = \left( \frac{W(x)}{z(x)} \right)^{1/2}
\]  
(3.2.17)
Solving for \( z(x) \) yields
\[
z(x) = \left( \frac{2}{3} \int_{x_0}^{x} W(x)^{1/2} \, dx \right)^{2/3}
\]  
(3.2.18)
where \( x_0 \) is a turning point. Note that \( z(x_0) = 0 \) so that the quantity in brackets in (3.2.17) is always positive. Its value at \( x_0 \) will be evaluated later. Thus the other transformation function \( u(x) \) is
\[
u(x) = z'(x)^{-1/2} = W(x)^{-1/2} \left( \frac{2}{3} \int_{x_0}^{x} W(x)^{1/2} \, dx \right)^{1/6}
\]  
(3.2.19)
The general solution for \( x \) far from the turning point is thus
\[
y(x) = W(x)^{-1/2} \left( \frac{2}{3} \int_{x_0}^{x} W(x)^{1/2} \, dx \right)^{1/6} \left[ a_1 Ai(z) + a_2 Bi(z) \right]
\]  
(3.2.20)
This is the solution obtained by the uniform JWKB method of solution to the Schroedinger equation, a modification of the Langer method. The Airy functions are regular so singularities can only occur if \( u(x) \to \infty \) so \( z' = 0 \). Since \( z'(x) = (W(x)/z(x))^{1/3} \) then \( z'(x) \) can only be zero at \( x = x_0 \) where \( W(x_0) = 0 \). However, \( z(x_0) = 0 \) so L'Hospital's rule must be used to evaluate \( z'(x_0) \) or equivalently \( [z'(x_0)]^2 \)

\[
\lim_{x \to x_0} [z'(x)]^2 = \lim_{x \to x_0} W(x) = \lim_{x \to x_0} W'(x) = W'(x_0)/z'(x_0) \quad (3.2.21)
\]

so

\[
z'(x_0) = [W'(x_0)]^{1/3} \quad (3.2.22)
\]

Thus no singularities exist in the uniform JWKB solution if \( W(x) \) has a leading linear term.

For the general case \( g(z) = z^p \) for integer \( p > 0 \) the model equation is

\[
\varphi''(z) = z^p \varphi(z) \quad (3.2.23)
\]

which has the independent solutions

\[
\varphi_1(z) = z^\xi J_\alpha(z) \quad (3.2.24)
\]

\[
\varphi_2(z) = z^\xi J_{-\alpha}(z)
\]

where \( J \)'s are the Bessel functions of the first kind, \( \xi = 2\alpha^{1/2}z \), and \( \alpha = (p+2)^{-1} \). The transformation for \( x \) far from the turning point is

\[
W(x) = z^p(x)z'(x)^2 \quad (3.2.25)
\]

which has solutions

\[
z(x) = \left[ \frac{p+2}{2} \int_{x_0}^{x} W(x)^{1/3} dx \right]^{2/(p+2)} \quad (3.2.26)
\]
\[ u(x) = W(x)^{-\alpha} \left( \frac{1}{2\alpha} \int_{x_0}^{x} W(x)^{\frac{\alpha}{2}} \, dx \right)^{\frac{p\alpha+1}{2}} \text{ (3.2.27)} \]

and the general solution for \( x \) far from the turning point is

\[ y_\alpha(x) = W(x)^{-\alpha} \left( \frac{1}{2\alpha} \int_{x_0}^{x} W(x)^{\frac{\alpha}{2}} \, dx \right)^{\frac{p\alpha+1}{2}} \left( a_1 J_\alpha(\xi) + a_2 J_{-\alpha}(\xi) \right) \text{ (3.2.28)} \]

From analysis similar to the uniform JWKB case, this approximate solution for \( p>0 \) will be regular everywhere, even at \( x=x_0 \), if \( W(x) \) has a lowest term of \( p \)th order in its Taylor expansion about \( x_0 \).

3.3 The Model Equation Used in This Work

For this work \( g(z)=z \) was chosen so the model equation is the Airy equation with the Airy functions as solutions. The choice \( g(z)=\pm i \) also seems suitable but no calculation involving these functions have yet been done. Such calculations are planned for the future.
Chapter 4

Methods of Solving the Transformation Equation

Almost all of the effort that it takes to solve the Schrödinger equation by this method goes into the solution of the transformation equation. The model equation is, in effect, already solved since \( g(z) \) is chosen to make \( \psi_1, \psi_2 \) well known functions. Once these functions have been expanded, no additional work need be done on other problems which share the same model equation.

The transformation equation (2.1.18) is a third order nonlinear differential equation. It may seem that the Schrödinger equation, a second order differential equation would be easier to solve than a third order equation but this need not be so in practice. The solution of the Schrödinger equation is often highly oscillatory, a situation that can cause significant errors to occur in numerical methods of solution.

In this method, the oscillatory part of the wave function is largely contained in the known functions which are solutions to the model equation. The transformation equation solution \( z(x) \) is a simple monotonically increasing or decreasing function, a situation usually well handled by numerical methods.

Three methods have been used to solve the transformation equation: the iteration method, the power series method, and the coupled differential equation method. They will be individually examined in the next three sections. The transformation equation used in these sections will have \( g(z) = z \) as discussed in section 3.3 but all the methods can be modified for use with any \( g(z) \).
In addition, all methods assume \( z'(x) > 0 \) so \( z(x) \) is
monotonically increasing. This causes no problem since if \( z'(x) < 0 \)
the equations are solved by reversing the orientation through the
use of regional coordinates. The relation between the global and
regional coordinates is

\[
x_{\text{global}} = A x_{\text{regional}} + B \tag{4.0.1}
\]

so

\[
\frac{d}{dx}_{\text{global}} = A \frac{d}{dx}_{\text{regional}} \tag{4.0.2}
\]

where \( A = \pm 1 \) is the orientation and \( B \) is some offset value. Often \( B \)
is chosen so that \( x_{\text{regional}} \) is zero at a turning point. After the
equations are solved using regional coordinates, the transform-
ation functions can be easily converted back to global coordinates.

4.1 The Iteration Method \(^{11}\)

Using the terminology in the above reference, the
transformation equation can be written

\[
W(x) = U(x) + \Delta[U, x] \tag{4.1.3}
\]

where

\[
U(x) = z(x)z'(x) \tag{4.1.4}
\]

\[
\Delta[U, x] = -\frac{1}{2}z(x) \tag{4.1.5}
\]

The term \( U(x) \) is called the substitute potential. This name
comes from the fact that \( U(x) \) replaces \( W(x) \) in the modified
uniform JWKB approximation discussed in section 3.2 and makes the
solution exact instead of an approximation.

The iteration starts with the substitute potential \( U(x) \)
equal to the potential \( W(x) \) as in the uniform JWKB approximation

\[
U_0(x) = W(x) \tag{4.1.6}
\]

and from (4.1.3).
\( \Delta[U_0, x] = 0 \) \hspace{1cm} (4.1.7)

where the subscript refers to the iteration step number. The 'potential defect' \( P(x) \) is defined as
\[ P_0(x) = W(x) - (U_0(x) + \Delta[U_0, x]) \] \hspace{1cm} (4.1.8)

For the first step, the substitute potential becomes
\[ U_1(x) = U_0(x) + \lambda P_0(x) \] \hspace{1cm} (4.1.9)

where \( \lambda \) is an arbitrary constant chosen to enhance the convergence. Typically \( \lambda = 0.01 \).

The iteration continues with the recursion relations for the \( n^{\text{th}} \) step
\[ P_n(x) = W(x) - (U_n(x) + \Delta[U_n, x]) \] \hspace{1cm} (4.1.10)
\[ U_{n+1}(x) = U_n(x) + \lambda P_n(x) \]

After \( m \) such steps
\[ W(x) = U_m(x) + \Delta[U_m, x] + P_m(x) \] \hspace{1cm} (4.1.11)

The iteration terminates when \( P_m(x) < \epsilon \) where \( \epsilon \) is the desired accuracy of the solutions. At this point the transformation function \( z(x) \) can be calculated knowing
\[ z'(x) = U_m(x)/z(x) \] \hspace{1cm} (4.1.12)

so
\[ z(x) = \left[ \frac{3}{2} \int_{x_0}^{x} U_m^2 \, dx \right]^{2/3} \] \hspace{1cm} (4.1.13)

where \( x_0 \) is the turning point. The solution in the region is

\[ y(x) = z^{-1/2} \left( a_1 \text{Ai}(z) + a_2 \text{Bi}(z) \right) \] \hspace{1cm} (4.1.14)

This method was successfully applied to the simple harmonic oscillator potential and the \( N \)-fold barrier potential (see section 5.4). Wave functions and eigenvalues were obtained.
The main problem with the iteration method of solution of the transformation equation is speed. The search for the energy level was so slow that even after a large amount of computer time (30 minutes on an IBM 3031 mainframe) the accuracy rarely exceeded 1%. This prompted the development of the faster methods of solution discussed in the next two sections.

4.2 Power Series Method

An often used method for solving differential equations involves the expansion of the solution in terms of a power series around some point \( x = x_s \). After writing out the terms of the Schwarzian, the transformation equation becomes

\[
W(x)z'(x)^2 + (1/2)z'(x)z'''(x) - (3/4)z''(x)^2 - z(x)z'(x)^4 = 0
\]

(4.2.15)

The expansions for the functions \( W(x) \) and \( z(x) \) around \( x = x_s \) are

\[
W(x) = \sum_{\alpha=0}^{\infty} w_{\alpha}(x-x_s)^{\alpha} \tag{4.2.16}
\]

\[
z(x) = \sum_{\alpha=0}^{\infty} z_{\alpha}(x-x_s)^{\alpha} \tag{4.2.17}
\]

so

\[
z'(x) = \sum_{\alpha=1}^{\infty} \alpha z_{\alpha}(x-x_s)^{\alpha-1} \tag{4.2.18}
\]

\[
z''(x) = \sum_{\alpha=2}^{\infty} \alpha(\alpha-1)z_{\alpha}(x-x_s)^{\alpha-2} \tag{4.2.19}
\]

\[
z'''(x) = \sum_{\alpha=3}^{\infty} \alpha(\alpha-1)(\alpha-2)z_{\alpha}(x-x_s)^{\alpha-3} \tag{4.2.20}
\]

In terms of these coefficients, the starting conditions at the
point. \( x=x_s \) become \( z(x_s)=z_0, \) \( z'(x_s)=z_1, \) and \( z''(x_s)=2z_2 \). The transformation equation with the above expansions substituted thus becomes

\[
\sum_{\gamma=0}^{\infty} \sum_{\alpha=1}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)z^\alpha \beta^4 z^\alpha (x-x_s)^{\alpha+\beta-4}
\]

\[
\sum_{\alpha=3}^{n+3} \alpha(\alpha-1)z^\alpha \beta^4 z^\alpha (x-x_s)^{\alpha+\beta-4}
\]

\[
-\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)z^\alpha z^{n-\alpha+4}
\]

\[
-\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

\[
-\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

Since the \((x-x_s)^n\) term must vanish

\[
\sum_{\alpha=1}^{n+1} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+4} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)z^\alpha z^{n-\alpha+4}
\]

\[
\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

\[
\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

and combining the 2nd and 3rd sums

\[
\sum_{\alpha=1}^{n+1} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+4} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(5\alpha-3n-13)z^\alpha z^{n-\alpha+4}
\]

\[
-\sum_{\alpha=1}^{n+1} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+4} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

\[
\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

\[
-\sum_{\alpha=2}^{n+4} \alpha z^2 \beta^4 z^\alpha (x-x_s)^{\alpha+\beta+2} + \sum_{\alpha=3}^{n+3} \alpha(\alpha-1)(\alpha-2)(n-\alpha+4)(n-\alpha+3)z^\alpha z^{n-\alpha+4}
\]

To obtain a general term involving \( n \) for use in a recursion formula, examine the upper limit of each sum. This general term must be non-vanishing.

For the first sum choose \( \alpha=1, \beta=n+1 \) (or vice versa) so the general term would be \((n+1)z_1z_{n+1}w_0\). If \( x_s=x_0 \) then \( w_0=W(x_0)=0 \)
and the term vanishes.

For the third sum choose \( \alpha = \beta = 1, \gamma = n + 1 \) so the general term would be \( (n+1)z_1^3z_{n+1}z_0 \). It could happen that \( z_0 = z(x_s) = 0 \) so the general term would vanish.

For the second sum the choice \( \alpha = n + 4 \) yields zero but \( \alpha = n + 3 \) yields \( \frac{1}{n+3}(n+2)(n+1)z_{n+3}z_1 \). Since \( z_1 = z'(x_s) \neq 0 \) in the transformation range then this term will not vanish. Using this term as the general term

\[
\frac{1}{n+3}(n+2)(n+1)z_{n+3}z_1
\]

\[
= - \sum_{\alpha, \beta = 1}^{n+1} \alpha^\beta z_\alpha \beta z_{n-\alpha-\beta+2}
\]

\[
\frac{1}{n+2} \sum_{\alpha = 2}^{n+2} \alpha(\alpha - 1)(n - \alpha + 4)(5\alpha - 3n - 13)z_\alpha z_{n-\alpha+4}
\]

\[
+ \sum_{\alpha, \beta, \gamma, \delta = 1}^{n+1} \alpha^\beta \gamma^\delta z_\alpha \beta \gamma \delta z_{n-\alpha-\beta-\gamma-\delta+4}
\]  

(4.2.24)

Using \( z_0, z_1, z_2 \) from the starting conditions all further \( z_n \)'s can be recursively obtained from this equation. For example \( n = 0 \) gives \( z_3 \).

\[
\frac{1}{3}(3)(2)(1)z_3z_1 = -z_1^2w_0 + 3z_2^2 + z_0z_1^4
\]  

(4.2.25)

Simplifying gives

\[
z_3 = (3z_2^2 - z_1^2w_0 + z_0z_1^4)/(3z_1)
\]  

(4.2.26)

Historically, this method was the successor to the iteration method. It proved to be very fast (about 1 second per integration) but the following problems occurred.

