A NEW APPROACH TO THE JWKB TREATMENT.

NASR YOUSSEF. SAAD

University of Windsor

Follow this and additional works at: https://scholar.uwindsor.ca/etd

Recommended Citation
https://scholar.uwindsor.ca/etd/681

This online database contains the full-text of PhD dissertations and Masters' theses of University of Windsor students from 1954 forward. These documents are made available for personal study and research purposes only, in accordance with the Canadian Copyright Act and the Creative Commons license—CC BY-NC-ND (Attribution, Non-Commercial, No Derivative Works). Under this license, works must always be attributed to the copyright holder (original author), cannot be used for any commercial purposes, and may not be altered. Any other use would require the permission of the copyright holder. Students may inquire about withdrawing their dissertation and/or thesis from this database. For additional inquiries, please contact the repository administrator via email (scholarship@uwindsor.ca) or by telephone at 519-253-3000ext. 3208.
Notice

The quality of this microfiche is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

If pages are missing, contact the university which granted the degree.

Some pages may have indistinct print especially if the original pages were typed with a poor typewriter ribbon or if the university sent us a poor photocopy.

Previously copyrighted materials (journal articles, published tests, etc.) are not filmed.

Reproduction in full or in part of this film is governed by the Canadian Copyright Act, R.S.C. 1970, c. C-30. Please read the authorization forms which accompany this thesis.

This dissertation has been microfilmed exactly as received.

Ottawa, Canada
K1A 0N4

Avis

La qualité de cette microfiche dépend grandement de la qualité de la thèse soumise au microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

S'il manque des pages, veuillez communiquer avec l'université qui a conféré le grade.

La qualité d'impression de certaines pages peut laisser à désirer, surtout si les pages originales ont été dactylographiées à l'aide d'un ruban usé ou si l'université nous a fait parvenir une photocopie de mauvaise qualité.

Les documents qui font déjà l'objet d'un droit d'auteur (articles de revue, examens publiés, etc.) ne sont pas microfilmés.

La reproduction, même partielle, de ce microfilm est soumise à la Loi canadienne sur le droit d'auteur, SRC 1970, c. C-30. Veuillez prendre connaissance des formulaires d'autorisation qui accompagnent cette thèse.

La thèse a été microfilmée telle que nous l'avons reçue.
A NEW APPROACH TO THE JWKB TREATMENT

by

Nasr Youssef Saad

A Dissertation
submitted to the Faculty of Graduate Studies
through the Department of
Physics in Partial Fulfillment
of the requirements for the Degree
of Doctor of Philosophy at
The University of Windsor

Windsor, Ontario, Canada

1980
TO LAUDY, MY WIFE.
ABSTRACT

The JWKB approximation is widely used in many problems in quantum mechanics for its simplicity and also because a closed-form solution often provides more insight than a numerical one. Unfortunately, like all approximations, the JWKB method has its limitations: Firstly, it may fail near or at a classical turning point, and secondly, it employs solutions for a potential which deviates from the actual potential \( W(x) \).

In this work, a new method is proposed to avoid the limitations of the JWKB method while keeping its advantages. First, the singularity around the classical turning point is resolved not only for a linear potential as proposed by Langer, but also for any potential with a linear leading term through the turning point, and second, a solution is constructed in closed form which is an exact solution for the actual potential \( W(x) \). The new method consists in finding a substitute potential \( U(x) \) in such a way that, together with its \( \delta [U, x] \), it is equal to the actual potential \( W(x) \). The solution is then based on \( U(x) \) but actually is the solution for \( W(x) \) because \( W(x) = U(x) + \delta [U, x] \).

The new method is first applied to potentials with only two turning points. The eigenvalue problem is reduced to the solution of a linear equation and the energy eigenvalues are exactly given. Then, potentials with more than two turning points are studied and the eigenvalue problem is again reduced to the solution of a polynomial equation whose order depends upon the number of turning points. Then the method is applied to the hindered or restricted rotation. The energy levels are found to be associated with the \( n \)-th roots of 1 in
the complex plane, i.e. on the unit circle.

The method described here is of rather general nature and can be used to solve a number of problems in quantum mechanics, where a solution for the Schrödinger equation in closed form is needed. The applications provided in this work are only given as examples of the applicability and the relative simplicity of the method.
ACKNOWLEDGEMENT

I am grateful to Dr. R. K. B. Helbing for suggesting this problem to me as dissertation and it is a great pleasure to acknowledge his constant guidance and supervision throughout the entire period of this work.

The financial support from the University of Windsor and grants from the National Research Council of Canada are gratefully acknowledged.
# TABLE OF CONTENTS

**ABSTRACT** ........................................................................................................ v &

**ACKNOWLEDGEMENTS** ..................................................................................... vii

**LIST OF TABLES** .......................................................................................... x

**LIST OF FIGURES** ........................................................................................ xi

**INTRODUCTION** ............................................................................................... 1

## CHAPTER

I. **THEORETICAL BACKGROUND**

1.1 The Schrödinger Equation ................................................................. 5

1.2 The JWKB Approximation ................................................................... 6

1.3 The Langer Modification .................................................................... 8

II. **THE METHOD PROPOSED**

II.1 Notations ............................................................................................... 11

II.2 Scaling Laws For $\Delta U_s x$ ........................................................... 11

II.3 Small $x$ Behaviour of $\Delta [U_s x]$ .................................................. 12

II.4 Large $x$ Behaviour of $\Delta [U_s x]$ .................................................. 14

II.5 Calculation of $\Delta [U_s x]$ ............................................................... 15

II.6 The Problem With Conventional JWKB Methods ....................... 18

II.7 The New Method ................................................................................... 23

II.8 Iteration Procedure And Results ..................................................... 25

III. **APPLICATION TO POTENTIALS WITH TWO TURNING POINTS: SINGLE BOWL POTENTIALS**

III.1 Method's Application .......................................................................... 30

III.2 Connection Matrix ............................................................................... 33

III.3 Classical Limit ...................................................................................... 38

III.4 Phase Shift ............................................................................................ 39

III.5 Eigenvalues ........................................................................................... 40

III.6 Results .................................................................................................. 42
## CHAPTER

### IV. APPLICATION TO POTENTIALS WITH MANY BOWLS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV.1</td>
<td>Decaying States</td>
<td>48</td>
</tr>
<tr>
<td>IV.2</td>
<td>Matrix Formalism For The General Case</td>
<td>51</td>
</tr>
<tr>
<td>IV.3</td>
<td>Eigenvalue Problem For Many Bowls</td>
<td>56</td>
</tr>
<tr>
<td>IV.4</td>
<td>Results for A Symmetric Double Potential Well</td>
<td>60</td>
</tr>
<tr>
<td>IV.5</td>
<td>Ring Structure For Many Bowls</td>
<td>61</td>
</tr>
</tbody>
</table>

## APPENDICES

<table>
<thead>
<tr>
<th>Appendix</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.</td>
<td>Taylor Expansion Method</td>
<td>72</td>
</tr>
<tr>
<td>B.</td>
<td>Gaussian Integration</td>
<td>76</td>
</tr>
<tr>
<td>C.</td>
<td>Matrix Formalism For The General Case</td>
<td>81</td>
</tr>
<tr>
<td>D.</td>
<td>Program Listings</td>
<td>84</td>
</tr>
</tbody>
</table>

## REFERENCES

- REFERENCES .......................................................... 91

## VITA AUCTORIS

- VITA AUCTORIS ...................................................... 95
LIST OF TABLES

III.1 Eigenfunctions of the harmonic oscillator. ............ 47
IV.1 Energy levels for a N-fold barrier ring potential ....... 70
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Int.</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Simple schematic classification of semi-classical methods</td>
<td>4</td>
</tr>
<tr>
<td>II.1</td>
<td>Large $x$ behaviour of $\Delta [U, x]$</td>
<td>16</td>
</tr>
<tr>
<td>II.2</td>
<td>$\Delta [U, x]$ evaluated for a potential with two turning points</td>
<td>19</td>
</tr>
<tr>
<td>II.3</td>
<td>The failure of the simple JWKB method.</td>
<td>20</td>
</tr>
<tr>
<td>II.4</td>
<td>Conventional JWKB method.</td>
<td>21</td>
</tr>
<tr>
<td>II.5</td>
<td>Conventional JWKB method.</td>
<td>22</td>
</tr>
<tr>
<td>II.6</td>
<td>Schematic of JWKB methods.</td>
<td>24</td>
</tr>
<tr>
<td>II.7</td>
<td>Schematic of the method proposed in this work.</td>
<td>27</td>
</tr>
<tr>
<td>II.8</td>
<td>The substitute potential of the method proposed.</td>
<td>28</td>
</tr>
<tr>
<td>II.9</td>
<td>The substitute potential of the method proposed.</td>
<td>29</td>
</tr>
<tr>
<td>III.1</td>
<td>The method proposed applied to a potential with two turning points.</td>
<td>31</td>
</tr>
<tr>
<td>III.2</td>
<td>Substitute potentials $U_1$ and $U_2$ between two turning points.</td>
<td>32</td>
</tr>
<tr>
<td>III.3</td>
<td>Energy levels for the harmonic oscillator.</td>
<td>44</td>
</tr>
<tr>
<td>III.4</td>
<td>Energy levels and eigenfunctions of the harmonic oscillator.</td>
<td>45</td>
</tr>
<tr>
<td>IV.1</td>
<td>The method applied to a potential with several turning points.</td>
<td>49</td>
</tr>
<tr>
<td>IV.2</td>
<td>The method applied to a double potential well (four turning points).</td>
<td>57</td>
</tr>
<tr>
<td>IV.3</td>
<td>The method applied to a potential with 6 turning points (three bowls) : overall matrix</td>
<td>59</td>
</tr>
<tr>
<td>IV.4</td>
<td>Energy levels of a symmetric double potential well</td>
<td>62</td>
</tr>
<tr>
<td>IV.5</td>
<td>Energy levels of a symmetric potential with three bowls.</td>
<td>63</td>
</tr>
</tbody>
</table>
IV.6 The method applied to the hindered rotation problem. ......................... 65
IV.7 Energy split-up pattern. ......................... 68
IV.8 Energy levels for a ring structure potential. ....... 70a
INTRODUCTION

In quantum mechanics, many problems are conveniently formulated in terms of coupled differential, or sometimes integro-differential, equations, such as electronic structure of atoms and molecules, molecular vibrations, perturbation theory, scattering of molecules, atoms, nuclei, etc. And dealing with atomic and molecular elastic scattering assuming central forces, it is found that, in many cases, the number of significant scattering phase shifts is in the order of hundreds and even thousands. Since, exactly speaking, each phase shift is given by the asymptotic behaviour of the solution of the radial Schrödinger equation, and numerical integration is not always possible, advantage is taken of approximations as much as possible.

There are a large number of methods proposed for solving this problem and trying to find closed-form solutions for the radial Schrödinger equation whenever possible rather than numerical solutions whose manipulation is limited.

If one wants to classify those methods, a first distinction can be made relative to the range of the potential energy: Some methods are covering the full spatial range of the potential. Other methods are dividing the range into several adjacent intervals depending upon the shape of the potential energy and the accuracy desired of the solution.