Using the non-linear simple potential (see section 5.1), an expansion around the turning point was obtained for the transformation function \( z(x) \). A comparison of the calculated
to the analytic solution showed that the results were highly accurate at $x_5 = x_0$ but away from this point the accuracy rapidly declined. By the time $|x - x_0| = 1$, the results were completely wrong. Since this small radius of convergence was not well understood at the time, this method was superceded by the coupled differential equation method discussed in the next section.

The success of the coupled differential equation method caused the power series method to be nearly forgotten. At this time, it is not clear whether the problems encountered were related to the choice of $x_5 = x_0$ the turning point or the choice of the potential or some inherent limitation in this method. Since the power series method is potentially more than ten times faster than the coupled differential equation method, a second look at it is planned for the future.

4.3 Coupled Differential Equation Method

The two equations involved in the transformation (2.1.12) and (2.1.20) can be written in the form of a coupled system of 3 first order ordinary differential equations. Each equation has the form

$$\frac{d}{dx} S_i(x) = f_i(x, S_1, S_2, \ldots, S_n), \quad i=1, n \tag{4.3.27}$$

where the $S_i$'s are the functions to be obtained. In this case, the functions $S_1(x), S_2(x), S_3(x)$ are chosen to be $z(x), u(x), u'(x)$ and the coupled set of equations are
\frac{d}{dx} z(x) = u(x)^{-2} \quad (4.3.28)

\frac{d}{dx} u(x) = u'(x) \quad (4.3.29)

\frac{d}{dx} u'(x) = u(x)W(x) - z(x)u(x)^{-3} \quad (4.3.30)

Although equation (4.3.29) looks artificial, it is needed to express the relationship between \( S_2'(x) \) and \( S_3(x) \).

These equations are solved by the subprogram DDFSYS\(^{12}\). The values of \( z(x) \), \( u(x) \), \( u'(x) \) at the point \( x_n \) and the distance \( h \) to the next point are required as inputs to calculate \( z(x_n+h) \), \( u(x_n+h) \), and \( u'(x_n+h) \).

At first some difficulties occasionally occurred when transformation functions grew very large, changed sign, and rapidly lost accuracy. This behavior can be easily corrected by starting a new region as discussed in section 4.4. Some other ideas for dealing with this are discussed in section 4.5.

This method has proven to be very successful in the solution of the transformation equation. The full program to solve the Eckart potential is presented in Appendix B. Often the accuracy of the eigenvalues and/or wavefunctions is 8 significant figures. Since the Airy function expansions used are accurate to about 8 significant figures, it is clear in these cases that the accuracy of the transformation function \( z(x) \) solved by this method must be at least that.

The search for a typical energy level and its associated wave function to an accuracy of about 7 significant figures takes about 1 minute on an IBM 3031 mainframe computer. To calculate the value of the eigenvalue condition \( m_{21} \) for a particular energy...
takes about 4 seconds.

4.4 Starting Conditions for the Transformation Equation

The starting condition for the solution of the transformation equation are not related to the eigenvalue conditions discussed in section 2.3. The transformation of the Schrödinger equation to the model equation is apparently free from constraints. As a result, the starting conditions of the transformation equation are completely arbitrary, and thus can be chosen at will.

In practice, however, the choice of the starting conditions seems to affect the size of the region over which the transformation is valid. Thus a "poor" choice of the starting conditions can seriously hamper the numerical solution of the transformation equation. Although the question of choosing the "best" starting conditions is currently unsolved, the remedies presented here and in section 4.5 effectively eliminate the problem.

Because problems can occur if the choice of the starting conditions is completely random, it makes sense to choose conditions which are closely related to the solution. For x far from the turning point x₀, the approximate solutions discussed in section 3.2 give a good estimate for the solution. Using the uniform JWKB approximation, the starting conditions at x=xₙ become

\[
\begin{align*}
z(xₙ) &= \left[ \frac{3}{2} \int_{x₀}^{xₙ} w(x)x dx \right]^{\frac{2}{3}} \quad (4.4.31) \\
z'(x) &= \left[ \frac{w(xₙ)}{z(xₙ)} \right]^{\frac{1}{2}} \quad (4.4.32)
\end{align*}
\]
\[ z^*(x_s) = \frac{1}{2} z'(x_s) \left[ \frac{W'(x_s)}{W(x_s)} - \frac{z'(x_s)}{z(x_s)} \right] \]  \hfill (4.4.33)

These starting conditions can be easily calculated everywhere except at \( x=x_o \).

At the turning point \( x=x_o \), a closely related set of conditions are used.

\[ W(x_o) = U(x_o) \]  \hfill (4.4.34)
\[ W'(x_o) = U'(x_o) \]  \hfill (4.4.35)
\[ W''(x_o) \neq U''(x_o) \]  \hfill (4.4.36)

where \( U(x)=z(x)z'(x)^2 \) is the substitute potential discussed in section 4.1. The derivatives of \( U(x) \) are

\[ U'(x) = z'(x)^3 + 2z(x)z'(x)z''(x) \]  \hfill (4.4.37)
\[ U''(x) = 3z'(x)2z''(x) + 2z'(x)2z''(x) + 2z(x)z''(x)^2 + 2z(x)z'(x)z''''(x) \]  \hfill (4.4.38)

At the turning point \( W(x_o)=0 \) and since \( z'(x) \neq 0 \) for any \( x \) then from (4.4.34) \( z(x_o)=0 \). Substituting into (4.4.37) and (4.4.38) and using (4.4.35), (4.4.36) yields

\[ W'(x_o) = z'(x_o)^3 \]  \hfill (4.4.39)
\[ W''(x_o) = 5z'(x_o)2z''(x_o) \]  \hfill (4.4.40)

Thus the starting conditions for \( x=x_o \)

\[ z(x_o) = 0 \]  \hfill (4.4.41)
\[ z'(x_o) = W'(x_o)^{1/3} \]  \hfill (4.4.42)
\[ z''(x_o) = (1/5)W''(x_o)W'(x_o)^{-2/3} \]  \hfill (4.4.43)

It is clear that other starting conditions based on other approximations of the Schrödinger equation could have been used.
4.5 Other Conditions

Although the relationship between the starting conditions and the range of validity of the transformation equation is only qualitatively understood the problem of where to start a new region has effectively been solved in the following way.

The derivative of the transformation function $z'(x)$ and the term of $u''/u$ in the transformation equation are closely monitored. As the range of validity of a region is ending, it seems that $z'(x) \to 0$. As this happens the quantity $u''/u$ increases enormously in magnitude, tending to $\infty$. A new transformation region begins when $z'(x)$ changes signs. At this point $u''/u$ abruptly changes signs and its magnitude decreases to a reasonable value.

A logical condition to start a new region is thus a large change in the quantity $u''/u$. The program in Appendix B starts a new region if $u''/u$ changes by a factor of 2 over one integration step. Normally $u''/u$ changes slowly so new regions are not frequently invoked.

When the importance of the term $u''/u = -\% (z, x)$ was understood, it seemed that the maximum range of a region might be obtained if the integral of $(u''/u)^2$ could be minimized. It is clear a minimum exists since $u''/u \neq 0$ for all $x$ (unless $W(x)$ is chosen as in section 5.1) and $u''/u = -\% (z, x)$ tends to zero far from the turning point. Using the calculus of variations (13), the equations for the integral to be a minimum were derived (see Appendix A). This introduced additional unknown functions from the Lagrange multipliers which could not be solved unless the transformation
functions were already known. As a result this idea was not pursued further.

Recently several other attempts have been made to better understand the effect of the starting conditions on the range of the transformation equation. One idea involves stability analysis of non-linear systems (14), (15). As of yet no results have been obtained since most of the available work deals with 2nd order differential equations and the generalization to 3rd order was not clear. The other idea involves the understanding of the transformation of the Schroedinger equation as a conformal mapping (16). So far this idea seems to confirm that multiple regions are needed to cover the real axis.
Chapter 5

Examples

Some examples involving a variety of potentials follow. Most of these potentials were chosen because their exact solutions are available for comparison with results from this method.

5.1 Potentials with \( (z,x) = 0 \)

The simplest transformation to solve with this method has the term \( k(z,x) = 0 \) for all \( x \). Potentials which fit this condition can be solved for directly using analytical methods. The transformation equation becomes

\[
W(x) = z(x)z'(x)^2
\]

(5.1.1)

and since \( u''/u = -k(z,x) = 0 \)

\[
u''(x) = 0
\]

(5.1.2)

This very simple differential equation can be solved yielding

\[
u(x) = C_1 x + C_2
\]

(5.1.3)

for arbitrary constants \( C_1, C_2 \).

If \( C_1 = 0 \) then \( u = C_2 \) so \( z' = u^{-2} = C_2^{-2} = A \) and \( z \) can be written as

\[
z(x) = A(x-x_0)
\]

(5.1.4)

for some constants \( A, x_0 \). Thus the corresponding potential \( W(x) \) can be calculated as

\[
W(x) = z(x)z'(x)^2 = A^3(x-x_0)
\]

(5.1.5)

the exactly linear potential. It thus has the general solution

\[
y(x) = a_1 Ai(A(x-x_0)) + a_2 Bi(A(x-x_0))
\]

(5.1.6)

If \( C_1 \neq 0 \) then the potential is more interesting. Now

\[
z'(x) = A(x-x_0)^{-2}
\]

(5.1.7)

and

30
\[ z(x) = A \left( \frac{1}{(x-x_p)} - \frac{1}{(x_0-x_p)} \right) \]  

(5.1.8)

where \( A, x_0, x_p \) are arbitrary constants. Thus the potential \( W(x) \) becomes

\[ W(x) = \frac{A^3}{(x-x_p)^4} \left( \frac{1}{(x-x_p)} - \frac{1}{(x_0-x_p)} \right) \]  

(5.1.9)

An examination of the constants shows that \( x=x_0 \) is the classical turning point since \( W(x_0)=0 \). In addition, a pole in the potential occurs at \( x=x_p \).

For physically interesting potentials, \( W(x) \) will have \( x_p \leq x_0 \) and preferably \( x_p \leq 0 \). The potential \( W(x) \) now has a minimum for \( A<0 \) (or a maximum for \( A>0 \)) at \( x_m \) given by

\[ x_m - x_p = (5/4)(x_0-x_p) \]  

(5.1.10)

At this point the value of the potential is

\[ W(x_m) = 4^4 A^3 [5(x_0-x_p)]^{-5} \]  

(5.1.11)

The general solution is

\[ y(x) = (x-x_p)(a_1Ai(z) + a_2Bi(z)) \]  

(5.1.12)

where \( z \) is given by equation (5.1.8). The specific solution depends on the boundary conditions.

To understand the problem just solved look more closely at the potential. In the limit as \( x \to \infty \) the potential \( W(x) \to 0 \). Since \( W(x) \) is energy adjusted, the solution (5.1.12) will be valid for the energy equal to the 'dissociation limit' of the potential. With the added requirement that the solution be an eigenstate, the boundary conditions applied to (5.1.12) become

\[ y(x_p) = 0 \]

\[ y(\infty) = 0 \]  

(5.1.13)

Recall that in the limit as \( z \to \infty \) the Airy function \( Ai \to 0 \) while
Bi\rightarrow\infty. Thus the condition \( y(x_p) = 0 \) means that \( a_2 \) in equation (5.1.12) must be zero. Also since

\[
\lim_{x \rightarrow \infty} z(x) = -\frac{A}{x_0 - x_p} = \text{constant} \tag{5.1.14}
\]

then the only way to make \( y(z(\infty)) = 0 \) is to have \( \text{Ai}(z(\infty)) = 0 \). Thus \( z(\infty) \) is a zero of the Airy function \( \text{Ai}(z) \). If \( z(\omega) \) is the \( n \)th zero of the Airy function \( \text{Ai} \) and thus of the wave function then the chosen potential will support \( n-1 \) eigenstates of less energy.

In figure 1 is an example of this potential for the dissociation limit corresponding to the 5th eigenenergy. The associated wave function and the transformation function \( z(x) \) are shown. The arbitrary constants are chosen as \( A = -16 \), \( x_p = 0 \). The 5th zero \(^{(17)} \) of \( \text{Ai}(z) \) occurs at \( z = -7.94413359 \) so \( x_0 = A/z = 2.014064821 \). This type of potential where \( (z, x) = 0 \) for all \( x \) can be obtained from any model equation of the form \( \psi''(z) = z^n \psi(z) \). Then the potential becomes

\[
W(x) = \frac{A^{n+2}}{(x-x_p)^4} \left[ \frac{1}{(x-x_p)} - \frac{1}{(x_0-x_p)} \right]^n \tag{5.1.15}
\]

with an extremum point at \( x_m \) where

\[
x_m - x_p = (4n)(x_0 - x_p)/4 \tag{5.1.16}
\]

and extremum value

\[
W(x_m) = 4^4 A^{n+2} n^n \left( (4n)(x_0 - x_p) \right)^{4+n} \tag{5.1.17}
\]
5.2 Harmonic Oscillator

The next logical choice for a test of the method is the harmonic oscillator potential \( V(x) = ax^2 \). It has energy levels \(^{(18)}\)

\[
E_n = \left( \frac{\hbar^2}{2m} \right)^{\frac{1}{2}} (2n+1) a^{\frac{1}{2}} \tag{5.2.18}
\]

with eigenfunctions

\[
\psi_n(x) = \left( \frac{C}{\pi^{\frac{1}{2}} 2^{n} n!} \right)^{\frac{1}{2}} e^{-\frac{x^2}{2C^2}} H_n(Cx) \tag{5.2.19}
\]

where

\[
C^2 = \left( \frac{2m}{\hbar^2} \right)^{\frac{1}{2}} \tag{5.2.20}
\]

and \( H_n \) are the Hermite polynomials of degree \( n \). For simplicity choose \( 2m/\hbar^2 = 1 \) and \( a = 1 \) so the energy adjusted potential is

\[
\tilde{V}(x) = (2m/\hbar^2) (V(x) - E) = x^2 - E \tag{5.2.21}
\]

and the energy levels become

\[
E_n = 2n + 1 \tag{5.2.22}
\]

In this case, the potential is arbitrarily broken up into 2 regions with the cut occurring at the minimum point. Because of reflection symmetry around this point, only one of the regions need be solved for the transformation functions. The transformation functions in the other regions can be obtained by realizing that the effect of the reflection is to change the sign of the derivative so

\[
\frac{d}{dx}\text{right} = -\frac{d}{dx}\text{left} \tag{5.2.23}
\]

where \( x_{\text{right}} \) and \( x_{\text{left}} \) are regional coordinates in the respective regions. Thus evaluated at the match point \( \xi_{(\text{right},\text{left})} \)
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Table 1:
Harmonic oscillator potential: Comparison of the exact and calculated energy level and wave function for the ground state n=0
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Table 1:

Harmonic oscillator potential: Comparison of the exact and calculated energy level and wave function for n=1.
\[ z_{\text{right}} = z_{\text{left}} \]
\[ z'_{\text{right}} = -z'_{\text{left}} \]  \( (5.2.24) \)
\[ z''_{\text{right}} = z''_{\text{left}} \]

The results of the calculations for \( n=0 \) are shown in Table 1 and for \( n=1 \) are shown in Table 2.

5.3 Eckart Potential

The non-symmetric Eckart potential \( (19) \) is next chosen. It has the form

\[ U(x) = \frac{A}{1+e^{-x}} + \frac{B}{1+e^{-x}} \]  \( (5.3.25) \)

The corresponding Schroedinger equation has the solution \( (20) \)

\[ \Psi(x) = e^{-i\alpha(1-s)} \]  \( (5.3.26) \)

where

\[ \alpha/C = -i(-E_n)^{\frac{1}{2}} \]  \( (5.3.27) \)
\[ \beta/C = i(A - E_n)^{\frac{1}{2}} \]  \( (5.3.28) \)

and \( F(a,b;c;s) \) is the hypergeometric function with the parameters \( a, b, \) and \( c \) given by

\[ a/C = (-E_n)^{\frac{1}{2}} + (A - E_n)^{\frac{1}{2}} + \frac{1}{2}(1 - (1-4B)^{\frac{1}{2}}) \]  \( (5.3.29) \)
\[ b/C = (-E_n)^{\frac{1}{2}} + (A - E_n)^{\frac{1}{2}} + \frac{1}{2}(1 + (1-4B)^{\frac{1}{2}}) \]  \( (5.3.30) \)
\[ c/C = 1 + 2(A - E_n)^{\frac{1}{2}} \]  \( (5.3.31) \)

with \( C^2=2m\hbar^2 \). Setting \( C=1 \) for convenience, the values chosen for the calculations are \( A=-1.922 \) and \( B=-1.2 \) for direct comparison with previous work \( (21) \).

The energy levels \( E_n \) of the bound states are characterized by wave functions which vanish at infinity. This forces the \( \alpha \) parameter of \( F(a,b;c;s) \) to be a negative integer and yields the energy levels

\[ 37 \]
\[ E_n = -\mathcal{W}^{-1}(T - A)^2 \]  \hspace{1cm} (5.3.32)

with

\[ T = \mathcal{W}[ (1 - 4B)^{\frac{1}{2}} - (2n+1)]^2 \]  \hspace{1cm} (5.3.33)

The results of calculations for \( n=0 \) and \( n=1 \) are shown in tables 3 and 4 respectively. Figures 2 and 3 show the potential \( W(x) \) and the transformation functions for \( n=0 \) and \( n=1 \) respectively. In both cases, the potential was divided into two regions by a cut near the minimum. No additional regions needed to be invoked as described in section 4.5.
--- Energy Level ---

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<td>-3.5113</td>
<td>8.217446 E-03</td>
<td>8.217498 E-03</td>
</tr>
<tr>
<td>-4.0624</td>
<td>3.201369 E-03</td>
<td>3.201389 E-03</td>
</tr>
<tr>
<td>-4.6135</td>
<td>1.228748 E-03</td>
<td>1.228756 E-03</td>
</tr>
<tr>
<td>-5.1646</td>
<td>4.675227 E-04</td>
<td>4.675255 E-04</td>
</tr>
<tr>
<td>-5.7158</td>
<td>1.769869 E-04</td>
<td>1.769875 E-04</td>
</tr>
<tr>
<td>-6.2669</td>
<td>6.680529 E-05</td>
<td>6.680421 E-05</td>
</tr>
<tr>
<td>-6.8180</td>
<td>2.517637 E-05</td>
<td>2.517257 E-05</td>
</tr>
</tbody>
</table>

Table 3:

Eckart potential: Comparison of the exact and calculated energy level and wave function for the lower (ground) level.
--- Energy Level ---

Calculated  Exact

-2.1084074538  -2.1084074165

--- Wave Function ---

\[
\begin{array}{ccc}
\text{x} & \text{Calculated} & \text{Exact} \\
11.1585 & 1.825204 \times 10^{-2} & 1.824907 \times 10^{-2} \\
10.4827 & 2.443178 \times 10^{-2} & 2.442962 \times 10^{-2} \\
9.8078 & 3.270276 \times 10^{-2} & 3.270122 \times 10^{-2} \\
9.1313 & 4.376885 \times 10^{-2} & 4.376780 \times 10^{-2} \\
8.4555 & 5.856516 \times 10^{-2} & 5.856450 \times 10^{-2} \\
7.7798 & 7.832449 \times 10^{-2} & 7.832419 \times 10^{-2} \\
7.1041 & 1.046474 \times 10^{-1} & 1.046474 \times 10^{-1} \\
6.4283 & 1.395459 \times 10^{-1} & 1.395462 \times 10^{-1} \\
5.7526 & 1.853736 \times 10^{-1} & 1.853742 \times 10^{-1} \\
5.0768 & 2.444083 \times 10^{-1} & 2.444093 \times 10^{-1} \\
4.4011 & 3.175089 \times 10^{-1} & 3.175104 \times 10^{-1} \\
3.7253 & 4.005864 \times 10^{-1} & 4.005882 \times 10^{-1} \\
3.0496 & 4.768317 \times 10^{-1} & 4.768341 \times 10^{-1} \\
2.3739 & 5.042917 \times 10^{-1} & 5.042942 \times 10^{-1} \\
1.6981 & 4.117384 \times 10^{-1} & 4.117405 \times 10^{-1} \\
1.0224 & 1.474158 \times 10^{-1} & 1.474166 \times 10^{-1} \\
0.8534 & 6.040970 \times 10^{-2} & 6.041004 \times 10^{-2} \\
0.7312 & -4.426915 \times 10^{-3} & -4.426918 \times 10^{-3} \\
0.3466 & -2.008887 \times 10^{-1} & -2.008898 \times 10^{-1} \\
-0.0425 & -3.472107 \times 10^{-1} & -3.472124 \times 10^{-1} \\
-0.4316 & -4.117619 \times 10^{-1} & -4.117640 \times 10^{-1} \\
-0.8207 & -3.962737 \times 10^{-1} & -3.962758 \times 10^{-1} \\
-1.2098 & -3.297778 \times 10^{-1} & -3.297796 \times 10^{-1} \\
-1.5989 & -2.445104 \times 10^{-1} & -2.445117 \times 10^{-1} \\
-1.9881 & -1.701896 \times 10^{-1} & -1.701905 \times 10^{-1} \\
-2.3772 & -1.108754 \times 10^{-1} & -1.108760 \times 10^{-1} \\
-2.7663 & -6.928831 \times 10^{-2} & -6.928867 \times 10^{-2} \\
-3.1554 & -4.204447 \times 10^{-2} & -4.204470 \times 10^{-2} \\
-3.5445 & -2.499408 \times 10^{-2} & -2.499422 \times 10^{-2} \\
-3.9336 & -1.464845 \times 10^{-2} & -1.464854 \times 10^{-2} \\
-4.3228 & -8.501619 \times 10^{-3} & -8.501678 \times 10^{-3} \\
-4.7119 & -4.901226 \times 10^{-3} & -4.901278 \times 10^{-3} \\
-5.1010 & -2.812697 \times 10^{-3} & -2.812753 \times 10^{-3} \\
-5.4901 & -1.609098 \times 10^{-3} & -1.609178 \times 10^{-3} \\
-5.8792 & -9.185397 \times 10^{-4} & -9.186689 \times 10^{-4}
\end{array}
\]

Table 4:

Eckart potential: Comparison of the exact and calculated energy level and wave function for the upper (excited) level.
5.4 N-fold Periodic Ring Potential

In this case, the basic sector potential
\[ U(x) = 1 - \cos x \]  \hspace{1cm} (5.3.34)
for 0 \leq x \leq 2\pi is repeated N times and then closes in on itself (see figure 4). As a result, the periodic boundary condition
\[ y(x) = y(x + 2\pi N) \]
\[ y'(x) = y'(x + 2\pi N) \]  \hspace{1cm} (5.3.35)
must be used instead of that discussed in section 2.3.

The highly symmetric nature of the potential suggests that a wise selection of cuts could effectively reduce the number of regions to be solved. If a cut occurs at each maximum or minimum point then 2N nearly identical regions will be formed. Neighbouring regions n, n+1 will have opposite orientation. Thus for the regional coordinates \( x_n, x_{n+1} \)
\[ \frac{d}{dx_{n+1}} = -\frac{d}{dx_n} \]  \hspace{1cm} (5.4.36)
so at the match point \( z_{n+1}^{(n+1,n)} \)
\[ z_{n+1} = z_n \]
\[ z'_{n+1} = -z'_n \]  \hspace{1cm} (5.4.37)
\[ z''_{n+1} = z''_n \]
The relation between the \( \mathcal{B} \) matrices of neighbouring regions comes about since
\[ b_{n+1} = b_n \]  \hspace{1cm} (5.4.38)
\[ b'_{n+1} = -b'_n \]
so
\[ \mathcal{B}_{n+1}(z_{n+1}^{(n+1,n)}) = \mathcal{E} \mathcal{B}_n(z_{n+1}^{(n+1,n)}) \]  \hspace{1cm} (5.4.39)
where
\[
E = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5.4.40}
\]
and note that \(E^{-1} = E\).

If regions of positive orientation are identified with '+' and regions of negative orientation with '-' then the \(B\) matrices at a given match point \(x = \xi\) are
\[
B_+ = E B_- B_+^{-1} = B_-^{-1} E \tag{5.4.41}
\]
\[
B_- = E B_+ B_-^{-1} = B_+^{-1} E
\]
The match matrix for the first sector is
\[
M_{31} = M_{32} M_{21} = B_0^{-1} (\xi^{(32)}) B_2 (\xi^{(32)}) B_2^{-1} (\xi^{(21)}) B_1 (\xi^{(21)}) \tag{5.4.42}
\]
or using (5.4.41)
\[
M_{31} = B_+^{-1} (\xi^{(32)}) E B_+ (\xi^{(32)}) B_+^{-1} (\xi^{(21)}) E B_+ (\xi^{(21)}) \tag{5.4.43}
\]
and the equation will remain true if \(B_+\) is replaced by \(B_-\).

The connection matrices of the other sectors will be equal to \(M_{31}\) for any sector potential \(V(x)\). Thus if \(M_{31}\) is defined as \(M\) the connection matrix around the ring (that is for \(N\) sectors) is \(M^N\).

The boundary conditions (5.4.35) imply that after going around the ring, the wave function will repeat itself exactly.
Thus
\[
a = M^N a \tag{5.4.44}
\]
so
\[
M^N = 1 \tag{5.4.45}
\]
As a result if \(\lambda\) is an eigenvalue of \(M\) then
\[
\lambda^N = 1 \tag{5.4.46}
\]
so
\[ \lambda_k = e^{2\pi i k/N} \]  \hspace{1cm} (5.4.47)
for \( k=0,1,\ldots,N-1 \) or alternately for integer \( k \) when
\(-N/2 \leq k \leq (N/2+1)\). All eigenvalues occur in complex conjugate pairs
on the unit circle except for \( \lambda_0 = 1 \) and \( \lambda_{N/2} = -1 \) for even \( N \), which
are real.

If the eigenvectors of \( M \) are \( a_k \) then
\[ M a_k = \lambda_k a_k \]  \hspace{1cm} (5.4.48)
This gives the coefficient vector in the first sector. The value
of the coefficient vector in a given sector \( S \) is obtained by
applying \( M \) a total of \( S \) times so
\[ a_{\text{sector } S} = M^S a_k \]  \hspace{1cm} (5.4.49)
A matrix theorem states
\[ \text{trace } M = \lambda_k + \lambda_{-k} \]  \hspace{1cm} (5.4.50)
so
\[ \text{trace } M = 2 \cos(2\pi k/N) \]  \hspace{1cm} (5.4.51)
is the condition for bound states. The quantity \( k^* \) is written for
\( k \) and \( k \) is redefined as
\[ k = 2\pi k^*/N \]
Since \( \text{trace } M \) is a function of energy then call \( P(E) = \text{trace } M \) so
the bound state condition becomes
\[ P(E) = 2 \cos k \]  \hspace{1cm} (5.4.52)
Now it can be seen that all energy levels of the same ratio \( k^*/N \)
are the same so that all levels are doubly degenerate except for
\( k=0 \) and \( k=\pm1 \).