The second classification can be said as being relative to the approach. Two ways are commonly used: one way consists of taking the actual potential without modification and either trying to find approximate
closed-form functions as the solution or to find numerical solutions; those numerical solutions can then be fitted by closed-form functions, adding correction terms when needed. (13, 20) The other way consists of approximating, over a certain range, the actual potential by another one for whom closed-form functions can be found as solutions. The range of each interval is large or small as prescribed by the accuracy desired; the range of integration is then divided into many intervals which are sufficiently small so that the potential energy of the problem may be approximated by a simple polynomial in each interval. The wave functions for the polynomial approximations to the potential are constructed in closed form and by suitably matching these wave functions at the boundaries between the intervals, the wave function for the entire range is constructed. (41, 60, 73, 76)

Both ways have their advantages and their disadvantages: By taking the actual potential (which one needs), one is not able to find exact closed-form solutions; and by using closed-form functions as solutions (which one wants to have), one is not exactly solving the problem for the actual potential but rather for an approximate one; besides, in almost all cases, the approximate potential is pieced together using a large number of intervals.

The method proposed in this work finds exact closed-form solutions for the actual potential. In principle the potential is not approximated and the solution is the exact one for the actual potential and in closed form. This method is different from the others; it is based on a new way of looking at the problem as will be shown in this work. It is valid for any number of classical turning points where a simple matrix formalism is developed in order to link up the coefficients of the solution between
each region containing a classical turning point. Besides, the inherent advantage of a closed-form solution is apparent when evaluating various matrix elements of interest involving the wave function, when treating the energy level problem for bound states.
Simple schematic classification of semi-classical methods.

Fig. (Int. 1)
CHAPTER I
THEORETICAL BACKGROUND

1.1: The Schrödinger Equation

For a particle of mass \( m \) moving in a potential \( V(q_1, q_2, q_3) \),

the Schrödinger equation has the form: \( (6,7,8) \)

\[ \nabla^2 \psi + \frac{2m}{\hbar^2} \left[ E - V(q_1, q_2, q_3) \right] \psi = 0 \]  

(1.1)

For that particle in a central potential, the Schrödinger equation can
be separated into an angular part \( Y(\theta, \phi) \) and a radial part \( R(r) \)

\[ \psi(r, \theta, \phi) = R(r) \cdot Y(\theta, \phi) \]  

(1.2)

where the functions \( Y(\theta, \phi) \) are the spherical harmonics given by:

\[ Y^m_l(\theta, \phi) = \frac{1}{\sqrt{2\pi}} \cdot e^{im\phi} \cdot \frac{2\ell + 1}{2} \cdot \left( \frac{\ell - |m|}{\ell + |m|} \right) \frac{1}{2} \cdot P^m_l \left( \cos \theta \right) \]  

(1.3)

\( \ell \) can take on the values of 0, 1, 2, 3, ... and \( m \) can take on the values
of 0, ±1, ±2, ... for any value of \( \ell \).

\( P^m_l(\cos \theta) \) is the associated Legendre polynomial corresponding to
quantum numbers \( \ell \) and \( m \) and is given by:

\[ P^m_l(x) = \frac{(1-x^2)^{m/2}}{2^\ell \ell!} \left( \frac{d}{dx} \left[ \frac{1}{(1-x^2)^{1/2}} \right] \right)^{\ell+|m|} \frac{1}{(1-x^2)^{1/2}} \]  

(1.4)

By using the substitution:

\[ R_l(r) = \frac{\partial E(r)}{\partial} \]  

(1.5)

the radial part follows the equation:

\[ \frac{d^2 \psi}{dr^2} + \left[ \frac{K}{r} - \bar{U}(r) - \frac{\ell(\ell + 1)}{r^2} \right] \psi = 0 \]  

(1.6)

where:

\[ K^2 = \frac{2mE}{\hbar^2} \]  

(1.7)
\[ \ddot{U}(r) = \frac{2m}{\hbar^2} V(r) \]  
(I.8)

Equation (I.6) is equivalent to a one-dimensional Schrödinger equation for a particle of mass \( m \) moving in an effective potential

\[ \ddot{U}(r) + \frac{\ell(\ell + 1)}{r^2} \]

where the second part is called the centrifugal potential, while the first part is the interaction potential.

For simplicity, we can write equation (I.6) as:

\[ \frac{d^2 \psi}{dr^2} + Q^2(r) \psi = 0 \]  
(I.9)

where

\[ Q^2(r) = \frac{k^2}{\hbar^2} \left( \ddot{U}(r) - \frac{\ell(\ell + 1)}{r^2} \right) \]  
(I.10)

The problem now is to find solutions for the radial Schrödinger equation: this problem is important especially when dealing with atomic and molecular physics assuming a central potential. In order to get results, one has to solve the radial Schrödinger equation for each value of \( \ell \). In many cases, the number of significant scattering phase shifts, for example, is so high that one has to use approximation methods. The JWKB approximation is often used in such cases.

1 - 2: The JWKB Approximation

Let us consider the case of a one-dimensional radial Schrödinger equation:

\[ Y'' + Q^2(x) Y = 0 \]  
(I.11)

where the \((')\) denotes the derivative with respect to \( x \).

a. If \( Q^2(x) = \text{constant} \), the solution is obvious:

\[ Y = \exp \left( \pm i Q x \right) \]  
(I.12)

b. If we consider a step potential which is pieced together from many steps and consists of many regions \( j \) where \( Q^2_j(x) = \text{constant} \) for \( x_j < x < x_{j+1} \) ; \( j = 1, 2, \ldots, N \) then, for each region, the solution will be:
\[ Y_j (x) = \exp \left[ \pm iQ_j x \right] \]  
(I.13)

The full solution would have to be pieced together from such basic solutions. For the solution, we would have a plane wave which adjusts its wavelength according to the changing \( Q_j^2 (x) \) according to:

\[ \lambda_j (x) = \frac{2\pi}{Q_j (x)} \]  
(I.14)

if we neglect reflection at each step.

c. For \( Q_j^2 (x) \) being a continuous function of \( x \), by trying the solution:

\[ Y(x) = s(x) \exp \left[ i \int Q(x) \, dx \right] \]  
(I.15)

one would have:

\[ Y' = \left( \frac{s'}{s} + iQ \right) Y \]  

and

\[ Y'' = \left[ \left( \frac{s'}{s} + iQ \right)^2 + \frac{s''}{s} - \left( \frac{s'}{s} \right)^2 + iQ^2 \right] Y \]

providing \( s \neq 0 \), the equation becomes:

\[ Y'' + Q^2 (x) Y = \frac{1}{a} \left( 2ia'Q + iaQ' + a'' \right) Y \]  
(I.16)

(I.16) gives two equations

1) \( a'' = 0 \) from the real part

2) \( 2a'Q + aQ' = 0 \) from the imaginary part.

Although these two equations are incompatible and consequently no solution of the intended form exists, usually the first equation is dropped and by solving the second equation, one has:

\[ a(x) = Q(x) \]  

which yields:

\[ a''(x) = -\frac{1}{4} \frac{Q''}{Q} (x) Q(x) + \frac{3}{4} Q''^2 (x) Q(x) \]

By inserting these expressions into equation (I.16) one gets:

\[ Y'' + \left[ \frac{Q^2}{4} - \frac{3}{4} \left( \frac{Q'}{Q} \right)^2 + \frac{1}{2} \frac{Q''}{Q} \right] Y = 0 \]  
(I.17)

The JWKB solutions are given as:
For $Q^2(x) > 0$, which corresponds to the classically allowed region:

$$Y_>(x) = Q(x)^{-\frac{1}{2}} \left[ c_1 \exp \left( i \int Qdx \right) + c_2 \exp \left( -i \int Qdx \right) \right] (1.18)$$

For $Q^2(x) < 0$, which corresponds to the classically forbidden region:

$$Y_<(x) = \left| Q(x) \right|^{-\frac{1}{2}} \left[ d_1 \exp \left( \int |Q| dx \right) + d_2 \exp \left( -\int |Q| dx \right) \right] (1.19)$$

where $c_1, c_2, d_1, d_2$ are constants which are determined by the boundary conditions.

This approximation is not valid anymore when one approaches the classical turning point: at a classical turning point, the solution is singular and has no longer a relation to the original Schrödinger equation:

From (1.10) we have: $Q(x) = \sqrt{2m[E - V(x)]}$ (1.20)

$Q(x_0) = 0$ yields the classical turning point $x_0$. One can see that for $Q(x) \rightarrow 0$, the solution is singular.

Due to that singularity, at the classical turning point $x_0$, the constants $c_1$ and $c_2$ on one side of the classical turning point cannot simply be taken as $d_1$ and $d_2$ on the other side.

In order to evaluate $c_1, c_2, d_1, d_2$ one needs to use the connection formulas: the method used to connect up the JWKB approximate solutions across the turning point is to fit an approximate potential function to the exact potential function $V(x)$ in the region of the turning point. (8)

1 - 3: The Langer Modification

In order to avoid the singularity of the wave function at the turning point and to find a solution which stays regular through the
turning point, Langer approximates the potential near the turning point by a linear one: (24)

The functions \( Y(x; \alpha, \beta) = S(x) \left[ \alpha J_{\gamma}(\gamma) + \beta J_{\gamma}(\gamma) \right] \) (I.21)

are solutions of the differential equations:

\[
Y'' + \left[ \frac{Q^2(x) + Q(x)}{x} \right] Y = 0
\]

(I.22)

where: \( Q(x) = \frac{S''(x)}{S(x)} \) (I.23)

\[
\gamma = \frac{1}{r + 2}
\]

(I.24)

and \( Q^2(x) \) has a Zero of order \( \gamma \).

Without loss of generality, we can assume \( x_0 = 0 \). \( x_0 \) is the Zero of \( Q^2(x) \) and thus the location of the classical turning point; \( \frac{1}{2} J_{\gamma} \)

are Bessel functions of order \( \gamma \), and \( S(x) = Q(x) \left[ x^\gamma \right] \) . (I.26)

Making the approximation of a linear potential (\( \gamma = 1; \gamma = \frac{1}{3} \))

one would have: \( S(x) = Q(x) \left[ x^\gamma \right] \) and

\[
S''(x) = \frac{3}{4} Q(x) Q^2(x) \left[ \frac{1}{2} \right] x^\gamma (x) - \frac{3}{2} Q(x) Q''(x) \left[ \frac{1}{2} \right] x^\gamma (x) - \frac{35}{36} Q(x) \left[ \frac{1}{2} \right] x^\gamma (x)
\]

(I.27)

This gives: \( Q(x) = \frac{3}{4} \left( \frac{Q'}{Q} \right)^2 - \frac{1}{2} \frac{Q''}{Q} - \frac{5}{36} \frac{Q^2}{x^2} \) (I.28)

Equation (I.22) becomes: \( Y'' + \left[ \frac{Q(x)}{x} - \frac{3}{4} \left( \frac{Q'}{Q} \right)^2 + \frac{1}{2} \frac{Q''}{Q} + \frac{5}{36} \frac{Q^2}{x^2} \right] Y = 0 \) (I.29)

solution (I.21) becomes: \( Y = Q(x) \left[ \frac{1}{2} \right] \left[ \alpha \frac{1}{2} \frac{J_{\gamma}}{x^\gamma} + \beta \frac{1}{2} \frac{J_{\gamma}}{x^\gamma} \right] \) (I.30)

That solution stays regular through the turning point. By comparison of equation (I.29) with the one given in the JWKB approximation (1.17), one can see that a single term is added: \( -\frac{5}{36} \frac{Q^2}{x^2} \)

This term vanishes for large distances from the turning point so it does no harm there and in the immediate neighbourhood of the turning
point, it affects the two other terms in (1.29). If one assumes a potential which is strictly linear through the turning point, this added term cancels exactly the two other terms: In fact, if $Q^2(x) = cx$ where $c$ is a constant, one can verify easily that:

$$-\frac{3}{4} \left( \frac{Q''}{Q} \right)^2 + \frac{1}{2} \frac{Q''}{Q} + \frac{5}{36} \frac{Q^2}{r^2} = 0$$

and equation (1.11) has an exact solution containing Bessel functions of order $1/3$ which stays regular through the turning point. Langer made the approximation of assuming the potential exactly linear through the turning point and proposed the modified equation (1.29) as an approximate radial equation.