At this point using the bound state condition, energy levels
and wave functions for specific \( N \) and \( k \) values can be solved for.
<table>
<thead>
<tr>
<th>N</th>
<th>level</th>
<th>This work</th>
<th>exact (23), (24) Mathieu Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>0.6215109</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>1.9180610</td>
<td>1.91806</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>0.6215109</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>0.6441334</td>
<td>0.64413</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>1.6492793</td>
<td>1.64928</td>
</tr>
<tr>
<td></td>
<td>A</td>
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<td>1.91806</td>
</tr>
<tr>
<td>4</td>
<td>A</td>
<td>0.6215109</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>E</td>
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</tr>
<tr>
<td></td>
<td>A</td>
<td>0.6523310</td>
<td>0.65233</td>
</tr>
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<td></td>
<td>A</td>
<td>1.5947995</td>
<td>1.59480</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>1.7130943</td>
<td>1.71309</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>1.9180610</td>
<td>1.91806</td>
</tr>
</tbody>
</table>

/----

A non-degenerate level
E doubly degenerate level
/----

Table 5:
Energy levels for a ring potential consisting of N repeating potential wells of the form \( V(x) = 1 - \cos(x) \). Comparison between proposed method and exact method (based on Mathieu functions). For \( N = 2 \) take the A levels of the \( N = 4 \) case. While the Mathieu function method is restricted to sinusoidal potentials, non-symmetric and non-repetitive multiple potential wells can now be treated under the proposed method.
Table 5 shows the results for \( N=1 \) to \( N=4 \) for all possible energy levels compared to exact results \(^{(23)}\), \(^{(24)}\) obtained by directly solving the Schroedinger equation. Figure 5 gives the wave function for \( k=\pi/2 \) corresponding to an energy of \( E=1.713094 \) and figure 6 gives the wave function for \( k=2\pi/3 \) corresponding to an energy \( E=1.6492793 \).

It is clear, however, that equation \( (5.4.52) \) contains more information. The solid state limit of \( N\to\infty \) can be obtained by considering \( k \) a continuous variable. Thus a Brillouin zone plot of energy \( E \) as a function of \( k \) can be obtained here (see figure 7).

Energy bands will be formed whenever there are real valued solutions \( k \) to equation \( (5.4.52) \) (see figure 8). The order of the levels in each band alternate from band to band, so that \( k=0 \) is the lowest level in the lowest band, but the highest level in the next band and so on. Each band is made up of doubly degenerate levels, except for the levels at the band edge where \( k=0, \pi \). Thus the case \( N=1 \) yields the number of bands supported by the potential and with the addition of the \( N=2 \) case establishes the band edges. Higher \( N \)'s fill in the band with doubly degenerate levels (see figure 9).

By obtaining the function \( P(E) \) to a high accuracy in the region covered by the energy bands, the case of any integer \( N \) can be solved easily by high accuracy interpolation methods. The case of \( N=60 \), chosen for its large number of level subsets, is shown in table 6.

The bound state condition \( (5.4.52) \) is valid for any given sector potential repeated \( N \) times. Thus even non-symmetric sector
potentials can be solved in this way.
<table>
<thead>
<tr>
<th>k*</th>
<th>Lower Band</th>
<th>Upper Band</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.62151081</td>
<td>1.9180582</td>
</tr>
<tr>
<td>1</td>
<td>0.62158871</td>
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</tr>
<tr>
<td>2</td>
<td>0.62182174</td>
<td>1.9104128</td>
</tr>
<tr>
<td>3</td>
<td>0.62220790</td>
<td>1.9014304</td>
</tr>
<tr>
<td>4</td>
<td>0.62274387</td>
<td>1.8897618</td>
</tr>
<tr>
<td>5</td>
<td>0.62342502</td>
<td>1.8760388</td>
</tr>
<tr>
<td>6</td>
<td>0.62424537</td>
<td>1.8608387</td>
</tr>
<tr>
<td>7</td>
<td>0.62519767</td>
<td>1.8446484</td>
</tr>
<tr>
<td>8</td>
<td>0.62627337</td>
<td>1.8278616</td>
</tr>
<tr>
<td>9</td>
<td>0.62746266</td>
<td>1.8107895</td>
</tr>
<tr>
<td>10</td>
<td>0.62875450</td>
<td>1.7936772</td>
</tr>
<tr>
<td>11</td>
<td>0.63013666</td>
<td>1.7767181</td>
</tr>
<tr>
<td>12</td>
<td>0.63159578</td>
<td>1.7600663</td>
</tr>
<tr>
<td>13</td>
<td>0.63311742</td>
<td>1.7438464</td>
</tr>
<tr>
<td>14</td>
<td>0.63468617</td>
<td>1.7281606</td>
</tr>
<tr>
<td>15</td>
<td>0.63628576</td>
<td>1.7130943</td>
</tr>
<tr>
<td>16</td>
<td>0.63789916</td>
<td>1.6987199</td>
</tr>
<tr>
<td>17</td>
<td>0.63950874</td>
<td>1.6850997</td>
</tr>
<tr>
<td>18</td>
<td>0.64109648</td>
<td>1.6722884</td>
</tr>
<tr>
<td>19</td>
<td>0.64264409</td>
<td>1.6603339</td>
</tr>
<tr>
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<td>0.64413334</td>
<td>1.6492792</td>
</tr>
<tr>
<td>21</td>
<td>0.64554622</td>
<td>1.6391625</td>
</tr>
<tr>
<td>22</td>
<td>0.64686524</td>
<td>1.6300182</td>
</tr>
<tr>
<td>23</td>
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<td>1.6219768</td>
</tr>
<tr>
<td>24</td>
<td>0.64915602</td>
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</tr>
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<td>25</td>
<td>0.65009792</td>
<td>1.6087075</td>
</tr>
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<td>26</td>
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</tr>
<tr>
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<td>1.5953600</td>
</tr>
<tr>
<td>30</td>
<td>0.65233091</td>
<td>1.5948000</td>
</tr>
</tbody>
</table>

Table 6:

Energy levels of an N-fold periodic sinusoidal ring potential $V(x) = 2m\hbar^2 (1 - \cos x)$ for $N = 60$ and $2m\hbar^2 = 1$. All levels are doubly degenerate, except the levels for $k* = 0$ and $k* = 30$ which are the ones at the band limit. Certain values of $N < 60$ yield appropriate subsets of the above list. Starting with $k* = 0$, increment $k*$ by $\Delta k* = 60/N$ until $k* = 30$ is surpassed. Thus, this table is valid for $N = 1, 2, 3, 4, 5, 6, 10, 12, 15, 20$ and 30.
Appendix A

Minimization of \( u''/u \)

The calculus of variations can be used to minimize the square of the quantity \( u''/u = W-zz'' \) over the interval \((x_1, x_2)\). Define the integral \( I \) as

\[
I = \int_{x_1}^{x_2} (W(x) - z(x)z'(x)^2)^2 \, dx \tag{A.1}
\]

subject to the conditions put on by the solution of the transformation equation

\[
u''/u - (W-zz') = 0 \tag{A.2}
\]

\[
u - (z')^{-2} = 0 \tag{A.3}
\]

The overall function to minimize \( \phi(x, z, z', u, u', u'') \) thus becomes

\[
\phi = (W-zz')^2 + \lambda_1 (u''/u - (W-zz')) + \lambda_2 (u - (z')^{-2}) \tag{A.4}
\]

for the Lagrange multipliers \( \lambda_1, \lambda_2 \).

The Euler equations to solve are

\[
\phi_z = (d/dx)\phi_{z'} = 0 \tag{A.5}
\]

\[
\phi_u - (d/dx)\phi_u' + (d/dx)^2 \phi_{u''} = 0 \tag{A.6}
\]

The needed partial derivatives of \( \phi \) are

\[
\phi_z = 2(W-zz')(z')^2 + \lambda_1 (z')^2 \tag{A.7}
\]

\[
\phi_{z'} = 2(W-zz')(z''z ') + \lambda_1 (2zz') + \lambda_2 (z')^{-3/2} \tag{A.8}
\]

\[
\phi_u = -\lambda_1 u'^{-2} + \lambda_2 \tag{A.9}
\]

\[
\phi_u' = 0 \tag{A.10}
\]

\[
\phi_{u''} = \lambda_1 u'^{-1} \tag{A.11}
\]

In this case, use the so-called natural boundary conditions

\[
\phi_z(x_{\text{end}}) = \phi_u''(x_{\text{end}}) = 0 \tag{A.12}
\]

for \( x_{\text{end}} = x_1 \) or \( x_{\text{end}} = x_2 \). The Lagrange multiplier functions thus have the value
\[ \begin{align*}
\lambda_1 &= 0 \quad \text{(if } u \neq 0) \quad \text{(A.13)} \\
\lambda_2 &= 8(\omega-\omega'^2)z(z')^{-5/2} \quad \text{(A.14)}
\end{align*} \]

at the endpoints \( x_1 \) and \( x_2 \).

Substituting (A.7) to (A.10) into (A.5) and (A.6) gives the differential equations

\[ \begin{align*}
-2(\omega-\omega'^2)z'^2 + \lambda_1 z'^2 & \quad \text{(A.15)} \\
-(d/dx)[4z(\omega-\omega'^2) + 2\lambda_1 \omega' + \lambda_2 z'^{-3/2}] &= 0 \\
-\lambda_1 u'u'^{-2} + \lambda_2 + (d/dx)^2[\lambda_1 u^{-1}] &= 0 \quad \text{(A.16)}
\end{align*} \]

Although the \( \lambda \)'s are in theory now specified, in practice their solution is extremely difficult. In order to solve (A.15) and (A.16) the transformation functions \( z, z', u, u', u'' \) must be known not only as functions of \( x \) but also functions of the starting conditions. This is clearly enormously more difficult than the current problem of determining the transformation functions for one given starting condition. When this was realized, the idea was not pursued further.
Appendix B

Computer Program using the Transformation Method

The following program solves for the energy level and the wave function of the ground state \((n=0)\) of the Eckart potential using the coupled differential method discussed in section 4.3. The model equation in all regions is the Airy equation thus solutions are in terms of the Airy function \(Ai, Bi\). A brief explanation of the program follows. Modifications needed for use with a different potential are also discussed.

The 'MAIN' program searches for a change in sign of the value of \(m_{21}\) as given by the function COND. When an interval where the sign changes is identified, the routine CONVER uses a modified Newton method to converge on the energy which makes \(m_{21}=0\). This energy value is used by the program WAVE to calculate the final wave function.

The function COND consists of two sections. The first half of the routine determines the regions and then for each region calls the routine SUBPOT to solve the coupled differential equations to obtain the transformation functions. The last half of the routine uses the endpoints of the regions to form the appropriate match matrix, taking into account regional coordinates. These matrices are multiplied together to get the overall match matrix and hence the value of \(m_{21}\).

Most of the remaining routines are self explanatory. The Airy function routine is based on an expansion of Chebyshev polynomials. Regular polynomial expansions can be found in references (1) and (2).

If the solution of a different potential is desired, certain
changes have to be made to the program. First of all, the potential and its derivatives must be available from \( V, V_P, V_{PP} \).

Major changes are needed in the COND routine to tell the program where the new arbitrarily defined regions are to be. Also changes often have to be made in MAIN to change the upper and lower limits of the search. Other minor changes may need to be done in TITLE, WAVE, and the routines used to calculate the exact value of the wave function if that is desired.
//ECKART JOB (XXXXXXXXXXX), 'ED BREWER'
// EXEC WATFIV
// GO.SYSIN DD %
$JOB WATFIV XXXXXXXXXX BREWER
C
MAIN
IMPLICIT REAL*8 (A-H, O-Z)
EXTERNAL COND
COMMON /POTENT/ ACOEFF, BCOEFF, EEXACT, NLEVEL
REAL*8 ACOEFF/-1.92200/, BCOEFF/-11.2000/
REAL*8 PI/3.14159265358979/, ACCUR/1.0D-8/

C
WMAX=ACOEFF-ACCUERR
WMIN=.2500*(ACOEFF+BCOEFF)**2/BCOEFF+ACCUERR
NLEVEL=1
CALL INIT

C
WMESH=DABS(WMIN-WMAX)/20.D0
WNEW=WMIN
WOLD=0
COLD=0

C
FIND AN AREA WHERE THE CONDITION CHANGES SIGN

C
WHILE (DABS(WMAX-WOLD).GT.1.D-14) DO
CNEW=COND(WNEW)
CALL WAVE(WNEW)
PRINT,’W=’,WNEW,’COND=’,CNEW
C
CONVERGE TO THE ZERO POINT IN THE SIGN CHANGE REGION

C
IF (COLD/CNEW,LT.0) THEN DO
CALL CONVER(COND,CNEW,WNEW,COLD,WOLD,0.D0,ACCUR,CBEST,WBEST)
CALL WAVE(WBEST)
STOP
END IF
WOLD=WNEW
COLD=CNEW
WNEW=WNEW+DMIN(DABS(WMAX-WNEW),WMESH)
END WHILE
STOP
END
C
FUNCTION COND(ENER)
C
CALCULATE THE VALUE OF M(2,1) SINCE THE EIGENVALUE CONDITION
IS M(2,1)=0
C
NOTE THAT THE ZEDUAL COMMON AREA CONTAINS INFORMATION
ABOUT ALL OF CALCULATED REGIONS:
C
ENERGY --- ENERGY AT WHICH Z, U, UP VALUES ARE CALCULATED
MAP(N) --- TYPE OF REGION N
TRANSF(N,M) --- TRANSFORMATION INFO FOR REGION N

60
GLOBAL X=TRANSF(N,1)+TRANSF(N,2)*LOCAL X
MATCH(N,I,J) -- MATCH MATRIX FOR REGION N
MAXREG ------- MAXIMUM NUMBER OF REGIONS

Each integration using SUBPOT will calculate values of 
Z,U,UP which depend only on the energy adjusted potential 
W(X) (where X is a local X). Different potentials W(X) 
define different "types" of regions. Often different regions 
will have the same W(X) so, instead of recalculation, those 
regions are assigned (in the vector "MAP") the same type as 
the first.