It is important to note here that the method described holds also for potentials which have a zero of order $\omega$ higher than one. Of course the modified equation (1.29) in that case will not be the same and the solutions will be a combination of Bessel functions of order

$$\gamma = \frac{1}{\sqrt{\omega + 2}}$$
CHAPTER II

THE METHOD PROPOSED

II - 1: Notations.

By introducing

\[ U(\kappa) = \frac{2}{3} Q(\kappa) \],

we can reformulate the essentials of Equations (I.29) and (I.30) in the following way:

The function

\[ Y(\kappa) = \left( \frac{2}{3} \right)^{\frac{1}{3}} \left[ a_0 A(\zeta) + a_1 B(\zeta) \right], \]

where

\[ \zeta = \left( \frac{2}{3} \kappa \right)^{\frac{1}{3}} \text{Sign}(U) \]

and

\[ \kappa = \int_{x_0}^{x} \left| U(x) \right| \frac{1}{2} dx \]

represents the general solution to the differential equation

\[ Y'' - \left[ U(x) + \Delta \left[ \frac{U}{x} \right] \right] = 0 \]

Here,

\[ \Delta \left[ \frac{U}{x} \right] = \frac{3}{4} \left( \frac{U}{x} \right)^2 - \frac{1}{2} \frac{U''}{Q} - \frac{5}{36} \frac{Q^2}{\kappa^2} \]

or, in terms of \( U(x) \),

\[ \Delta \left[ \frac{U}{x} \right] = \frac{5}{16} \left[ \left( \frac{U'}{U} \right)^2 \right] - \frac{1}{4} \left( \frac{U''}{U} \right) - \frac{5}{36} \left( \frac{U}{x} \right) \]

The first zero of \( U(x) \) is at \( x = x_0 \), assumed to be at \( x_0 = 0 \) without loss of generality.

II - 2: Scaling Laws for \( \Delta \left[ \frac{U}{x} \right] \)

In order to carry out the method, one has to study first the behaviour of \( \Delta \left[ \frac{U}{x} \right] \) for any \( U(x) \).

Two scaling laws greatly extend the applicability of already known values of \( \Delta \left[ \frac{U}{x} \right] \):
a - The first law is concerned with potentials which differ only by a multiplicative constant \( c \). Let us suppose a potential \( U(x) \) for whom \( \Delta[U, x] \) is known; one can obtain directly, for any other potential \( CU(x) \), the corresponding \( \Delta[CU, x] \). One gets:

\[
\Delta[CU, x] = \Delta[U, x]
\]  (II.8)

b - The second law is concerned with potentials where the variable \( x \) is multiplied by a constant \( A \). By introducing a new variable defined as:

\[
x = Ax
\]  (II.9)

Then \( dx = Ad\bar{x} \). This can be generalised to give:

\[
A^n \frac{d^{(m)}}{dx^n} = \frac{d^{(m)}}{d\bar{x}^n}
\]  (II.10)

where \( d^{(m)} \) represents the \( n \)th derivative.

By looking into the expression of \( \Delta[U, x] \) and using (II.9) and (II.10) we find:

\[
\Delta[U, Ax] = \frac{1}{A^2} \Delta[U, \bar{x}]
\]  (II.11)

Similarly we have:

\[
\int (Ax) = A \int (\bar{x})
\]  (II.12)

\[
Z(Ax) = A^{2/3} Z(\bar{x})
\]  (II.13)

\[
U(Ax) = \frac{1}{A^2} U(\bar{x})
\]  (II.14)

With these two scaling laws, one is able to handle a wide range of potentials, with only one effort.

II - 3: Small \( x \) Behaviour Of \( \Delta[U, x] \)

Without loss of generality we assume the turning point at \( x = 0 \),
so that the small $x$ behaviour of $\Delta [U, x]$ will be the behaviour of $\Delta [U, x]$ near the classical turning point. Let us recall here that for the original JWKB approximation (section 1.2) $\Delta [U, x]$ is singular near the classical turning point. In section 1.3, for the approximation with the Langer modification assuming a strictly linear potential, $\Delta [U, x]$ was equal to zero.

In our general case, let us study the behaviour of $\Delta [U, x]$ near a classical turning point:

Let us consider a potential $U(x)$ with a linear leading term; the assumption we made for the potential to have a linear leading term near the classical turning point is valid in almost all the cases since the potential functions in all practical cases are continuous and Taylor-expandable which make the treatment valid for any potential.

We can expand $U(x)$ as:

$$U(x) = a_1 x^1 + a_2 x^2 + \ldots + a_n x^n$$  \hspace{1cm} \text{(II.15)}

without loss of generality, we can set $a_1 = 1$, and expand $\sqrt{U(x)}$ as:

$$\sqrt{U(x)} = \sqrt{x} \left[ 1 + b_1 x + b_2 x^2 + \ldots + b_m x^m \right]$$  \hspace{1cm} \text{(II.16)}

where the coefficients $b_i$ are related to the $a_i$'s by (1):

$$b_m = \frac{1}{m} \sum_{k=1}^{m} (mk - m + k)a_k b_{m-k}$$  \hspace{1cm} \text{(II.17)}

for $m > 1$ and $n = \frac{1}{2}$

$U'(x)$ and $U''(x)$ can be expanded from (II.17) and by making use of (II.19) with $n = 2$, $n = -1$ and $n = -2$, one is able to expand $\left[U'(x)\right]^2$, $U^{-1}(x)$ and $U^{-2}(x)$. $H(x)$ can be expanded also, using (II.18) as:

$$H(x) = \frac{2}{3} x^{3/2} \left[ 1 + \frac{3}{5} b_1 x + \frac{3}{7} b_2 x^2 + \ldots + \frac{3}{(2m + 3)} b_m x^m \right]$$  \hspace{1cm} \text{(II.18)}

and $H^{-2}(x)$ can also be obtained from (II.17).
Having now all the terms in the expression of \( \Delta[U,x] \) with series expansions, one can express \( \Delta[U,x] \) by a series expansion using the multiplication of power series relation given by: \( (1) \)

\[
\sum_{k=0}^{\infty} a_k x^k \sum_{k=0}^{\infty} b_k x^k = \sum_{k=0}^{\infty} c_k x^k \quad \text{with} \quad c_k = \sum_{k=0}^{\infty} a_k b_{m-k} \quad (II.19)
\]

the result obtained is:

\[
\Delta[U,x] = \frac{d_{-2}}{x^2} + \frac{d_{-1}}{x} + d_0 + d_1 x + \ldots + d_m x^m \quad (II.20)
\]

with \( d_{-2} = 0 \) and \( d_{-1} = 0 \) \( (II.21) \)

This is to say that \( \Delta[U,x] \) is not singular any more around the turning point for any potential providing that the potential can be expanded by a series with a linear leading term near the classical turning point. The term introduced in the expression of \( \Delta[U,x] \) according to the Langer modification (section I.3) and which was originally derived assuming a strictly linear potential, happens to be useful for any potential with a linear leading term: It takes out the singularity at the classical turning point.

With this result, \( \Delta[U,x] \) can be expressed by:

\[
\Delta[U,x] = d_0 + d_1 x + \ldots + d_m x^m \quad (II.22)
\]

The coefficients \( d_m \) are related to the \( a's \) in \( (II.15) \). Of course, it is always possible to put restrictions on the \( a's \) (which means on the potential itself) in order to make one or more coefficients of \( \Delta[U,x] \) equal to zero. This may be one way (though not general) to ensure a \( \Delta[U,x] \) which is small. A more detailed study of this possibility is given in Appendix A where \( U(x) \) was expanded as a polynomial of the 7th degree.

\(-4:\) **Large \( x \) Behaviour of \( \Delta[U,x] \)**

We can have a look at the asymptotic behaviour of \( \Delta[U,x] \) for large value of \( x \) by noting that in equation \( (II.7) \), all the three terms
in the expression of \( \Delta[U, x] \) behave like \( \frac{1}{x^2} \) asymptotically.

\[
\Delta[U, x] \xrightarrow[x \to \infty]{} \frac{1}{x^2}
\]

This behaviour is shown in Figures (II.1)'

**II - 5: Calculation Of \( \Delta[U, x] \)**

In order to evaluate \( \Delta[U, x] \) for a given \( U(x) \), the direct use of equation (II.7) presents limitations which one can avoid by a suitable numerical approach:

a - The most important limitation is that the classical turning point at \( x = 0 \) cannot be handled, although it should according to the result obtained in (section II.3). \( \Delta[U, x] \) cannot be evaluated for \( x = 0 \) in the form given in equation (II.7), because each individual term in (II.7) has a singular behaviour at \( x = 0 \).

b - Because of that, and in order to get accurate results, one has to use a double precision calculation which makes the computation time longer.

In order to avoid these limitations, let us introduce a function \( f(x) \) defined by:

\[
[U(x)]^{\frac{1}{2}} = x^{\frac{1}{2}} f(x) \tag{II.23}
\]

Since \( U(x) \) has a linear leading term near the turning point, we have:

\[
f(x = 0) = \text{constant which can be set to 1 without loss of generality.}
\]

\( f(x) \) can then be expanded as:

\[
f(x) = 1 + b_1 x + b_2 x^2 + \ldots + b_n x^n \tag{II.24}
\]

By squaring (II.23), one gets:

\[
U(x) = x f^2(x) \tag{II.25}
\]

\( U'(x) \) and \( U''(x) \) can be obtained as:

\[
U'(x) = f^2(x) + 2x f(x) f'(x) \tag{II.26}
\]
Large $x$ behaviour of $\Delta[u,x]$

Fig. (II.1)
\[ U''(x) = 4 f(x) f'(x) + 2x f(x) f''(x) + 2x^2 f'(x) \]  

(II.27)

\[ \mu(x) \text{ will be expressed as:} \]

\[ \mu(x) = \int_0^x \sqrt{x} f(x) \, dx \]  

(II.28)

Let us mention here that in order to calculate \( \mu(x) \) with enough accuracy, a Gauss integration of the type \( \int_0^x \sqrt{1+t^2} f(x) \, dx \) has been developed for polynomials \( f(x) \) up to the 7th degree. The Gauss integration method is given in Appendix B along with a general recursion formula for higher degrees of \( f(x) \).

Integrating (II.28) by parts gives:

\[ \mu(x) = \frac{2}{3} x^{3/2} f(x) - \frac{2}{3} \int_0^x \frac{3}{2} f'(x) \, dx \]  

(II.29)

or

\[ \mu(x) = \frac{2}{3} x^{3/2} \left[ f(x) - x \Omega_o(x) \right] \]  

(II.30)

with

\[ \Omega_o(x) = x^{-5/4} \int_0^x \frac{3}{2} f'(x) \, dx \]  

(II.31)

For \( \Delta \left[ \mu(x) \right] \) we find

\[ \Delta \left[ \mu(x) \right] = \frac{3}{4} \left[ \frac{f'(x)}{f(x)} \right]^2 - \frac{1}{2} \frac{f''(x)}{f(x)} + C(x) \]  

(II.32)

with

\[ C(x) = \frac{f(x) \cdot \Omega_1(x) - 2 \cdot \Omega_o(x) \left[ \frac{f'(x)}{f(x)} - \frac{5}{8} \Omega_o(x) \right] + x f'(x) \Omega_2^2(x) f(x)}{4 \Omega_2^2(x)} \]  

(II.33)

Here

\[ \Omega_1(x) = \left[ \frac{f'(x)}{f(x)} - \frac{5}{8} \Omega_o(x) \right] \]  

(II.34)

\[ \Omega_2(x) = f(x) - x \Omega_o(x) \]  

(II.35)

For \( f(x) = \sum_{n=0}^\infty b_n x^n \), one gets

\[ \Omega_o(x) = \sum_{n=0}^{N-1} \frac{2(n+1)}{12(n+2)} b_{n+1} x^{n+1} \]

\[ \Omega_1(x) = \sum_{n=0}^{N-1} \frac{2(n+1)(n+2)}{(2m+7)} b_{m+1} x^{m+1} \]

\[ \Omega_2(x) = \sum_{n=0}^{N} \frac{b_m}{(2n+3)} x^n \]  

(II.36)
With this new approach, a single precision calculation is used and gives accurate results. But mostly, the difficulties arising near \( x = 0 \) have been removed: In fact, one can now cover a range in \( x \) from negative values through Zero to positive values in a single effort.

Let us mention here that the singularity in the behaviour of \( \Delta [U, x] \) has been removed from the classical turning point at \( x = 0 \). However the singularity remains as one approaches the next turning point, if there is one. That is why, for each turning point, this method is valid around one turning point only.

For the case where there are many turning points, we can apply this approach at each turning point separately.

In summary, we can say here that, around each turning point, \( \Delta [U, x] \) is well behaved as long as it is not close to another turning point. Figure (II.2) shows an example of how to treat the many turning points problem using this approach.

**II - 6: The Problem With Conventional JWKB Methods**

In order to see the consequences of \( \Delta [U, x] \) let us recall here that in the JWKB approximation, \( \Delta [U, x] \) is singular near the classical turning point. An example is shown in Figure (II.3). With the larger modification, we have seen (section I.3) that, even though the singularity at the classical turning point has been taken care of and the solution is regular through the turning point, one problem still remained unsolved in the conventional JWKB method: the solution is not for the original potential \( U(x) \) but for a modified one which we denote by \( \widetilde{U}(x) = U(x) + \Delta [U, x] \). The larger \( \Delta [U, x] \) is compared to \( U(x) \), the more the solution given deviates from representing the
\[ U(x) \]

\[ \Delta[U, x] \]

\[ \Delta[U, x] \] evaluated for a potential with two turning points:

Each turning point region is treated separately, with the origin at the turning point.

Fig. (II.2)
The failure of the simple JWKB method:

The simple JWKB method implies a modification of the potential $U(x)$ (solid line) into another potential $U(x) + \Delta[U,x]$ (dotted line). At the turning point, $\Delta[U,x]$ is singular.

Fig. (II.3)
The conventional JWKB method incorporates Langer's modification and thus removes the singularity of \( \Delta[U, x] \) at the turning point. However, the original potential \( U(x) \) is still modified into \( U(x) + \Delta[U, x] \). The turning point is shifted to \( x_o = \tilde{x}_o \).

Fig. (11.4)
Conventional JWKB method:
The conventional JWKB method incorporates Langer's modification and thus removes the singularity of $\Delta[U,x]$ at the turning point. However, the original potential $U(x) = x(x + 1)$ is still modified into $U(x) + \Delta[U,x]$. Note that in this case the turning point $x_0$ has disappeared altogether.

Fig. (II.5)
solution for the original potential $U(x)$.

Figures (II.4) and (II.5) show for given potentials $U(x)$, the deviation due to $\Delta[U(x)]$. That deviation has as consequences:
- Wrong wave function near the turning point,
- Wrong tunneling behaviour,
- Energy level shifts,
- Shifts in the turning point location,
- Phase shift errors.

II - 7: The New Method

Suppose we wanted to solve the equation:

$$Y'' - W(x)Y = 0,$$  \hfill (II.37)

where $W(x)$ is the reduced, energy adjusted potential, i.e. the reduced actual potential less the reduced total energy so that the Zeroes of $W(x)$ are the classical turning points.

Up to now, the typical JWKB approach is to ask for

$$W(x) \approx U(x),$$

or, in other words, to require that

$$\Delta[U(x)] \approx 0$$

in order to have (II.2) as the approximate solution. However, it is and remains an approximation, even when other corrections are applied. A study of this possibility is given in Appendix A.

In contrast to the above we now require

$$W(x) = U(x) + \Delta[U(x)]$$  \hfill (II.38)

even if $\Delta[U(x)]$ is very large.\footnote{Note that the turning points of $W(x)$ and $U(x)$ are at different values of $x$. As before, we will continue to choose the turning point of $U(x)$ as $x = x_0 = 0$ without loss of generality. Thus, e.g. the lower integration limit in (II.3) is the classical turning point of $U(x)$ and not of $W(x)$. However, this "shift" in the turning point is easily taken into account by a "shift" in the $x$ - origin.}
Schematic of JWKB methods:

Use of JWKB methods imply a modification of the original potential $W(x)$ by a term $\Delta(W, x)$. Therefore, the analytical solution $Y$ is a good approximate solution only as long as $\Delta(W, x)$ remains small.
With equation (II.38) valid, we now have as solutions the functions of equation (II.2) provided we have found a "substitute potential" $U(x)$ which indeed obeys equation (II.38).

Therefore, our effort is to:

1. Show that $\Delta[U, X]$ is a well behaved function everywhere; this is done in section (II.3), and

2. Show that equation (II.38) can indeed be solved to any accuracy desired.

Thus, the problem of solving the Schrödinger equation is equivalent to solving the integro-differential equation (II.38). This looks at first like a more difficult task when looking at the equation. However, the following points are to be considered:

- There is no oscillatory behaviour in the $U(x)$ involved. This allows much lower degree polynomials for representing $U(x)$ within a certain accuracy.

- It is already a known fact the $\Delta[U, X]$ will become negligible far away from the turning point, thus making $W(x) \approx U(x)$ asymptotically.

- From the above it follows that, in practice, one has to solve equation (II.38) for only a limited region around the turning point, but still covers the whole range of $x$.

II - 8: Iteration Procedure And Results

Various methods may be employed in the effort to find the "substitute potential" $U(x)$. In this work, an iteration method has proved successful in all cases treated so far.

The iteration starts with $U_o(x) = U_o(x) + \Delta[U_o, X]$ where $U_o(x) = W(x)$

The potential defect $P_o(x)$ is:
\[ P_0(x) = U(x) - \left[ U_0(x) + \Delta [U_0, x] \right] \]  

(II.39)

We anticipate this defect by using a new potential \( U_1(x) \) such that:

\[ U_1(x) = U_0(x) + \lambda P_0(x) \]  

(II.40)

The value of \( \lambda \) is arbitrary and is used in order to enhance the convergence.

After \( m \) iterations, the modified potential will be:

\[ \tilde{U}_m(x) = U_m(x) + \Delta [U_m, x] \]  

(II.41)

and

\[ P_m(x) = U(x) - \left[ U_m(x) + \Delta [U_m, x] \right] \]

At the end we would have:

\[ V(x) = U(x) + \Delta [U, x] + P(x) \]  

(II.42)

Once \( V(x) < \epsilon \) for all values of \( x \) is reached the analytic solution which is given for \( U(x) \) with Airy functions, will then be the exact solution for the differential equations with the originally wanted potential \( U(x) \) given in (II.37).

A schematic figure is presented to summarize the idea described here in Figure (II.7).

Some of the results are shown in Figures (II.8) and (II.9).

One can make some remarks at this point:

a - The convergence of the iteration procedure has (so far) been successful for any of the various potentials used having a linear leading term through the classical turning point. However a rigorous study of the convergence properties of the iteration procedure is still to be done.

b - Varying the value of \( \lambda \), which is arbitrary, within limits, leads to faster or slower convergence in practice, depending upon \( U_0(x) \) and \( \Delta [U_0, x] \)

c - At all times, the analytical solution (II.2) is the exact solution for the potential \( U_m(x) + \Delta [U_m, x] \) Thus, all deviations from other
exact theoretical values are solely due to the potential difference $P(x)$ between $U_m(x) + \Delta [U, x]$ and $W(x)$, i.e. the accuracy set or achieved in solving equation (II.38). There are no other errors of uncontrolled origin.

- For any function $U(x)$ which is analytic in the complex $x$ plane, $\Delta [U, x]$ is also analytic except for singularities due to "turning points" $x_\pm$ (for which $U(x_\pm) = 0$) other than the one at the origin. When such points $x_\pm$ lie on the real axis, a separate treatment is carried out at each such point (see following chapters). One could not imagine the case where such a point $x_\pm$ lies close, but not on, the real axis. This situation could possibly arise when the energy is "slowly being taken over a potential hump", i.e. when two classical turning points in $W(x)$ merge and then disappear from the real axis and wander off into the complex plane.

Again, a more detailed study of this physical situation is planned for the near future. It should be noted however that, in all cases so far studied, $U(x)$ tended to "straighten out" $W(x)$ (e.g. see Fig. II.4, II.5, II.8 and II.9). Thus, a double turning point in $W(x)$ will still lead to a $U(x)$ with a leading linear term and its turning point shifted by quite a bit. And it is the turning point of $U(x)$ and not of $W(x)$ which count in this method.

- The iteration method used here is hopefully only one of many successful methods to solve equation (II.38). One avenue yet to be explored (among others) is to set up an equivalent system of coupled differential equations.
Schematic of the method proposed in this work:

Rather than using the original potential \( W(x) \) when constructing the analytical solution \( Y \), one now takes a substitute potential \( U(x) \) which satisfies \( W(x) = U(x) + \Delta [U, x] \).
The substitute potential of the method proposed:

The substitute potential $U(x)$ found by the method proposed compared to the original potential $W(x)$ of Figure (II.4).
The substitute potential of the method proposed:

The substitute potential \( U(x) \) found by the method proposed compared to the original potential \( W(x) \) of Figure (II.5).

Fig. (II.9)
CHAPTER III
APPLICATIONS TO POTENTIALS WITH TWO TURNING POINTS:
SINGLE BOWL POTENTIALS

III - 1: Methods Application

After we presented the method, we are going to apply it, in this chapter, to study a potential which has only two turning points for each energy level. Let us call this potential \( W(x) \).

The corresponding reduced and energy adjusted potential will again be called \( U(x) \).

We denote the classical turning points by \( 1 \), \( 2 \) starting from the innermost one to the outermost. We also denote the regions around each turning point by the indices 1 and 2.