ZED(I,J,K) -- I=REGION TYPE
   --- J=VALUES OF X,Z,U,UP
      J=1 IS LOCAL X
      J=2 IS Z
      J=3 IS U
      J=4 IS UP
   --- K=POINT #

NP(I)------- NUMBER OF POINTS IN ZED(I,J,K) IN REGION TYPE I
ORDER(I)----- ORDERING OF POINTS IN ZED(I,J,K) IN REGION TYPE I
             ORDER(I)=+1 IF POINTS ORDERED SMALLEST TO LARGEST
             ORDER(I)=-1 IF POINTS ORDERED LARGEST TO SMALLEST
MAXTYP ------ MAXIMUM NUMBER OF REGION TYPES
MAXPT ------ MAXIMUM NUMBER OF POINTS IN A REGION

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ERROR/ IERROR
COMMON /POTENT/ ACOEFF,SCOEFF,EXACT,NLEVEL
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
INTEGER MAXTYP/20/,MAXREG/20/,MAXPT/20/
REAL*8 B(2,2),B1(2,2),M(2,2)
REAL*8 ONE(2,2)/1.D0,0.D0,0.D0,1.D0/
CALCULATE Z, U, UP FOR RIGHT REGION

XSTART=6.0D0
XEND=XCUT-XRIGHT
CALL INTER(XSTART,XEND,XRIGHT,1.0D0)

CALCULATE Z, U, UP FOR LEFT REGION

XSTART=4.0D0
XEND=XLEFT-XCUT
CALL INTER(XSTART,XEND,XLEFT,-1.0D0)

CALCULATE THE OVERALL MATCH MATRIX AND ASSIGN REGION TYPES

LASREG=REGION-1

CALCULATE MATRIX IN FIRST REGION

REGION=1
CALL ENDMAT(B,BI,+1,IER)
IF (IER.NE.0) RETURN
CALL MATMUL(M,B,ONE)
REGION=REGION+1

MULTIPLY BY B\times B INVERSE) UNTIL LAST REGION

WHILE (REGION.LT.LASREG) DO
CALL ENDMAT(B,BI,+1,IER)
IF (IER.NE.0) RETURN
CALL MATMUL(M,BI,M)
EXECUTE SMATCH
CALL MATMUL(M,B,M)
REGION=REGION+1
END WHILE

CALCULATE MATRIX FOR LAST REGION

REGION=LASREG
CALL ENDMAT(B,BI,+1,IER)
IF (IER.NE.0) RETURN
CALL MATMUL(M,BI,M)
EXECUTE SMATCH

IERERROR=0
PRINT, 0
PRINT, 'M MATRIX='
CALL MATPR(M)
COND=M(2,1)
RETURN

REMOTE BLOCKS

REMOTE BLOCK SMATCH
DO 11 IVAL=1,2
DO 11 JVAL=1,2
MATCH(REGION-1,IVAL,JVAL)=M(IVAL,JVAL)
END BLOCK
END

SUBROUTINE INTER(XFIRST,XLAST,SHIFT,SENSE)

ROUTINE TO CALCULATE Z,U,UP OVER SOME INTERVAL

NOTE: NEW REGIONS MAY BE INVOKED IF CONDITION DESCRIBED IN ULIMIT IS VIOLATED

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
X
MAP,NP,ORDER,REGION,TYPE,MAXREG,MAXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
REAL*8 PAR(10)
INTEGER NPOINT/10/
EXTERNAL ZEROPTH,ULIMIT

STEP=DABS(XFIRST-XLAST)/NPOINT
XSTART=XFIRST
XEND=XLAST
INTREG=REGION

IER=-1
WHILE (IER.NE.0) DO
EXECUTE NEWREG

IF DELTA U CANNOT BE MADE EQUAL TO 0 AT A POINT THEN
START INTEGRATION AT 0 AND GO TO THAT POINT

IF (IER.EQ.2) THEN DO
MIDREG=REGION
XSTART=0
XEND=ZED(MAP(REGION-1),1,NP(MAP(REGION-1)))

MAKE SURE END POINT IS POSITIVE

WHILE (XEND.LT.0) DO
PRINT,'FORCED TO STEP BACK ONE POINT'
NP(MAP(REGION-1))=NP(MAP(REGION-1))-1
XEND=ZED(MAP(REGION-1),1,NP(MAP(REGION-1)))
END WHILE
PRINT,'STARTING AT ZERO'

INTEGRATE OUT TO XEND MAKING NEW REGIONS AS NECESSARY

EXECUTE NEWREG

PUT REGIONS BACK IN CORRECT ORDER

CALL SWITCH(MIDREG,LASREG)
CONTINUE OLD INTEGRATION FROM ZERO

PRINT,'OLD INTEGRATION CONTINUES'
XSTART=0
XEND=XLAST
END IF

END WHILE

SWITCH ORDER OF REGIONS IF IN NEGATIVE SENSE AREA

IF (SENSE.LT.0) CALL SWITCH(INTREG,LASREG)
RETURN

REMOTE BLOCK NEWREG

PROCEDURE TO CHOOSE ARGUMENTS FOR AND EXECUTE ROUTINE SUBPOT

IER=-1
WHILE (IER.NE.0.AND.IER.NE.2) DO

TRANSF(REGION,1)=SHIFT
TRANSF(REGION,2)=SENSE

IF (IER.EQ.1) THEN DO
MR=MAP(REGION-1)
XSTART=ZED(MR,1,NP(MR))
Z =ZED(MR,2,NP(MR))
U =ZED(MR,3,NP(MR))
UP =ZED(MR,4,NP(MR))
IOP=2
ELSE DO
IOP=1
ENDIF

CALL SUBPOT(XSTART,XEND,STEP,Z,U,UP,ZEROTH,ULIMIT,PAR,IOP,IER)

IF (IER.NE.2) THEN DO
MAP(REGION)=TYPE
LASREG=REGION
TYPE=TYPE+1
REGION=REGION+1
ENDIF

END WHILE
END BLOCK
END

SUBROUTINE SWITCH(IREG,LREG)

REVERSE THE ORDER OF REGIONS IREG THROUGH LREG

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
X MAP,NP,ORDER,REGION,TYPE,MAXREG,MAXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)

IF (LREG.GT.IREG) THEN DO
  I=IREG
  L=LREG
ELSE DO
  I=IREG
  L=IREG
END IF

WHILE (L.GT.I)
  ISAVE=MAP(I)
  MAP(I)=MAP(L)
  MAP(L)=ISAVE
  I=I+1
  L=L-1
END WHILE
RETURN
END

SUBROUTINE ENDMAT(B,BI,ISW,IER)

CALCULATE THE B AND B INVERSE MATRICES AT END POINTS

IMPLICIT REAL*8(A-H,O-Z)
REAL*8 B(2,2),BI(2,2)
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
X MAP,NP,ORDER,REGION,TYPE,MAXREG,MAXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
INTEGER RIGHT,LEFT,PB,PBI

FIND RIGHT AND LEFT ENDPOINTS OF EACH REGION
  USING TRANSF(REGION,2)*(POINT ORDERING OF REGION)

MR=MAP(REGION)
RIGHT=LEFT=1
IF (TRANSF(REGION,2)*ORDER(MR).GT.0) THEN DO
  RIGHT=NP(MR)
ELSE DO
  LEFT=NP(MR)
END IF

IF ISW=+1 THEN CALCULATE B AT LEFT ENDPOINT
  AND B INVERSE AT RIGHT ENDPOINT
IF ISW=-1 THEN CALCULATE B AT RIGHT ENDPOINT
  AND B INVERSE AT LEFT ENDPOINT
IF (ISW.EQ.1) THEN DO
PB =LEFT

PBI=RIGHT
ELSE DO
PB =RIGHT
PBI=LEFT
END IF

CALL BMAT(B,ZED(MR,2,PB),ZED(MR,3,PB),ZED(MR,4,PB),
TRANSF(REGION,2),IER)
IF (IER.NE.0) RETURN
CALL BIMAT(BI,ZED(MR,2,PBI),ZED(MR,3,PBI),ZED(MR,4,PBI),
TRANSF(REGION,2),IER)
RETURN
END

FUNCTION WAVEF(N(X))

CALCULATE THE EXACT WAVEFUNCTION (HYPERGEOMETRIC FUNCTIONS)

IMPLICIT REAL*8(A-H,O-Z)
COMMON /EXWAVE/ WNORM,ALPHA,BETA,AW,BW,CW,N
Y=1.D0/(1.D0+DEXP(X))
FACTOR=Y**BETA**(1.D0-Y)**(A+B)
HYPER=TERM**1.D0
IF (N.NE.0) THEN DO
A=A+1.D0
B=B+1.D0
C=C+1.D0
HYPER=HYPER**TERM
END IF
WAVEF=WAVEF*FACTOR*HYPER
RETURN
END

SUBROUTINE INIT
IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/ ACOEFF,BCOEFF,EXACT,NLEVEL
COMMON /EXWAVE/ WNORM,ALPHA,BETA,AW,BW,CW,N

BETA(N(X),B)=DZGAMA(A)*DZGAMA(B)/DZGAMA(A+B)

N=NLEVEL
ELEVEL=2.D0*NLEVEL+1.D0
T=.25D0*(DSQRT(1.D0-4.D0*BCOEFF)-ELEVEL)**2
EXACT=-.25D0*(T-ACOEFF)**2/T

CALCULATE VARIOUS CONSTANTS ASSOCIATED WITH
A PARTICULAR VALUE OF N

ALPHA=DSQRT(-EXACT)
BETA=DSQRT(ACOEFF-EEXACT)
N=1.
BW=ALPHA+BETA+.5D0*(1.D0+DSQRT(1.D0-4.D0*BCOEFF))
CW=1.D0+2.D0*BETA

WINORM IS THE NORMALIZATION FACTOR

WINORM=BETAFN(2.D0*BETA,2.D0*ALPHA)
IF (N.EQ.1) THEN DO
WINORM=WINORM-2.D0*BW*BETAFN(2.D0*BETA+1.D0,2.D0*ALPHA)/CW
WINORM=WINORM+BW**2*BETAFN(2.D0*BETA+2.D0,2.D0*ALPHA)/CW**2
END IF
WINORM=1.D0/DSQRT(DABS(WINORM))
RETURN
END

SUBROUTINE ENDPT(ENERGY,XRIGHT,XLEFT,XMIN,IER)

CALCULATE THE TURNING POINTS FOR A GIVEN VALUE OF ENERGY
ALSO XMIN=THE VALUE OF X WHERE THE MINIMUM OF
POTENTIAL OCCURS

IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/ ACOEFF,BCOEFF,EEXACT,NLEVEL
AX=ACOEFF-ENERGY
BX=2.D0*ENERGY-ACOEFF-BCOEFF
CX=ENERGY
IER=1
DISC=BXX**2-4.D0*AX*CX
IF (DISC.LT.0) RETURN
ROOT=DSQRT(DISC)
XE1=(-BX-ROOT)/2.D0/AX
XE2=(-BX+ROOT)/2.D0/AX
IF (XE1.GE.0.OR.XE2.GE.0) RETURN
XRIGHT=DLOG(-XE1)
XLEFT=DLOG(-XE2)
XMIN=DLOG((BCOEFF+ACOEFF)/(BCOEFF-ACOEFF))
IER=0
RETURN
END

FUNCTION V(X)

CALCULATE THE VALUE OF THE POTENTIAL AT THE GLOBAL X

IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/ ACOEFF,BCOEFF,EEXACT,NLEVEL
ZETA=DEXP(X)
FACTOR=ZETA/(1.D0-ZETA)
V=-ACOEFF*FACTOR-BCOEFF*FACTOR/(1.D0-ZETA)
RETURN
END

FUNCTION VP(X)
CALCULATE THE 1ST DERIV OF THE POTENTIAL AT THE GLOBAL X

IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/, ACOEFF, BCOEFF, EEXACT, NLEVEL
ZETA=-DEXP(X)
FACTOR=ZETA/(1.0D0-ZETA)
VP=(V(X) - BCOEFF*FACTOR*X2)/(1.0D0-ZETA)
RETURN
END

FUNCTION VPP(X)

CALCULATE THE 2ND DERIV OF THE POTENTIAL AT THE GLOBAL X

IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/, ACOEFF, BCOEFF, EEXACT, NLEVEL
ZETA=-DEXP(X)
FACTOR=ZETA/(1.0D0-ZETA)
VPP=2.0D0*(VP(X) - BCOEFF*FACTOR*X3/ZETA*X2)/(1.0D0-ZETA)
RETURN
END

SUBROUTINE WAVE(ECALC)

CALCULATE THE WAVE FUNCTION

IMPLICIT REAL*8(A-H,O-Z)
COMMON /POTENT/, ACOEFF, BCOEFF, EEXACT, NLEVEL
COMMON /ZEDUAL/ ENERGY, ZED, TRANSF, MATCH,
X MAP, NP, ORDER, REGION, TYPE, MAXREG, MAXTYP, MAXPT,
INTEGER REGION, TYPE, MAP(20), NP(20), ORDER(20)
REAL*8 ZED(20, 4, 20), TRANSF(20, 2), MATCH(20, 2, 2)
REAL*8 B(2, 2), A(2)

CALL TITLES(ECALC)