Around the turning point \( 1 \) we choose a region 1, and a region 2 around the turning point \( 2 \), in such a way that the two regions overlap. (See Fig. III.1)

By using the iteration procedure described previously in section II.8, one can find, for each region, the corresponding reduced, energy adjusted potentials \( U_i(x) \) and \( U_\omega(x) \) in each region.

The overlapping region is used in order to find the point \( x_\omega \) where the values of \( Z_1 \) and \( Z_\omega \), corresponding respectively to \( U_i(x) \) and \( U_\omega(x) \), are equal. At this location, i.e. at \( x = x_\omega \), we finally place the "cut" i.e. the boundary between region 1 and 2. (See Fig. III.2)

According to (II.8), the solution in region 1 is given by:

\[
Y_1(x) = \left| Z_1 \right|^\frac{k}{2} \left[ a_{1,1} A_1(Z_1) + a_{2,1} B_1(Z_1) \right] \quad \text{(III.1)}
\]

where \( Z_1 \) corresponds to \( U_1(x) \)

and in region 2 we have the solution:

\[
Y_\omega(x) = \left| Z_\omega \right|^\frac{k}{2} \left[ a_{1,2} A_1(Z_\omega) + a_{2,2} B_1(Z_\omega) \right] \quad \text{(III.2)}
\]

where \( Z_\omega \) corresponds to \( U_\omega(x) \).
The method proposed applied to a potential with two turning points:
Around each turning point, the original potential \( W(x) \) is substituted by the potentials \( U_1(x) \) and \( U_2(x) \), both of which satisfy \( W(x) = U_1(x) + U_2(x) \) within the overlapping regions.

Fig. (III.1)
Substitute potentials $U_1$ and $U_2$ between two turning points:

The location of the cut between region 1 and 2 is chosen so that $Z_1 = Z_2$ at the cut. $x_{0,1}$ and $x_{0,2}$ are the origins for $U_1$ and $U_2$ respectively.

Fig. (III.2)
III - 2: Connection Matrix

In order to connect the coefficients $a_1$ and $a_2$ in both regions, we use a connection matrix. At the cut, we also have $\mu_1 = \mu_2$ according to (II.5). In that case, the Airy functions $A_1$ and $B_1$ which are functions of their argument $Z$ will also be equal at the cut. If we add the subscript $c$ to denote the respective values at the cut, we would have:

\[
\begin{align*}
Z_{1,c} &= Z_{2,c} = Z \\
\mu_{1,c} &= \mu_{2,c} = \mu \\
A_1(Z_{1,c}) &= A_1(Z_{2,c}) = A \\
B_1(Z_{1,c}) &= B_1(Z_{2,c}) = B \\
A''_1(Z_{1,c}) &= A''_1(Z_{2,c}) = A'' \\
B''_1(Z_{1,c}) &= B''_1(Z_{2,c}) = B''
\end{align*}
\]  

(III.3)

where the (\('\) denotes the derivative with respect to $Z$.

At the cut, the wave function and its first derivative in region 1 are equal to those in region 2. This leads to:

\[
\begin{align*}
a) & \quad Y_1(x_{1,c}) = Y_2(x_{2,c}) \\
b) & \quad \frac{dy_1(x_{1,c})}{dx} = \frac{dy_2(x_{2,c})}{dx}
\end{align*}
\]

where $x_1$ and $x_2$ are the abscissas corresponding to the origins for $U_1(x)$ and $U_2(x)$ respectively. If we denote by $x_{o,1}$ and $x_{o,2}$ the abscissas of the turning points $1$ and $2$ and by $x_{1,2}$ the distance between the two turning points, we can introduce new coordinates $x_i$ $(i = 1, 2)$ for each turning point which serve just like the $x$-coordinate in Chapter II.

\[
\begin{align*}
x_{1} &= x - x_{o,1} \\
x_{2} &= x - x_{o,2} \\
x_{1,2} &= x_{o,2} - x_{o,1}
\end{align*}
\]

(III.4)

this leads to: $dx_1 = dx_2 = dx$
Condition (a) yields:

\[
|U_1|^{-k} \left[ a_{1,1} A + a_{2,1} B \right] = |U_2|^{-k} \left[ a_{1,2} A + a_{2,2} B \right] (III.5)
\]

In order to evaluate condition (b), we first take the derivative of the wave function with respect to \(x\), denoted by \(\dot{}\).

We denote \(\text{sign} \left[ U(x) \right]\) by \(s\), and obtain from

\[
Y(\alpha) = |Z|^\frac{k}{2} |U|^{-k} \left[ a_1 A + a_2 B \right]
\]

the following relations:

\[
Y' = Y Z' \\
Y^* = \frac{s}{4} \left[ |Z|^\frac{k}{2} |U|^{-k} \right] \left[ a_1 A + a_2 B \right] + |Z|^\frac{k}{2} |U|^{-k} \left[ a_1^* + a_2^* \right]
\]

\[
Y' = |Z|^\frac{k}{2} |U|^{-k} \left[ \frac{1}{4} \left( \frac{Z_1^* - U_1^*}{Z} \right) (a_1 A + a_2 B) + Z_1^* (a_1^* + a_2^* B) \right] (III.6)
\]

Then condition (b) results in:

\[
|U_1|^{-k} \left[ \frac{1}{4} \left( \frac{Z_1^* - U_1^*}{Z} \right) (a_1,1 A + a_2,1 B) + Z_1^* (a_1,1 A^* + a_2,1^* B) \right] = (III.7)
\]

\[
|U_2|^{-k} \left[ \frac{1}{4} \left( \frac{Z_2^* - U_2^*}{Z} \right) (a_2,1 A + a_2,2 B) + Z_2^* (a_2,1 A^* + a_2,2^* B) \right]
\]

The two equations which connect the coefficients in both regions can be written as:

\[
a_{1,1} b_1 + a_{2,1} b_2 = a_{1,2} b_3 + a_{2,2} b_4
\]

\[
a_{1,1} c_1 + a_{2,1} c_2 = a_{1,2} c_3 + a_{2,2} c_4
\]

(III.8)

where:

\[
b_1 = |U_1|^{-k} A
\]

\[
b_2 = |U_1|^{-k} B
\]

\[
b_3 = |U_2|^{-k} A
\]

\[
b_4 = |U_2|^{-k} B
\]

\[
c_1 = |U_1|^{-k} \left[ \frac{1}{4} \left( \frac{Z_1^* - U_1^*}{Z} \right) \right] A + Z_1^* A^*
\]

(III.9)

\[
c_2 = |U_1|^{-k} \left[ \frac{1}{4} \left( \frac{Z_1^* - U_1^*}{Z} \right) \right] B + Z_1^* B^*
\]

\[
c_3 = |U_2|^{-k} \left[ \frac{1}{4} \left( \frac{Z_2^* - U_2^*}{Z} \right) \right] A + Z_2^* A^*
\]
\[ c_4 = \left| U_2 \right|^{-1} \left[ \frac{1}{4} \left( \frac{Z_{1,2}}{Z_1} - \frac{U_{1,2}}{U_2} \right) B + \frac{Z_{1,2}}{Z_2} B^* \right] \]

Equations (III.8) will give us:

\[ a_{1,1} = \frac{b_1 c_2 - b_2 c_1}{b_1 c_2 - b_2 c_1} a_{1,2} + \frac{b_2 c_1 - b_1 c_2}{b_1 c_2 - b_2 c_1} a_{2,2} \]

\[ a_{2,1} = \frac{b_1 c_2 - b_2 c_1}{b_1 c_2 - b_2 c_1} a_{1,2} + \frac{b_2 c_1 - b_1 c_2}{b_1 c_2 - b_2 c_1} a_{2,2} \]

Equations (III.10) give the coefficients in region 1 as a function of those in region 2. Those equations can be expressed as a matrix equation by:

\[ \tilde{a}_1 = \begin{bmatrix} M_{1,2} \end{bmatrix} \tilde{a}_2 \] (III.11)

with:

\[ \tilde{a}_1 = \begin{pmatrix} a_{1,1} \\ a_{2,1} \end{pmatrix}, \quad \tilde{a}_2 = \begin{pmatrix} a_{1,2} \\ a_{2,2} \end{pmatrix} \]

\[ \begin{pmatrix} A & B^2 \\ -A & -AB \end{pmatrix} \neq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

\[ [M_{1,2}] = D_{1,2} \begin{pmatrix} \pi G_{1,2} \begin{pmatrix} A & B \\ -A & -AB \end{pmatrix} + \pi(1 - C_{1,2}) \end{pmatrix} + \begin{pmatrix} A & B \\ -A & -AB \end{pmatrix} \]

(III.12)

and:

\[ D_{1,2} = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} \]

\[ C_{1,2} = \frac{Z_{1,2}^*}{Z_1} \]

\[ G_{1,2} = \frac{1}{4Z_{1,2}^*} \left( \frac{Z_{1,2}^*}{Z_1} - \frac{U_{1,2}}{U_1} - \frac{Z_{1,2}^*}{Z_2} + \frac{U_{1,2}}{U_2} \right) \]

If we call:

\[ \alpha_{1,2} = \pi \left[ G_{1,2} A + (1 - C_{1,2}) A^* \right] \] (III.14)

\[ \beta_{1,2} = \pi \left[ G_{1,2} B + (1 - C_{1,2}) B^* \right] \] (III.15)
one gets:

\[
[M_{1,2}] = D_{i,2} \begin{pmatrix} B \alpha_{1,2} & B\beta_{1,2} \\ -A\alpha_{1,2} & -A\beta_{1,2} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{III.16}
\]

We can obtain similarly the coefficients in region 2 as function of those in region 1. The connection matrix will be denoted by \([M_{2,1}]\) and given by:

\[
[M_{2,1}] = D_{2,1} \begin{pmatrix} B\alpha_{2,1} & B\beta_{2,1} \\ -A\alpha_{2,1} & -A\beta_{2,1} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{III.17}
\]

with:

\[
D_{2,1} = \frac{U_2}{U_1}
\]

\[
\alpha_{2,1} = \pi \left[ G_{2,1} A + (1 - C_{2,1}) A^T \right]
\]

\[
\beta_{2,1} = \pi \left[ G_{2,1} B + (1 - C_{2,1}) B^T \right]
\]

\[
C_{2,1} = \frac{Z_1^T}{Z_2^T}
\]

\[
G_{2,1} = \frac{1}{4Z_2^T} \left( Z_1^T - \frac{U_2^T}{Z} - \frac{Z_2^T}{Z} + \frac{U_1^T}{Z} \right)
\]

We can see from (III.13) and (III.18) that:

\[
D_{2,1} = \frac{1}{D_{i,2}}
\]

\[
C_{2,1} = \frac{1}{C_{i,2}} \tag{III.19}
\]

\[
G_{2,1} = - \frac{G_{i,2}}{C_{i,2}}
\]

one can verify that:
\[ \text{det} \left( M_{1,2} \right) = D_{1,2} \quad C_{1,2} \]
\[ \text{det} \left( M_{2,1} \right) = D_{2,1} \quad C_{2,1} \]
\[ \left[ M_{1,2} \right]_5 \left[ M_{2,1} \right]_5 = \left[ M_{2,1} \right]_5 \left[ M_{1,2} \right]_5 = I \]

where \( I \) is the unit matrix defined by:
\[
I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

If we consider now a potential symmetric about the cut, those results become simpler, namely:
\[
U_1 \quad (x_1, c) = U_2 \quad (x_2, c) = U
\]
\[
Z_1^* = -Z_2^* = Z^*
\]
\[
U_1^* = -U_2^* = U^*
\]

We add the label \( s \) for the symmetric case.