CHOOSE COEFFICIENT VALUES IN REGION 1 TO BE (1,0)
A(1)=1.0D0
A(2)=0.0D0

RUN OVER ALL REGIONS

IMAX=REGION
DO 1 IREG=1, IMAX

CALCULATE WAVE FUNCTION IN AT EACH POINT IN REGION

NT=NP(MAP(IREG))
MREG=MAP(IREG)
DO 2 N=1, NT
NN=N
IF (TRANSF(IREG, 2)*ORDER(MREG), GT, 0) NN=NT-N+1
CALL BMAT(B,ZED(MREG,2,NN),ZED(MREG,3,NN))
X,ZED(MREG,4,NN),TRANSF(IREG,2),IER)
WAVEF=A(1)*X*B(1,1)+A(2)*X*B(1,2)
X=TRANSF(IREG,1)+ZED(MREG,1,NN)*TRANSF(IREG,2)
CALL WAVEOUT(X,WAVEF,ZED(MREG,2,NN),ZED(MREG,3,NN),ENERGY)
CONTINUE

WRITE(6,200) A
200 FORMAT(''/'',''A(1)=''''D22.12,'''A(2)=''''D22.12,/)'''

GET COEFFICIENTS FOR NEXT REGION

IF (IREG.NE.IMAX) THEN DO
A(1)=MATCH(IREG,1,1)
A(2)=MATCH(IREG,2,1)
END IF

GO TO NEXT REGION

CONTINUE

RETURN

END

SUBROUTINE TITLES(ECALC)
IMPLICIT REAL*8(A-H,O-Z)
COMMON /Potent/Acoeff,Bcoeff,Eexact,Nlevel

WRITE(6,10) NLEVEL
10 FORMAT(''/'',''WAVEFUNCTIONS OF ECKART POTENTIAL FOR N='''I2)'''

PRINT TITLES'''

WRITE(6,120) Eexact
120 FORMAT(''AND FOR EXACT ENERGY LEVEL=''''F15.10)'''
WRITE(6,100) ECALC
100 FORMAT(''WITH CALCULATED ENERGY LEVEL=''''F15.10/)'''
WRITE(6,101)
101 FORMAT(''7X,'''7X,2X,'''CALCULATED',3X,
X 8X,'''Z',8X,5X,'''SMALL U',5X,
X ,8X,'''U',8X,8X,1X,'''W',8X)

RETURN

END

SUBROUTINE WAVOUT(X,WAVEF,Z,U,ENERGY)

PRINT OUT THE CALCULATED WAVE FUNCTIONS

IMPLICIT REAL*8(A-H,O-Z)
ZP=1.00/UX*X2
WRITE(6,1) X,WAVEF,Z,U,Z/UX*X4,V(X)-ENERGY
1 FORMAT(1X,F12.7,3X,1(I1D14.7,1X),4(D17.10))
RETURN

END
SUBROUTINE BMAT(BM,Z,U,UP,XSIGN,IER)

CALCULATE THE B MATRIX GIVEN THE Z,U,UP VALUES

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION BM(2,2)

XSIGN IS THE ORIENTATION OF THE LOCAL X RELATIVE TO
THE GLOBAL X (+1 FOR SAME,-1 FOR OPPOSITE)

CALL AIRY(AI,BI,AIP,BIP,Z,IER)
IF (IER.NE.0) RETURN
BM(1,1)=UXAI
BM(1,2)=UXBI
BM(2,1)=XSIGN*(UP*AI+AIP/U)
BM(2,2)=XSIGN*(UP*BI+BIP/U)
RETURN
END

SUBROUTINE BIMAT(BIM,Z,U,UP,XSIGN,IER)

CALCULATE THE B INVERSE MATRIX GIVEN THE Z,U,UP VALUES

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION BIM(2,2)
REAL*8 PI/3.14159265358979/

XSIGN IS THE ORIENTATION OF THE LOCAL X RELATIVE TO
THE GLOBAL X (+1 FOR SAME,-1 FOR OPPOSITE)

CALL AIRY(AI,BI,AIP,BIP,Z,IER)
IF (IER.NE.0) RETURN

WRONSK= INVERSE OF THE WRONSKIAN OF THE AIRY FUNCTIONS (1/PI)

WRONSK=XSIGN*PI
BIM(1,1)= XSIGN*(UP*BI+BIP/U)*WRONSK
BIM(1,2)=-(UXBI)*WRONSK
BIM(2,1)=-XSIGN*(UP*AI+AIP/U)*WRONSK
BIM(2,2)=(UXAI)*WRONSK
RETURN
END

SUBROUTINE MATMUL(A,B,C)

DO A 2 BY 2 MATRIX MULTIPLICATION A=B*C

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION A(2,2),B(2,2),C(2,2),TEMP(2,2)
DO 1 I=1,2
DO 1 J=1,2
TEMP(I,J)=0.DO
DO 1 K=1,2
1 TEMP(I,J)=TEMP(I,J)+B(I,K)*C(K,J)
DO 2 I=1,2
DO 2 J=1,2
A(I,J)=TEMP(I,J)
RETURN
END

SUBROUTINE MATPRT(A)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION A(2,2)
WRITE(6,1) ((A(I,J),J=1,2),I=1,2)
1 FORMAT(2(' ',D22.12,3X,D22.12,' /'))
RETURN
END

SUBROUTINE SUBPOT(XSTART,XEND,STEP,Z,U,UP,ICOND,ERCOND,PAR
,IOPIER)

CALCULATE THE Z VALUES FOR THE ENERGY NOW IN COMMON
STARTING INTEGRATION AT XSTART AND GOING TO XEND

IMPLICIT REAL*8 (A-H,O-Z)
REAL*4 EPS/1E-6/,STEP*8/10.D0/,HMAX*8
DIMENSION Y(5),DY(5),PAR(10)
EXTERNAL LANGER

FIND THE INITIAL CONDITIONS USING ROUTINE ICOND

IF (IOPIER.EQ.2) RETURN

USING ZP=1/U**2, SET UP INITIAL CONDITIONS FOR NEW
EQUATIONS WHERE U=Y(1),UP=Y(2),Z=Y(3)
AND Y(4)=INTEGRAL OF (DELTA U)**2

Y(1)=U
Y(2)=UP
Y(3)=Z
Y(4)=0.00
X=XSTART

PRINT, '
PRINT,'AT UPPER POINT'
PRINT,'Z=',Z
PRINT,'U=',U,'UP=',UP

LOOP CONDITIONS

H=(XEND-XSTART)/STEP
HMAX=DABS(H)
IER=-1
CALL ERECOND(X,Y,PAR,IER)

N=4 IF INTEGRAL OF DELTA U SQUARED WANTED
N=3 IF NOT
N=3

LOOP

WHILE (DABS(XEND-X) GT.1.D-14.AND.IER.EQ.0) DO
  H=DSIGN(DMIN1(DABS(H),DABS(XEND-X),DABS(HMAX)),H)
  PRINT
  PRINT,'X=',X
  PRINT,'Z=',Y(3)
  PRINT,'U=',Y(1),',UP=',Y(2)
  CALL SAVZED(X,Y,PAR)
  CALL DDFSYS(N,LANGER,EPS,H,X,Y,PAR)
  CALL ERCOND(X,Y,PAR,IER)
END WHILE

THE VALUES OF Z,U,UP,ZP,ZPP AT THE END POINT ARE NOW KNOWN

PRINT
IF (IER.NE.0) THEN DO
PRINT, 'CONDITION FORCED PREMATURE END OF REGION AT'
ELSE DO
PRINT, 'AT LOWER POINT'
END IF
U=Y(1)
UP=Y(2)
Z=Y(3)
PRINT,'Z=',Z
PRINT,'U=',U',UP=',UP
RETURN
END

SUBROUTINE SAVZED(X,Y,PAR)
SAVE VALUES OF U,Z,ZP ETC. NEEDED LATER TO CALCULATE THE
WAVEFUNCTION

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ZEDVAL/,ENERGY,ZED,TRANSF,MATCH,
   X MAP,NP,ORDER,REGION,TYPE,MAXREG,MAXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
DIMENSION Y(5),DY(5),PAR(10)

IF (NP(TYPE).LT.MAXPT) NP(TYPE)=NP(TYPE)+1
N=NP(TYPE)
IF (N.EQ.2) THEN DO
  IF (X.GE.ZED(TYPE,1,1)) THEN DO
      ORDER(TYPE)=+1
   ELSE DO
      ORDER(TYPE)=-1
  END IF
END IF
ZED(TYPE,1,N)=X
ZED(TYPE,2,N)=Y(3)
ZED(TYPE,3,N)=Y(1)
ZED(TYPE,4,N)=Y(2)
RETURN
END

SUBROUTINE ULIMIT(X,Y,PAR,IER)
CHECK IF INTEGRATION SHOULD BE STOPPED AND
A NEW REGION STARTED

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION Y(5),YSAVE(5),PAR(10)
DATA RANGE/2.0D0/

IF IER=-1 ON ENTRANCE THEN USE X,Y,PAR VALUES
TO SET LIMITS

IER=0
U=Y(1)
IF (IER.EQ. -1) THEN DO
U_UPPER=U*RANGE
U_LOWER=U/RANGE
ELSE DO
IF (U.GT.U_UPPER,OR.U.LT.U_LOWER) IER=1
END IF
RETURN
END

SUBROUTINE ZEROTH(XSTART,XEND,Z,U,UP,PAR,IOP,IER)
GET THE INITIAL CONDITIONS AT XSTART USING THE ZERO TH ORDER
APPROXIMATION ZXZP**2=W(X),U=1/Z**2 (DELTA U=0)

ON ENTRANCE IOP=1  --> INTEGRATE FROM 0 TO XSTART
TO FIND VALUES OF Z,U,UP
IOP=2  --> USE THE VALUE OF Z TO GET
VALUES OF U,UP

NOTE: IF XSTART=0 THEN VALUES OF Z,U,UP ARE FROM
ABOVE EQUATION EVALUATED IN THE LIMIT AS
X APPROACHES ZERO.

IMPLICIT REAL*8 (A-H,O-Z)
REAL*4 EPS/1E-5/
DIMENSION Y(5),DY(5),PAR(10)
EXTERNAL ZPRIME

IER=0
IF (XSTART.EQ.0) THEN DO
Z=0
ZP=W0*DO)**(1.DO/3.DO)
ZPP = ZP*WP(0.0)/((3.0*WP(0.0))
U = 1.0/ZP**2
UF = -.5D0*ZPP*UX**3
RETURN
END IF

IF (IOP.EQ.1) THEN DO

FIRST FIND THE VALUE OF Z,ZPRIME AT XSTART

X = .001D0*XSTART
Y(1) = X*WP(0.0)**(1.0/3.0)
H = .1D0*XSTART
N = 1

INTEGRATE FROM 0 TO XSTART VIA ROUTINE DDFSYS

WHILE ((ABS(XSTART-X) .GT. 1.0D-14) DO
H = DSIGN(DMIN1(ABS(H),DABS(XSTART-X)),H)
CALL DDFSYS(N,ZPRIME, EPS,H,X,Y,PAR)
END WHILE

Z = Y(1)
END IF

IF (IOP.EQ.2) THEN DO
IF (W(XSTART)/2.GT.0) THEN DO
X = XSTART
Y(1) = Z
ELSE DO
IER = 2
RETURN
END IF
END IF

CALL ZPRIME(X,Y,DY,PAR)
ZP = DY(1)
ZPP = .5D0*ZP*(WP(X)/W(X)-ZP/Z)
U = 1.0/DSQRT(ZP)
UF = -.5D0*ZPP*UX**3
RETURN
END

FUNCTION W(X)

CALCULATE THE VALUE OF THE POTENTIAL AT A LOCAL COORD X

IMPLICIT REAL*8(A-H,S-Z)
COMMON /ZEDUAL, ENERGY, ZED, TRANSF, MATCH,
X MAP, NP, ORDER, REGION, TYPE, MAXREG, MAXTYP, MAXPT
INTEGER REGION, TYPE, MAP(20), NP(20), ORDER(20)
REAL*8 ZED(20,4,20), TRANSF(20,2), MATCH(20,2,2)
W = U*(TRANSF(REGION,1)+TRANSF(REGION,2)**2-ENERGY
RETURN

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FUNCTION WP(X)

CALCULATE THE 1ST DERIV OF THE POTENTIAL AT A LOCAL COORD X

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
X MAP,NP,ORDER,REGION,TYPE,MAXREG,MXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
WP=TRANSF(REGION,2)XVP(TRANSF(REGION,1)+TRANSF(REGION,2)XX)
RETURN
END

FUNCTION WPP(X)

CALCULATE THE 2ND DERIV OF THE POTENTIAL AT A LOCAL COORD X

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ZEDVAL/ENERGY,ZED,TRANSF,MATCH,
X MAP,NP,ORDER,REGION,TYPE,MAXREG,MXTYP,MAXPT
INTEGER REGION,TYPE,MAP(20),NP(20),ORDER(20)
REAL*8 ZED(20,4,20),TRANSF(20,2),MATCH(20,2,2)
WPP=UPP(TRANSF(REGION,1)+TRANSF(REGION,2)XX)
RETURN
END

CPRINTOFF

SUBROUTINE CONVER(FUN,HI,XHI,LOH,XLOH,TARGET,TOL,BEST,XBEST)

ROUTINE TO FIND X GIVEN F(X)

ON ENTRANCE
  FUN = FUNCTION F
  XHI = AN UPPER BOUND FOR X
  HI = F(XHI)
  XLOH = A LOWER BOUND FOR X
  LOH = F(XLOH)
  TARGET = THE GIVEN F(X)
  TOL = RELATIVE TOLERANCE

ON EXIT
  XBEST = AN ESTIMATE OF THE TARGET X WITHIN TOLERANCE
          BOUNDS
  BEST = F(XBEST)

NOTE:
(1)  TARGET-TOL < BEST < TARGET+TOL
(2)  FUNCTION FUN SHOULD PLACE VALUES IN COMMON ERROR
        IF NO ERROR    ==> IERROR=0
        IF ERROR       ==> IERROR=1