The connection matrix will be given by:
\[
\left[ M_{1,2} \right]_5 = \left[ M_{2,1} \right]_5 = \begin{pmatrix} B(\alpha_{1,2})_s & B(\beta_{1,2})_s \\ -A(\alpha_{1,2})_s & -A(\beta_{1,2})_s \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

with:
\[
(\alpha_{1,2})_s = (\alpha_{2,1})_s = \tau \left[ (G_{1,2})_s A + 2A^* \right]
\]
\[
(\beta_{1,2})_s = (\beta_{2,1})_s = \tau \left[ (G_{1,2})_s B + 2B^* \right]
\]
\[
(D_{1,2})_s = (D_{2,1})_s = 1
\]
\[
(C_{1,2})_s = (C_{2,1})_s = -1
\]
\[
(G_{1,2})_s = (G_{2,1})_s = \frac{1}{2Z^*} \left( \frac{Z^*}{Z} - \frac{U^*}{U} \right)
\]

we can verify also that:
\[
\text{det} \left( M_{1,2} \right)_s = \text{det} \left( M_{2,1} \right)_s = -1
\]
\[
\left[ M_{1,2} \right]_5 \left[ M_{2,1} \right]_5 = \left[ M_{2,1} \right]_5 \left[ M_{1,2} \right]_5 = I
\]
III - 3: Classical Limit

The classical limit is obtained for values of $Z \gg 1$. We can use the asymptotic expressions of the Airy functions and their derivatives. For $Z$ large, we have (1):

\[
\begin{align*}
A_1 (Z) &\rightarrow \frac{1}{2} \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} e^{-\frac{Z}{2}} \\
B_1 (Z) &\rightarrow \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} e^{\frac{Z}{2}} \\
A_1^* (Z) &\rightarrow -\frac{1}{2} \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} e^{\frac{Z}{2}} \\
B_1^* (Z) &\rightarrow \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} e^{\frac{Z}{2}} \\
A_1 (-Z) &\rightarrow \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} \sin \left( \frac{Z}{2} + \frac{\pi}{4} \right) \\
B_1 (-Z) &\rightarrow \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} \cos \left( \frac{Z}{2} + \frac{\pi}{4} \right) \\
A_1^* (-Z) &\rightarrow -\pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} \cos \left( \frac{Z}{2} + \frac{\pi}{4} \right) \\
B_1^* (-Z) &\rightarrow \pi^{-\frac{1}{2}} |Z|^{-\frac{1}{2}} \sin \left( \frac{Z}{2} + \frac{\pi}{4} \right)
\end{align*}
\]

a) The classically allowed region:

For the case where $U(x) < 0 \Rightarrow Z < 0$, the connection matrix will be given by:

\[
[M_{1,2}]_{<0} = \frac{1}{2} D_{1,2} \left( \begin{array}{cc}
\sin \vartheta & \cos \vartheta \\
\cos \vartheta & -\sin \vartheta
\end{array} \right) + \left( \begin{array}{c}
0 \\
1
\end{array} \right)
\]

\[
\left( 1 - C_{1,2} \right) \left( \begin{array}{cc}
\cos \vartheta & -\sin \vartheta \\
-\sin \vartheta & -\cos \vartheta
\end{array} \right) + \left( \begin{array}{c}
1 \\
0
\end{array} \right) \left( \begin{array}{c}
0 \\
1
\end{array} \right)
\]

with $\vartheta = \frac{Z}{2} + \frac{\pi}{2}$ (III.24)

b) The classically forbidden region:

For the case where $U(x) > 0 \Rightarrow Z > 0$, we will have:
\[
\left[ N_{1, 2} \right]_{\gamma_0} = D_{1, 2} \left( \frac{G - 2}{\pi \nu} \left[ Z - \left( 1 - C_{1, 2} \right) \right] \right) \left( \begin{array}{c}
1 \\
2e^{2^k}\end{array}\right) + \left( \begin{array}{c}
1 \\
0\end{array}\right)
\]

(III.25)

III - 4: Phase Shifts

If we assume that for large values of x, the function \( Q^2(x) \) approaches a constant value \( Q_{\infty}^2 > 0 \), then \( U(x) \) will approach a negative constant. In this case \( Z \) will be negative, and the asymptotic behaviour of the wave function will be obtained by using the asymptotic behaviour of the Airy functions and their derivatives where \( Z \) is large and negative. (see III.24)

Let us denote the coefficients of the wave function in that region by \( a_{1, \infty} \) and \( a_{2, \infty} \) then:

\[
Y(x \to \infty) = \left[ \begin{array}{c}
\pi^{-\frac{1}{4}} |U|^{-\frac{1}{4}} \\
\end{array}\right] \left[ a_{1, \infty} \sin (\gamma + \eta_{\infty}) + a_{2, \infty} \cos (\gamma + \eta_{\infty}) \right]
\]

(III.26)

This can be written as:

\[
Y(x \to \infty) = \left[ \begin{array}{c}
\pi^{-\frac{1}{4}} |U|^{-\frac{1}{4}} \\
\end{array}\right] A_{\infty} \cos (\gamma + \eta_{\infty} + \eta_{im})
\]

(III.27)

where \( A_{\infty} \) is the amplitude of the wave function at \( x \to \infty \) and \( \eta_{im} \) is a phase shift.

Comparing (III.27) and (III.26) gives:

\[
\begin{align*}
A_{\infty}^2 & = a_{1, \infty}^2 + a_{2, \infty}^2 \\
\tan \eta_{\infty} & = -\frac{a_{1, \infty}}{a_{2, \infty}}
\end{align*}
\]

(III.28) (III.29)

The JWKB phase shift is given by:

\[
\eta_{JWKB} = \lim_{x \to \infty} \left( \int_{x_0}^{x} \sqrt{|U|} \, dx - \int_{x_0}^{x} \sqrt{|U_0|} \, dx \right)
\]

(III.30)

where \( \sqrt{|U_0|} \) represents the case without interaction potential and \( x_0 \) and \( x_{\infty} \) represent the respective outermost classical turning points, respectively, and
\( \sqrt{|U|} \) represents the case with interaction potential.

The total phase shift will then be given by:

\[
\eta = \lim_{x \to \infty} \left( \int_{x}^{x} \sqrt{|U|} \, dx - \int_{x}^{x} \sqrt{|U_0|} \, dx \right) + \eta_{in} \quad (III.31)
\]

We can see that, in addition to the well known JWKB phase shift, there is another contribution to it, \( \eta_{in} \), due to effects arising from inner potential bowls.

**III - 5: Eigenvalues**

By applying the method proposed, we will see that the eigenvalues for a potential with two turning points, are obtained by solving a polynomial equation of degree 1. The potentials with more than two turning points will be studied in Chapter IV and the results will be similarly simple.

It is known that, in order to obtain a stationary state with given energy (eigenvalue), the wave function must vanish in the limit \( x \to \pm \infty \).

If we say that, without loss of generality, in region 1 (containing the first turning point), the coefficients of the wave function are for \( x \to \pm \infty \):

\[
a_1, 1 = 1 \quad \text{and} \quad a_2, 1 = 0
\]

then, in region 2 (containing the second turning point), the coefficients of the wave function should be:

\[
a_1, 2 = R \quad \text{and} \quad a_2, 2 = 0
\]

where \( R \) is a constant, if and only if the energy is an eigenvalue.
The quantum condition for eigenvalues is then:

\[
\begin{pmatrix}
\mathbf{X} \\
\mathbf{0}
\end{pmatrix} = 
\begin{bmatrix}
\mathbf{M}_{2,1}
\end{bmatrix}
\begin{pmatrix}
1 \\
0
\end{pmatrix}
\]  

(III.32)

(III.32) gives two equations:

\( a) \quad D_{2,1} \cdot (B \cdot \alpha_{2,1} + 1) = R \)  

(III.33)

\( b) \quad -D_{2,1} \cdot A \cdot \alpha_{2,1} = 0 \)  

(III.34)

equation (III.34) is satisfied for:

\[ \alpha_{2,1} = 0 \]  

(III.35a)

or \[ A = 0 \]  

(III.35b)

For \( \alpha_{2,1} = 0 \), equation (III.35) will give:

\[ R = D_{2,1} > 0 \]

For \( A = 0 \), equation (III.33) becomes:

\[ D_{2,1} \left[ \frac{\pi B A^\prime (1 - C_{2,1}) + 1}{\pi} \right] \mathbf{X} = R \]

Since the Wronskian \( W(A, B) = \frac{1}{\pi} \), this leads (for \( A = 0 \)) to

\[ B A^\prime = \frac{1}{\pi} \]

Finally, equation (III.33) gives:

\[ R = D_{2,1} \cdot C_{2,1} < 0 \]

One finds that \( \alpha_{2,1} = 0 \) corresponds to an eigenvalue whenever the wave function is symmetric and \( A = 0 \) corresponds to an eigenvalue whenever the wave function is antisymmetric. The solutions alternate starting from \( \alpha_{2,1} = 0 \). It is clear that the polynomial in \( \xi \) of degree one to be solved is:

\[ \xi - A \alpha_{2,1} = 0 \]  

(III.36)

For the symmetric case where \( D_{2,1} = 1 \) and \( C_{2,1} = -1 \) we would have:

\[ R = \pm 1 \]

We can also derive the well known semi-classical condition for
eigenstates by solving (III.36) in the classical limit using the connection matrix \( [M_r^s] \) given in (III.24).

\[-G_{22}^i \left\{ 2 \pi \frac{1}{\sqrt{n}} \sin \left( \frac{\beta}{n} + \frac{n}{2} \right) + \sin \left( \frac{\beta}{n} + \frac{n}{2} \right) \cos \left( \frac{\beta}{n} + \frac{n}{2} \right) \right\} = 0 \quad (III.37)\]

which yields for \( |z| \gg 1 \):

\[\beta = (n + \frac{1}{2}) \pi \quad (III.38)\]

and knowing that \( \beta = \int_{x_{01}}^{x_{n2}} \frac{1}{\sqrt{|U|}} \, dx \), this gives the semi-classical condition for eigenstates:

\[\int_{x_{01}}^{x_{n2}} \frac{1}{\sqrt{|U|}} \, dx = (n + \frac{1}{2}) \pi \quad (III.39)\]

III - 6: Results

The eigenvalue condition has been applied to an harmonic oscillator and the results have been compared to the ones given by theoretical methods and also to the ones obtained using the solutions based on the original potential \( W(x) \).

The condition for eigenvalues given in (III.36) was derived independently of the choice of the potential. It is based on the fact that the solution of the Schrödinger equation consists of a combination of Airy functions \( A_1 \) and \( B_1 \). That condition will be applied to two cases: first to the solution based on the originally wanted potential \( W(x) \) and then to the solution based on the potential \( U(x) \) found by using the iteration method. The eigenvalues in both cases will be compared to the exact theoretical values.

Condition (III.36) will be expressed in the symmetric case by:

\[\tau \left[ \frac{1}{2} \left( \frac{1}{Z} - \frac{U^*}{Z^*U} \right) A^2 + 2AA^* \right] = 0 \quad (III.40)\]

the left hand quantity is a function of the energy \( E \). The solutions of (III.40) correspond to the eigenvalues. Let us call that quantity \( \Sigma(E) \).
\[ \varepsilon(E) = n \left[ \frac{1}{2} \left( \frac{1}{2} - \frac{V^p}{Z^2 U^2} \right) A^2 + 2 AA^* \right] \]  

(III.41)

Let us assume an harmonic oscillator interaction potential

\[ V_0(x) = \frac{1}{2} fx^2. \]

The reduced, energy adjusted potential is:

\[ W(x) = \frac{2m}{\hbar^2} \left[ \frac{1}{2} fx^2 - E \right] \]

(III.42)

It is known that the energy levels of an harmonic oscillator are given by:

\[ E_n = \left( n + \frac{1}{2} \right) \hbar \sqrt{\frac{f}{m}} \]

(III.43)

By making a suitable substitution of variable so that the zeroes of \( W(x) \) will correspond to the classical turning points, (III.42) becomes:

\[ W(x) = \frac{mE}{\hbar^2} x \left( x + 2 \sqrt{\frac{2E}{f}} \right) \]

(III.44)

One can choose for simplicity \( m = \frac{\hbar^2}{2} \) and \( f = 2 \).

This yields:

\[ W(x) = x \left( x + 2 \sqrt{E} \right) \]

(III.45)

According to (III.43) the exact theoretical energy levels are:

\[ E_0 = 1; \quad E_1 = 3; \quad E_2 = 5 \]

(see Fig. III.4)

Equation (III.41) can be solved for different values of \( W(x) \) which corresponds to different values of the energy. The zeroes of (III.41) which correspond to the eigenvalues can be found, in practice, by approximating \( g(E) \) by a linear function of \( E \) in a small interval on both sides of the expected energy eigenvalues. \( g(E) \) is then found by linear interpolation. By plotting the results obtained in (Fig. III.3), we find that, by using the originally wanted potential, there is a shift in the first energy level by an amount of 14%. If \( U(x) \) is used, the shift is less than 1%. In practice, this small shift of 1% is
EXACT
USING $W(x)$
USING $U(x)$

Energy levels for the harmonic oscillator:

Energy levels for the harmonic oscillator, using the conventional JWKB method ($\ldots\ldots\ldots$), using method proposed ($\ldots\ldots\ldots$), and exact values ($\ldots\ldots\ldots$). A moderate accuracy of 1% was chosen for $U(x)$ in order to show its influence upon the eigenenergies.

Fig. (III.3)
Energy levels and eigenfunctions of the harmonic oscillator:

The exact Hermite polynomial solution was compared to the eigenfunctions produced by the proposed method. The differences are too small to be shown here. See table (III.1) for more detailed comparison.

Fig. (III.4)
attributed to the degree of accuracy in the calculations. If necessary, higher degrees of accuracy are easily accessible.

The same technique has been applied to higher energy levels. It appears that the shift caused by the use of \( W(x) \) becomes smaller and smaller. In that particular case, for the second energy level, the amount of the shift is about 4%. For the third energy level and higher, the shift is smaller than that.

The eigenfunctions for the harmonic oscillator have also been evaluated with the proposed method and compared with the exact Hermite polynomial solutions (Fig. III.3).

Since the differences are too small to be shown on the plot, table (III.1) is given for a more detailed comparison.
### HERMITE POLYNOMIAL

<table>
<thead>
<tr>
<th>x</th>
<th>Y₀</th>
<th>x</th>
<th>Y₁</th>
<th>x</th>
<th>Y₂</th>
<th>x</th>
<th>Y₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.751125</td>
<td>0.1</td>
<td>0.144345</td>
<td>0.2</td>
<td>0.151951</td>
<td>0.3</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.053563</td>
<td>0.746472</td>
<td>0.15</td>
<td>0.144345</td>
<td>0.25</td>
<td>0.151951</td>
<td>0.35</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.0153126</td>
<td>0.742457</td>
<td>0.25</td>
<td>0.259979</td>
<td>0.35</td>
<td>0.259979</td>
<td>0.45</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.0314699</td>
<td>0.7381707</td>
<td>0.35</td>
<td>0.259979</td>
<td>0.45</td>
<td>0.259979</td>
<td>0.55</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.062251</td>
<td>0.734257</td>
<td>0.45</td>
<td>0.259979</td>
<td>0.55</td>
<td>0.259979</td>
<td>0.65</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.0933164</td>
<td>0.730597</td>
<td>0.55</td>
<td>0.259979</td>
<td>0.65</td>
<td>0.259979</td>
<td>0.75</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.123203</td>
<td>0.727023</td>
<td>0.65</td>
<td>0.259979</td>
<td>0.75</td>
<td>0.259979</td>
<td>0.85</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.1535953</td>
<td>0.723620</td>
<td>0.75</td>
<td>0.259979</td>
<td>0.85</td>
<td>0.259979</td>
<td>0.95</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.183823</td>
<td>0.720429</td>
<td>0.85</td>
<td>0.259979</td>
<td>0.95</td>
<td>0.259979</td>
<td>1.05</td>
<td>-0.531120</td>
</tr>
<tr>
<td>0.213919</td>
<td>0.717490</td>
<td>0.95</td>
<td>0.259979</td>
<td>1.05</td>
<td>0.259979</td>
<td>1.15</td>
<td>-0.531120</td>
</tr>
</tbody>
</table>

#### METHOD PROPOSED

- **Eigenfunctions of the harmonic oscillator:**
  - The exact Hermite polynomial solutions are given along with the eigenfunctions produced by the method proposed.

---

*Table (III.1)*
CHAPTER IV
APPLICATION TO POTENTIALS WITH MANY BOWLS

IV - 1: Decaying States

In contrast to eigenstates (where we have an even number of
turning points), for the decaying states we have an odd number of
turning points, at least three. We start by considering the case of a
potential \( V(x) \) with only three turning points. As before, we use the
same method in order to have the corresponding reduced, energy adjusted
potential \( W(x) \) so that its zeroes are the classical turning points.
As before also, for each turning point, we apply the iteration procedure
in order to find the corresponding potentials \( U_1(x) \), \( U_2(x) \) and \( U_3(x) \).
For three turning points, we have two connecting matrices: \([M_{1,2}]\)
connecting regions 1 and 2 and \([M_{2,3}]\) connecting regions 2 and 3, it is
obvious that: (See Fig. IV.1)

\[
[M_{1,3}] = [M_{1,2}] [M_{2,3}]
\]  

(IV.1)

Let us label all the values of \( z, z', a, b, a', b' \) at the cut between
regions 1 and 2 by the index 1 and at the cut between regions 2 and 3
by the index 2. We get:

\[
[M_{1,2}] = D_{1,2} \begin{pmatrix} B_{1} \alpha_{1,2} & B_{1} \beta_{1,2} \\ -A_{1} \alpha_{1,2} & -A_{1} \beta_{1,2} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]  

(IV.2)

with \( D_{1,2} \), \( \alpha_{1,2} \) and \( \beta_{1,2} \) defined as in (III.13,14,15) and

\[
[M_{2,3}] = D_{2,3} \begin{pmatrix} B_{2} \alpha_{2,3} & B_{2} \beta_{2,3} \\ -A_{2} \alpha_{2,3} & -A_{2} \beta_{2,3} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]  

(IV.3)
The method applied to a potential with several turning points:

Fig. (IV.1)
where:
\[
\alpha_{2,3} = \pi \left[ G_{2,3} A_2 + (1 - C_{2,3}) A_2^* \right] \\
\beta_{2,3} = \pi \left[ G_{2,3} B_2 + (1 - C_{2,3}) B_2^* \right]
\] (IV.4)

with:
\[
D_{2,3} = \left| \begin{array}{c} u_2 \\ u_3 \end{array} \right| \\
C_{2,3} = \frac{Z_{1,2}^* Z_{1,3}}{Z_{1,3}} \\
G_{2,3} = \frac{1}{4Z_{1,2}^*} \left( \frac{Z_{1,3}}{2} \frac{Z_{1,2}}{2} \left( \frac{u_2}{u_2} \right)^* - \frac{u_3^2}{u_3} \right)
\] (IV.6)

This gives:
\[
[M_{1,3}] = D_{1,2} D_{2,3} \begin{pmatrix} B_2 \alpha_{1,2} - A_2 \beta_{1,2} \\ B_1 \alpha_{2,3} \end{pmatrix} + \begin{pmatrix} B_1 \alpha_{2,3} & B_1 \beta_{2,3} \\ -A_1 \alpha_{2,3} & -A_1 \beta_{2,3} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\] (IV.7)

One can also obtain \([M_{3,1}]\) by:
\[
[M_{3,1}] = [M_{3,2}] [M_{2,1}]
\] (IV.8)

It can be easily verified that:
\[
[M_{1,3}] [M_{3,1}] = [M_{3,1}] [M_{1,3}] = \mathbb{1}
\] (IV.9)

In this potential, the particle has the possibility to tunnel out of the inner potential bowl and the wave function does not vanish at infinity. Thus, we have no boundary condition in the outer region. Nevertheless we can define a decaying state by its relative minimum for the asymptotic amplitude \(A_{\infty}\) which describes the probability to find the particle far outside the potential bowl.

Without loss of generality, the coefficient vector \(z_1\) in region
1 can be set to \((1,0)\), the coefficient vector \(\mathbf{a}_3\) in region 3 is then given by:

\[
\begin{pmatrix}
\mathbf{a}_{1,3} \\
\mathbf{a}_{2,3}
\end{pmatrix} = \begin{bmatrix} M_{3,1} \end{bmatrix} \begin{pmatrix} 1 \\
0
\end{pmatrix}
\]

This gives:

\[
\begin{align*}
\mathbf{a}_{1,3} &= D_{2,1} \cdot D_{3,2} \left[ B_2 \alpha_{2,1} \left( B_1 \alpha_{3,2} - A_1 \beta_{3,2} \right) + B_1 \alpha_{2,1} + B_2 \beta_{3,2} + 1 \right] \\
\mathbf{a}_{2,3} &= -D_{2,1} \cdot D_{3,2} \left[ A_2 \alpha_{2,1} \left( B_1 \alpha_{3,2} - A_1 \beta_{3,2} \right) + A_1 \alpha_{2,1} + A_2 \beta_{3,2} \right]
\end{align*}
\]

\[
A_\infty = \mathbf{a}_{1,3} + \mathbf{a}_{2,3}
\]

\[
\begin{align*}
\mathbf{a}_{1,3} &= D_{2,1}^2 \cdot D_{3,2}^2 \left[ (B_1 \alpha_{3,1} + 1) (B_2 \alpha_{3,2} + 1) - A_1 B_2 \alpha_{2,1} \beta_{3,2} \right] \\
\mathbf{a}_{2,3} &= D_{2,1}^2 \cdot D_{3,2}^2 \left[ -\xi (B_2 \alpha_{3,2} + 1) + A_2 \alpha_{3,2} (B_1 \alpha_{3,1} + 1) \right]
\end{align*}
\]

with \(\xi = A_1 \alpha_{2,1}\)

The condition for a decaying state is given by:

\[
\left( \frac{dA_\infty}{dE} \right)^2 = \left( \frac{dA_{2,1}}{d\xi} \right)^2 = 0
\]

\[
\frac{dA_\infty}{d\xi} = 0 \quad \text{yields} \quad \xi = D_{2,1} \cdot D_{3,2} \frac{A_2 \alpha_{3,2} (B_1 \alpha_{3,1} + 1)}{B_2 \alpha_{3,2} + 1}
\]

One can see that in the limit of a high barrier, \(B_2\) is large compared to the other terms and condition (IV.11) is then reduced to condition (III.36).