IMPLICIT REAL*8(A-H,O-Z)
COMMON /ERROR/IERROR
REAL*8 LOH, LOW, LOWER
DATA MAXISW/2/

INITIALIZE

IF (HI.GT.TARGET) THEN DO
  HIGH=HI
  XHIGH=XHI
  LOW=LOH
  XLOW=XLOH
ELSE DO
  HIGH=LOH
  XHIGH=XLOH
  LOW=HI
  XLOW=XHI
END IF

LOWER=TARGET-TOL
UPPER=TARGET+TOL
BEST=2.DOXUPPER
IVAL=ISW=0

LOOP

WHILE (BEST.LT.LOWER.OR.BEST.GT.UPPER.OR.ISW.EQ.0) DO
  XBEST=XLOW+(TARGET-LOW)*(XHIGH-XLOW)/(HIGH-LOW)
  BEST=FUN(XBEST)
  IVAL=IVAL+1
  WRITE(6,10) XBEST,BEST,XHIGH,HIGH,XLOW,LOW
  FORMAT(9X,'XBEST=','D22.10,',BEST=','D22.10,/
         X'XHIGH=','D22.10,',HIGH=','D22.10,/
         X'XLOW=',D22.10,',LOW=',D22.10,/
         X')
  IF (BEST.LT.LOW.OR.BEST.GT.HIGH) IERROR=2
  IF (IERROR.NE.0) RETURN
  IF (BEST.GE.TARGET) THEN DO
    IF (ISW.NE.MAXISW) THEN DO
      IF (ISW.LT.0) ISW=0
      ISW=ISW+1
    ELSE DO
      ISW=0
      XLOW=XBEST-(XHIGH-XBEST)
      LOW=FUN(XLOW)
      IVAL=IVAL+1
    END IF
    HIGH=BEST
    XHIGH=XBEST
  ELSE DO
    IF (ISW.NE.-MAXISW) THEN DO
      IF (ISW.GT.0) ISW=0
      ISW=ISW-1
    ELSE DO
      ISW=0
      XHIGH=XBEST+(XBEST-XLOW)
      HIGH=FUN(XHIGH)
      IVAL=IVAL+1
    END IF
  END IF

76
END IF
LOW=BEST
XLOW=XBEST
END IF
END WHILE

C
WRITE(6,40) IVAL
40 FORMAT(' A TOTAL OF',I4, ' FUNCTION EVALUATIONS NEEDED')
RETURN
END

C
SUBROUTINE DDFSYS(N,F,EPS,H,X,Y,PAR)
C
C 'EPS' IS SINGLE PRECISION (REAL*4), WHEREAS 'X', 'Y' AND 'H' ARE
C DOUBLE PRECISION (REAL*8)
C N=NUMBER OF FIRST ORDER DIFF. EQU. (N.LE.5), WHICH ARE OF THE FORM
C DZ=F(X,Y1,Y2,......) AND ARE PROVIDED BY SUBROUTINE F(X,Y,DZ,PAR)
C 'PAR'-UPTO 10 DOUBLE PRECISION PARAMETERS
C EPS=ACCURACY PER STEP, SHOULD BE LARGER THAN 10.XX(-D+3)
C WHERE D IS THE NUMBER OF DIGITS OF THE MACHINE REPRESENTATION.
C H=SUGGESTED STEP WIDTH, H IS AUTOMATICALLY ADJUSTED.
C RETURNING FROM DIFSYS (X,Y) IS REPLACED BY (X+H,Y(X+H))
C H IS THEN USED AS SUGGESTED STEP SIZE FOR NEXT INTEGRATION STEP
C
C IMPLICIT REAL*8 (A-H,0-2)
EXTERNAL F
REAL*4 EPS
REAL*8 DT(5)/5*0.0D00/, DT(5,6)/30*0.0D00/, Y(5), D(6), YA(5),
1 YD(5), D2(5), YG(8,5), YH(8,5), YL(5), YM(5), S(5), PAR(10)
INTEGER R, SR
LOGICAL KCONV, BO, BH
EP=ABS(EPS)
N1=N
H=H
IF(EP.LT.5.E-9) EP=5. E-9
CALL F(X,Y,DZ,PAR)
BH=.FALSE.
DO 1 I=1, N1
1 YA(I)=Y(I)
2 A=HH+X
FC=1.5
BO=.FALSE.
M=1
R=2
SR=3
JJ=0
DO 3 J=1, 10
3 IF(BO) GO TO 10
D(1)=2.25
D(3)=9.
D(5)=36.
GO TO 12
10 D(1)=1.7777777777777778
D(3)=7.111111111111111

77
D(5)=28.44444444444444
12 KONV=J,GT.5
13 IF(J.GT.7) GO TO 13
14 L=J-1
15 IF(L-1) 15,15,16
16 D(L)=MXM
17 GO TO 15
18 L=6
19 D(6)=64.
20 FC=.6*FC
21 M=M+M
22 G=HH/M
23 B=G+G
24 IF(BH.AND.J.LT.9) GO TO 17
25 GO TO 18
26 DO 19 I=1,N1
27 YM(I)=YH(J,I)
28 YL(I)=YG(J,1)
29 GO TO 25
30 KK=(M-2)/2
31 M=M-1
32 DO 20 I=1,N1
33 YL(I)=YA(I)
34 YM(I)=G*XZ(I)+YA(I)
35 DO 21 K=1,M
36 CALL F(X+K*G,YM,DY,P1)
37 DO 22 I=1,N1
38 U=BDY(I)+YL(I)
39 YM(I)=U
40 S(I)=U
41 IF(U-S(I)) 22,22,23
42 S(I)=S(I)
43 CONTINUE
44 IF(K.EQ.KK.AND.K.NE.2) GO TO 24
45 GO TO 21
46 JJ=I+JJ
47 DO 26 I=1,N1
48 YH(JJ,I)=YM(I)
49 YG(JJ,I)=YL(I)
50 CONTINUE
51 CALL F(A,YM,DY,P1)
52 D 30 I=1,N1
53 U=DTT(I)
54 C=.5*(YM(I)+YL(I)+6*XZ(I))
55 T4=C
56 DTT(I)=C
57 L=MAX0(L,1)
58 DO 31 K=1,L
59 B1=D(K)*X
60 B=B1-C
61 U=U
62 IF(B.NE.0) GO TO 32
63 GO TO 33
64 B=(C-U)/B
65 78
U=CB\times B \\
C=BI\times B \\
33 \quad V=DT(I,K) \\
DT(I,K)=U \\
31 \quad TA=U+TA \\
IF(DABS(Y(I)-TA) .GT. EPS(I)) KONV=.FALSE. \\
30 \quad Y(I)=TA \\
IF(KONV) GO TO 50 \\
D(2)=4. \\
D(4)=16. \\
BO=.NOT.BO \\
M=R \\
R=SR \\
3 \quad SR=M+M \\
BH=.NOT.BH \\
HH=HH/2. \\
GO TO 2 \\
50 \quad H=FC\times HH \\
X=A \\
RETURN \\
END \\
C \\
SUBROUTINE LANGER(X,Y,DZ,PAR) \\
C \\
A DDFSYS COMPATIBLE ROUTINE USED TO CALCULATE THE EXACT VALUES OF Z ETC. \\
C \\
IMPLICIT REAL*8 (A-H,O-Z) \\
DIMENSION Y(5),DZ(5),PAR(10) \\
DZ(1)=Y(2) \\
DZ(2)=Y(3)\times Y(2) \\
DZ(3)=2.00\times(ax-x)\times Y(2)\times Y(2) + .500\times Y(3)\times Y(3) + 2 \\
DZ(4)=0. \\
RETURN \\
END \\
C \\
SUBROUTINE ZPRIME(X,Y,DZ,PAR) \\
C \\
A DDFSYS COMPATIBLE ROUTINE USED TO CALCULATE THE ZEROTH ORDER APPROXIMATION OF Z ETC. \\
C \\
IMPLICIT REAL*8 (A-H,O-Z) \\
DIMENSION Y(5),DZ(5),PAR(10) \\
DZ(1)=DSQRT(W(X) / Y(1)) \\
RETURN \\
END
SUBROUTINE AIRY(AI,BI,AIP,BIP,Z,IER)

AIRY FUNCTIONS AI(Z), BI(Z)
AND THEIR DERIVATIVES AIP(Z), BIP(Z).

WRITTEN BY TIM SCHOLL

SEE REFERENCE (17) FOR EXPLANATION OF SOME EXPANSIONS

ON ENTRANCE
IER=0 ...... DON'T PRINT ERROR MESSAGES
IER=1 ...... PRINT ERROR MESSAGES

ON EXIT
IER=0 ...... NO ERRORS
IER=1 ...... OVERFLOW AI=AIP=0, BI=BIP=1E75
IER=-1 ...... ARGUMENT TO TRIG FUNCTION TOO LARGE

IMPLICIT REAL*8 (A-H,O-Z)
IF (Z.LE.-80.0D00) CALL AREA4(AI,BI,AIP,BIP,Z,IER,&99)
IF (Z.LE.-3.60D00) CALL AREA3(AI,BI,AIP,BIP,Z,IER,&99)
IF (Z.LE.1.0D00) CALL AREA2(AI,BI,AIP,BIP,Z,IER,&99)
CALL AREA1(AI,BI,AIP,BIP,Z,IER)
99 RETURN
END

C

SUBROUTINE AREA1(AI,BI,AIP,BIP,Z,IER)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CVAI(12), CVBI(14), CVAIP(12), CVBIP(14)

COEFFICIENT VECTOR--AIXXXXX
DATA CVAI( 1)/-5.445045903973671D-02/
DATA CVAI( 2)/ 1.228202483907300D-02/
DATA CVAI( 3)/-2.10799475153601D-03/
DATA CVAI( 4)/ 4.499311380490556D-04/
DATA CVAI( 5)/-1.107885512234551D-04/
DATA CVAI( 6)/ 3.029414769197648D-05/
DATA CVAI( 7)/-8.581599138196050D-06/
DATA CVAI( 8)/ 3.124271524032183D-06/
DATA CVAI( 9)/-5.899825616934007D-07/
DATA CVAI(10)/ 5.786979221922356D-07/
DATA CVAI(11)/ 4.449623915138266D-08/
DATA CVAI(12)/ 1.155036393855280D-07/

COEFFICIENT VECTOR--BIXXXXX
DATA CVBI( 1)/ 8.2279556360447162D-02/
DATA CVBI( 2)/-6.316641547042471D-03/
DATA CVBI( 3)/-1.913197185955132D-02/
DATA CVBI( 4)/ 1.720510408372530D-03/
DATA CVBI( 5)/ 2.383041346077916D-03/
DATA CVBI( 6)/-1.134023234668820D-03/
DATA CVBI( 7)/ 1.233865816914231D-03/
DATA CVBI( 8)/ 1.579050652106840D-03/
DATA CVBI( 9)/ 9.623176146072881D-04/
DATA CVBI(10)/ 1.074857412313187D-03/
DATA CVBI(11)/ 6.974912380788279D-04/
DATA CVBI(12)/ 3.194142054489408D-04/
DATA CVBI(13)/ 1.7394425478044740-04/
DATA CVBI(14)/ 2.472984890990492D-05/
C COEFFICIENT VECTOR---AIP
DATA CVAIP( 1)/ 7.897729009600677D-02/
DATA CVAIP( 2)/ -1.510260266172028D-02/
DATA CVAIP( 3)/ 2.46327938831557D-03/
DATA CVAIP( 4)/ -5.01404093621199D-04/
DATA CVAIP( 5)/ 1.235657928041223D-04/
DATA CVAIP( 6)/ -3.686442633555789D-05/
DATA CVAIP( 7)/ 2.841490054306729D-06/
DATA CVAIP( 8)/ -1.28387874251164D-05/
DATA CVAIP( 9)/ -6.395677045695181D-06/
DATA CVAIP(10)/ -8.177544529803375D-06/
DATA CVAIP(11)/ -2.946959206582392D-06/
DATA CVAIP(12)/ -2.767821448973843D-06/
C COEFFICIENT VECTOR---BIP
DATA CVBIP( 1)/ -1.15546316390965D-01/
DATA CVBIP( 2)/ 2.649705118599784D-03/
DATA CVBIP( 3)/ 2.131461302832706D-02/
DATA CVBIP( 4)/ -1.325904771351788D-03/
DATA CVBIP( 5)/ -2.703662585231253D-03/
DATA CVBIP( 6)/ 1.150856772259972D-03/
DATA CVBIP( 7)/ -1.280847875449697D-03/
DATA CVBIP( 8)/ -1.720672591436791D-03/
DATA CVBIP( 9)/ -1.0577134410854480D-03/
DATA CVBIP(10)/ -1.158533819253664D-03/
DATA CVBIP(11)/ -7.377105071484384D-04/
DATA CVBIP(12)/ -3.497253573830967D-04/
DATA CVBIP(13)/ -1.88797391127985D-04/
DATA CVBIP(14)/ -2.894453443570144D-05/
C OTHER COEFFICIENTS
DATA SQRTP1/1.772453850905516/
C
C LARGE Z, Z > 1.0
IF (Z.GT.40.8D00) THEN DO
  IF (IER,EQ.1) THEN DO
    WRITE (6,1)
1 FORMAT(1-A " WARNING!!! EXPONENT OVERFLOW. ",/)
    * AI EQUALS 0/*
    * AIP EQUALS 0/*
    * BI EQUALS 1.0E+75/*
    * BIP EQUALS 1.0E+75)
  END IF
  AI=AIP=0.0D00
  BI=BIP=1.0D+75
  IER=+1
ELSE DO
  SUB=.666666666666666667Z*DSQRT(Z)
  Z0=1.000/SUB
  ZCOR=1.333333333333333D 00*Z0-1.0D00
  CALL CNPS(Y,ZCOR,CVAI,12)
  Y=(Y/SUB)+1.0D00
  AI=+0.5000000*Y*XEXP((-DSQRT(DSQRT(Z))*SQRTP1))
  CALL CNPS(Y,ZCOR,CVAI,12)
  Y=(Y/SUB)+1.0D00
END IF
81
AIP=-0.50D00*Y*DEXP(-SUB)*DSQRT(DSQRT(Z))/SQRTP1
ZCOR=1.376873969378290D 00*Z0-1.065310864067434
CALL CNPS(Y,ZCOR,CVBi,14)
Y=(Y/SUB)+1.0D00
B1=Y*DEXP(SUB)/(DSQRT(DSQRT(Z)))*SQRTP1
CALL CNPS(Y,ZCOR,CVBiP,14)
Y=(Y/SUB)+1.0D00
B1=Y*DEXP(SUB)/(DSQRT(DSQRT(Z)))*SQRTP1
IER=0
END IF
RETURN
END

SUBROUTINE AREAS(AI,B1,AIP,BIP,Z,IER,x)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CVAI(16),CVBI(16),CVAIP(16),CVBiP(16)

COEFFICIENT VECTOR--AIXXXXXX
DATA CVAI(1)/8.353676583513726D-02/
DATA CVAI(2)/2.32624057241384D-01/
DATA CVAI(3)/-2.94545305195283D-01/
DATA CVAI(4)/-7.848440599679570D-02/
DATA CVAI(5)/1.232075953712138D-01/
DATA CVAI(6)/-2.497793206372120D-02/
DATA CVAI(7)/1.158731541242598D-02/
DATA CVAI(8)/6.28174915835338D-03/
DATA CVAI(9)/-4.731488472076063D-04/
DATA CVAI(10)/-4.069834887026604D-04/
DATA CVAI(11)/1.25318105974273D-04/
DATA CVAI(12)/-1.596034427055931D-06/
DATA CVAI(13)/-6.478601227972824D-06/
DATA CVAI(14)/1.321405553651502D-06/
DATA CVAI(15)/3.815480415977664D-08/
DATA CVAI(16)/-5.872827832431077D-08/

COEFFICIENT VECTOR--BIXXXXXX
DATA CVBI(1)/2.890781856566552D-01/
DATA CVBI(2)/6.018552281473439D-01/
DATA CVBI(3)/4.121103023807179D-01/
DATA CVBI(4)/-1.674068616700080D-01/
DATA CVBI(5)/3.162375338106135D-02/
DATA CVBI(6)/5.288176479310745D-02/
DATA CVBI(7)/-1.360446821927808D-02/
DATA CVBI(8)/-7.6895839564037D-04/
DATA CVBI(9)/1.989127261940178D-03/
DATA CVBI(10)/-3.158790170775661D-04/
DATA CVBI(11)/4.885337970872278D-05/
DATA CVBI(12)/3.403901248098371D-05/
DATA CVBI(13)/-3.410106414046498D-06/
DATA CVBI(14)/-8.430603277137648D-07/
DATA CVBI(15)/3.302966882264039D-07/
DATA CVBI(16)/-2.013749214127708D-08/

COEFFICIENT VECTOR--AIPXXXXX
DATA CVAIP(1)/5.470559688919087D-03/
DATA CVAIP(2)/-1.464288889259264D-01/
DATA CVAIP(3)/-2.78297407363954D-01/
DATA CVAIP(4)/3.658238191524662D-01/
DATA CVAIP( 5)/-7.355548107104228D-02/
DATA CVAIP( 6)/-6.272432747214548D-02/
DATA CVAIP( 7)/ 3.505053039582666D-02/
DATA CVAIP( 8)/-2.268760121033407D-03/
DATA CVAIP( 9)/-3.186200110356446D-03/
DATA CVAIP(10)/ 1.022713653099007D-03/
DATA CVAIP(11)/-1.112740955366838D-06/
DATA CVAIP(12)/-6.700088905496098D-05/
DATA CVAIP(13)/ 1.416872314179926D-05/
DATA CVAIP(14)/ 5.942349252532730D-07/
DATA CVAIP(15)/-7.625956182743886D-07/
DATA CVAIP(16)/ 1.155578036520587D-07/
C
COEFFICIENT VECTOR--BIP XXXX
DATA CVBIP( 1)/ 1.548618316819235D-01/
DATA CVBIP( 2)/ 7.69102354013728D-01/
DATA CVBIP( 3)/-2.136267063043775D-01/
DATA CVBIP( 4)/ 5.239661663024924D-02/
DATA CVBIP( 5)/ 2.230848421926327D-01/
DATA CVBIP( 6)/-5.75990977237984D-02/
DATA CVBIP( 7)/-6.935976313120824D-03/
DATA CVBIP( 8)/ 1.338090814244242D-02/
DATA CVBIP( 9)/-2.156270198902540D-03/
DATA CVBIP(10)/-4.565047617742590D-04/
DATA CVBIP(11)/ 3.15826492108724D-04/
DATA CVBIP(12)/-3.170102485956567D-05/
DATA CVBIP(13)/-9.768927175521692D-06/
DATA CVBIP(14)/ 3.896608455151422D-06/
DATA CVBIP(15)/-2.408393901199891D-07/
DATA CVBIP(16)/-1.071314679028117D-07/
C
SMALL Z, -3.6 < Z < 1.0 XXXXXXXXXXX
CORZ=.4347826036956521D 000X+.5652173913043479D 00
CALL CNPS(AI,CORZ,CVAI,16)
CALL CNPS(BI,CORZ,CVBI,16)
CALL CNPS(AIP,CORZ,CVAIP,16)
CALL CNPS(BIP,CORZ,CVBIP,16)
IER=0
RETURN 1
END
C
SUBROUTINE AREA3(AI,BI,AIP,BIP,Z,IER,*)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CVCHI(7),CVPSI(7),CVFAI(6),CVGAX(6)
C
COEFFICIENT VECTOR--FAIXXXXXXXXX
DATA CVFAI( 1)/ 9.984079740170277D-01/
DATA CVFAI( 2)/-1.566213391555130D-03/
DATA CVFAI( 3)/ 2.441839992342595D-05/
DATA CVFAI( 4)/-1.009622526114867D-06/
DATA CVFAI( 5)/ 7.192640017489443D-08/
DATA CVFAI( 6)/-7.880984124842139D-09/
C
COEFFICIENT VECTOR--GAIXXXXXXXXX
DATA CVGAX( 1)/ 1.002246049711181D 00/
DATA CVGAX( 2)/ 2.215105970219821D-03/
DATA CVGAX( 3)/-2.928594564290988D-05/
DATA CVGAX( 4)/ 1.141573497352018D-06/
DATA CVGAX(5) = -7.878499032736654D-08
DATA CVGAX(6) = 8.563234193601136D-09
C

COEFFICIENT VECTOR = CHI
DATA CVCHI(1) = -1.544954187712260D-01
DATA CVCHI(2) = 1.703052732415939D-03
DATA CVCHI(3) = -4.856159837236686D-05
DATA CVCHI(4) = 2.843599961858338D-06
DATA CVCHI(5) = -2.516391153404993D-07
DATA CVCHI(6) = 2.319432723458549D-08
DATA CVCHI(7) = -2.863613493894515D-08
C

COEFFICIENT VECTOR = PSI
DATA CVPSI(1) = 2.164073298813229D-01
DATA CVPSI(2) = -2.279929742637604D-03
DATA CVPSI(3) = 5.938956347398345D-05
DATA CVPSI(4) = -3.318493529119677D-06
DATA CVPSI(5) = 3.883196691495894D-07
DATA CVPSI(6) = -1.296251363114941D-07
DATA CVPSI(7) = 4.834436265690296D-08
C

OTHER COEFFICIENTS
DATA PI4 = 7853981633974483
DATA PI = 3.141592653589793

C

LARGE Z , -80.0 < Z < -3.6 XXXXXXX
Z = DABS(Z)
ZCUB = 1.000/Z^3
CORZ = 9.331200000000020D0 01*ZCUB = 1.000
CALL CNPS(CHIVAL,CORZ,CVCHI,7)
CALL CNPS(PSIVAL,CORZ,CVPSI,7)
CORZ = 9.33205038301146D0 01*ZCUB = 1.0001822660945D 00
CALL CNPS(FMXVAL,CORZ,CUFAX,6)
CALL CNPS(GMXVAL,CORZ,CVGAX,6)
CHIVAL = (CHIVAL*ZCUB) + 1.000
PSIVAL = (PSIVAL*ZCUB) + 1.000
PSIVAL = 6666666666666667*Z*XDSQRT(Z)*CHIVAL + PI4
PSIVAL = 6666666666666667*Z*XDSQRT(Z)*PSIVAL - PI4
FMXVAL = DSGRT(FMXVAL/(PI*XDSQRT(Z)))
GMXVAL = DSGRT(GMXVAL*XDSQRT(Z)/PI)
AI = FMXVAL*XDSIN(CHIVAL)
BI = FMXVAL*XDCOS(CHIVAL)
AIP = GMXVAL*XDSIN(PSIVAL)
BIP = GMXVAL*XDCOS(PSIVAL)
Z = -Z
IER = 0
RETURN 1
END
C

SUBROUTINE AREA4(AI,BI,AIP,BIP,Z,IER,X)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CVCHI(7),CVPSI(7),CUFAX(3),CVGAX(5)
C

COEFFICIENT VECTOR = FAX
DATA CVFAX(1) = -1.509179214180789D-01
DATA CVFAX(2) = 4.761985614359914D-03
DATA CVFAX(3) = 1.125942924075128D-05
C

COEFFICIENT VECTOR = GAX
DATA CVGAX(1) = 2.125390533066555D-01
DATA CVGAX ( 2) = -5.950776056239688D-03/
DATA CVGAX ( 3) = 2.540058457241702D-04/
DATA CVGAX ( 4) = -2.480352429183556D-05/
DATA CVGAX ( 5) = 8.063094016067059D-06/
COEFFICIENT VECTOR—CHI******
DATA CVCHICI ( 1) = -1.544954187712260D-01/
DATA CVCHICI ( 2) = 1.703052732415939D-03/
DATA CVCHICI ( 3) = -4.856159372364868D-05/
DATA CVCHICI ( 4) = 2.843599961858338D-06/
DATA CVCHICI ( 5) = -2.516391153404093D-07/
DATA CVCHICI ( 6) = 2.319432723458549D-08/
DATA CVCHICI ( 7) = -2.863613493894515D-08/
COEFFICIENT VECTOR—PSI******
DATA CVPSI ( 1) = 2.164073298813229D-01/
DATA CVPSI ( 2) = -2.279929742637604D-03/
DATA CVPSI ( 3) = 5.938956347398345D-05/
DATA CVPSI ( 4) = -3.18493352811967D-06/
DATA CVPSI ( 5) = 3.883196491495894D-07/
DATA CVPSI ( 6) = -1.296251363114941D-07/
DATA CVPSI ( 7) = 4.834436265690296D-08/
OTHER COEFFICIENTS
DATA PI4 = .7853981633974483/
DATA PI = 3.141592653589793/

C

LARGE Z , Z < -80.0 ************
IF (Z.LT. -1.0D+10) THEN DO
IF (IER.EQ.1) THEN DO
WRITE (6,1) FMXVAL,GMXVAL
1 FORMAT(' -WARNING!!! OUT OF RANGE FOR TRIG FUNCTIONS./, ' ,
ABS(AI,BI) <= ,1PD23.16/, ,
ABS(AIP,BIP) <= ,1PD23.16)
END IF
AI=AIP=BI=BIP=0.0000
IER=-1
ELSE DO
Z=DABS(Z)
ZCUB=1.000/ZXX3
CORZ=9.33120000000002D 01%ZCUB-1.0000
CALL CNPS(CHIVAL, CORZ, CVCHI, 7)
CALL CNPS(PSIVAL, CORZ, CVPSI, 7)
CALL CNPS(FMXVAL, CORZ, CVFAX, 3)
CALL CNPS(GMXVAL, CORZ, CVGAX, 5)
CHIVAL=(CHIVAL*ZCUB)+1.0000
CHIVAL=(CHIVAL*ZCUB)+1.0000
PSIVAL=(PSIVAL*ZCUB)+1.0000
PSIVAL=(PSIVAL*ZCUB)+1.0000
FMXVAL=(FMXVAL*ZCUB)+1.0000
FMXVAL=(FMXVAL*ZCUB)+1.0000
GMXVAL=(GMXVAL*ZCUB)+1.0000
GMXVAL=(GMXVAL*ZCUB)+1.0000
GMI=FMXVAL/GMXVAL/DSRT(Z)/PI
AIP=FMXVAL*DSIN(CHIVAL)
BIP=FMXVAL*DCOS(CHIVAL)
AIP=GMXVAL*DSIN(PSIVAL)
BIP=GMXVAL*DCOS(PSIVAL)
Z=-Z
IER=0
END IF
RETURN 1
END

C SUBROUTINE CNPS(Y,X,C,N)
C
DIMENSION C(N)
DOUBLE PRECISION C,Y,X,H0,H1,H2,ARG

C TEST OF DIMENSION
IF (N) 1,1,2
RETURN

1 IF (N-2) 3,4,4
Y=C(1)
RETURN

C INITIALIZATION
ARG=X+X
H1=0.000
H0=0.000

C DO 5 I=1,N
K=N-1
H2=H1
H1=H0
5 H0=ARG*H1-H2+C(K+1)
Y=0.5D00*C(1)-H2+H0
RETURN
END

.C$PRINTON
$ENTRY
$IBSYS
$STOP
///
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8. N. Froman and P.O. Froman, JWKB Approximation, North Holland Publishing Co., Amsterdam, 1965
12. R. Bulirsch and J. Stoer, Numerische Mathematik 8, 1966


Vita Auctoris

I was born in Windsor on April 26, 1958. In 1981, I received a B.Sc. in Physics from the University of Windsor. In that same year, I began work on an M.Sc. degree.