**IV - 2: Matrix Formalism For The General Case**

In order to apply the method described to a higher number of turning points and to the case of restricted or hindered rotations, it is useful to develop a more general matrix formalism.

For each turning point \((i)\) between two regions \(i\) and \(i+1\), we
label all the values given previously by the index \( i \) only. With this convention, the matrix which connects the coefficient vectors \( \mathbf{a}_i^T \) of the solutions in regions \( i \) and \( i + 1 \) on both sides of the turning point \( \Omega \), will be denoted by \( \left[ M_i \right] \).

\[
\left[ M_i \right] = D_i \begin{bmatrix}
    \left( \begin{array}{cc}
        B_i^T & B_i^T \\
        -A_i^T & -A_i^T \\
    \end{array} \right)
    \right) + \begin{bmatrix}
    1 \\
    0 \\
    0 \\
    1 \\
\end{bmatrix}
\]

(IIV.12)

where:

\[
D_i = \begin{bmatrix}
    U_i^T \\
    U_{i+1}^T \\
\end{bmatrix}
\]

\[
\alpha_i^T = \pi \left[ G_i^T \left( A_i^T + (1 - C_i) - A_i^T \right) \right]
\]

\[
\beta_i^T = \pi \left[ G_i^T \left( B_i^T + (1 - C_i) B_i^T \right) \right]
\]

(IIV.13)

with:

\[
G_i = \frac{1}{4Z_i^T} \left( Z_i^T - \frac{U_i^T}{Z_i^T} - \frac{Z_{i+1}^T + \frac{U_{i+1}}{Z_{i+1}^T}}{Z_i^T} \right)
\]

\[
C_i = \frac{Z_{i+1}^T}{Z_i^T}
\]

The inverse matrix \( \left[ M_i \right]^{-1} \) is given by:

\[
\left[ M_i \right]^{-1} = \frac{1}{D_i} \begin{bmatrix}
    \left( \begin{array}{cc}
        B_i^T & B_i^T \\
        -A_i^T & -A_i^T \\
    \end{array} \right)
    \right) + \begin{bmatrix}
    1 \\
    0 \\
    0 \\
    1 \\
\end{bmatrix}
\]

(IIV.14)

where:

\[
\alpha_i^T = \frac{1}{C_i} \alpha_i^T
\]

(IIV.15)

and

\[
\beta_i^T = \frac{1}{C_i} \beta_i^T
\]

(IIV.16)

Let us call now:
\[
\begin{bmatrix}
R_{ij} \\
R_{ij}
\end{bmatrix} =
\begin{pmatrix}
B_i \alpha_j & B_i \beta_j \\
-A_i \alpha_j & -A_i \beta_j
\end{pmatrix}
\]

\[
\begin{bmatrix}
\overline{R_{ij}} \\
\overline{R_{ij}}
\end{bmatrix} =
\begin{pmatrix}
B_i \overline{\alpha}_j & B_i \overline{\beta}_j \\
-A_i \overline{\alpha}_j & -A_i \overline{\beta}_j
\end{pmatrix}
\]  

\[\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\]

with this we can write:

\[
[M_{ij}^\perp] = D_i \begin{bmatrix}
R_{ii} & 1
\end{bmatrix}
\]

\[\begin{bmatrix}
M_{ij}^\perp
\end{bmatrix}^{-1} = \frac{1}{D_i} \begin{bmatrix}
\overline{R_{ii}} & 1
\end{bmatrix}
\]  

Let us first evaluate \( [R_{ii}]^2 \).

\[
[R_{ii}]^2 = (B_i \alpha_i - A_i \beta_i) [R_{ii}]
\]

If we write \( \gamma_{ij} = (B_i \alpha_j - A_i \beta_j) \)  
we can write: \[ [R_{ii}]^2 = \gamma_{ii} [R_{ii}] \]

Using the fact that the Wronskian \( W(A, B) = \frac{1}{n} \), in the expression of \( \gamma_{ii} \), we get:

\[
\gamma_{ii} = (C_i - 1)
\]

This leads to: \[ [R_{ii}]^2 = (C_i - 1) [R_{ii}] \]

the result can be generalized to give:

\[
[R_{ii}]^n = (C_i - 1)^{n-1} [R_{ii}] \text{ for } n \geq 1
\]

From (IV.17) one can get:

\[
[R_{ii}] = -\frac{1}{C_i} [R_{ii}]
\]

we can get a similar result for \( [R_{ii}] \) as:
\[
\left[ R_{i,i} \right]^n = \left( -\frac{1}{C_i} \right)^{n-1} \left[ R_{i,i} \right]^{n-1} \left( C_i - 1 \right)^{m-1} \left[ R_{i,i} \right] \text{ for } n \gg 1.
\] (IV.27)

We also have:
\[
\left[ R_{i,i} \right] \left[ R_{i,i} \right] = \left[ R_{i,i} \right] \left[ R_{i,i} \right] = -\frac{1}{C_i} \left( C_i - 1 \right) \left[ R_{i,i} \right]
\] (IV.28)

This can be generalized to give:
\[
\left( \left[ R_{i,i} \right] \left[ R_{i,i} \right] \right)^n = \left( \left[ R_{i,i} \right] \left[ R_{i,i} \right] \right)^n = \left( -\frac{1}{C_i} \right)^n \left( C_i - 1 \right)^{2m-1} \left[ R_{i,i} \right] \] (IV.29)

With these results one can verify that:
\[
\left[ M_{i,i} \right] \left[ M_{i,i} \right]^{-1} = \left[ M_{i,i} \right]^2 \left[ M_{i,i} \right] = 1
\] (IV.30)

Without symmetry, we have the following results:
\[
\left[ M_{i,i} \right]^2 = D_i \left[ \left( C_i + 1 \right) \left[ R_{i,i} \right] + 1 \right]
\]
\[
\left[ M_{i,i} \right]^3 = D_i \left[ \left( C_i + 1 \right) \left[ R_{i,i} \right] + 1 \right] + \left[ \left( C_i + 1 \right) \left[ R_{i,i} \right] + 1 \right]
\]
\[
\left[ M_{i,i} \right]^n = D_i \left( C_i^{-1} + C_i^{-2} + \ldots + C_i^{-n} \right) \left( C_i^{-1} + C_i^{-2} + \ldots + C_i^{-n} \right)
\] (IV.31)

\[
\left( \left[ M_{i,i} \right]^{-1} \right)^2 = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^2 \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^3 = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^3 \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^n = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^n \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^{2(n-1)} = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^{2(n-1)} \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^{2(n-2)} = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^{2(n-2)} \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^{2(n-3)} = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^{2(n-3)} \right)
\]
\[
\left( \left[ M_{i,i} \right]^{-1} \right)^{2(n-4)} = \left( \frac{1}{D_i} \right) \left( \left( \left[ R_{i,i} \right]^{-1} \right)^{2(n-4)} \right)
\]

These results for \( \left[ R_{i,i} \right] \) are simpler for the case where the cut is at the symmetry axis of the potential:
\[
\begin{align*}
C_i & = -1 \\
D_i & = 1
\end{align*}
\]
\[(\alpha_i)_s = (\overline{\alpha}_i)_s\]
\[(\beta_i)_s = (\overline{\beta}_i)_s\]
\[(\gamma_{i,i})_s = -2\]
\[
\begin{align*}
[R_{i,i}]_s &= [R_{i,i}]_s \\
[R'_{i,i}]_s &= (-2)^{n-1}[R'_{i,i}]_s \\
(R_{i,i})_s [R_{i,i}]_s &= (-2)^{2n-1}[R_{i,i}]_s
\end{align*}
\]  

(IV.32)

Using those relations for \([R_{i,i}]_s\) and \([R_{i,i}]_s\) we can find similar relations for \([M_{i,i}]_s\) and \([M_{i,i}]_s^{-1}\):

\[
[M_{i,i}]_s^2 = I
\]
\[
[M_{i,i}]_s^3 = [M_{i,i}]_s
\]
\[
[M_{i,i}]_s^{2n} = I; [M_{i,i}]_s^{2n+1} = [M_{i,i}]_s
\]  

(IV.33)

The same result is obtained for \([M_{i,i}]_s^{-1}\) since \([M_{i,i}]_s^{-1} = [M_{i,i}]_s\).

We can now give some relations which can be verified easily and which will be useful later on:

\[
[R_{11}]_i^2 = (C_i - 1) [R_{11}]
\]
\[
[R_{22}]_i^2 = (C_2 - 1) [R_{22}]
\]
\[
[R_{12}]_i^2 = \gamma_{1,2} [R_{12}]
\]
\[
[R_{21}]_i^2 = \gamma_{2,1} [R_{21}]
\]
\[
[R_{11}]_i [R_{22}]_i = \gamma_{2,1} [R_{12}]
\]
\[
[R_{11}]_i [R_{12}]_i = (C_i - 1) [R_{12}]
\]
\[
[R_{11}]_i [R_{21}]_i = \gamma_{2,1} [R_{11}]
\]
\[
[R_{22}]_i [R_{11}]_i = \gamma_{1,2} [R_{21}]
\]
\[
[R_{22}]_i [R_{12}]_i = \gamma_{1,2} [R_{22}]
\]
\[
[R_{22}]_i [R_{21}]_i = (C_2 - 1) [R_{21}]
\]
\[
[R_{12}]_i [R_{11}]_i = \gamma_{1,2} [R_{11}]
\]
\[
[R_{12}]_i [R_{21}]_i = (C_2 - 1) [R_{11}]
\]
\[
[R_{12}]_i [R_{22}]_i = (C_2 - 1) [R_{12}]
\]  

(IV.34)
\[
\begin{bmatrix}
R_{21} & R_{31}
\end{bmatrix}
\begin{bmatrix}
R_{11}
\end{bmatrix}
= (C_1 - 1)
\begin{bmatrix}
R_{21}
\end{bmatrix}
\]
\[
\begin{bmatrix}
R_{21} & R_{12}
\end{bmatrix}
= (C_1 - 1)
\begin{bmatrix}
R_{22}
\end{bmatrix}
\]
\[
\begin{bmatrix}
R_{21} & R_{22}
\end{bmatrix}
= \gamma_{21}
\begin{bmatrix}
R_{22}
\end{bmatrix}
\]

**IV - 3: Eigenvalue Problem For Many Bowls**

Let us start by trying to apply the method to find the eigenvalues of a symmetric double potential well. In this case, we have four turning points and four corresponding regions with three cuts and three connection matrices. Assuming the axis of symmetry along the cut 2 leads to:

\[
\begin{bmatrix}
M_1
\end{bmatrix}
= \begin{bmatrix}
M_3
\end{bmatrix}
\quad \text{(See Fig. IV.2)}
\]

we have:

\[
\begin{bmatrix}
M_1
\end{bmatrix}
= \begin{bmatrix}
R_{11} + 1
\end{bmatrix}
\]

and

\[
\begin{bmatrix}
M_2
\end{bmatrix}
= \begin{bmatrix}
R_{22} + 1
\end{bmatrix}
\]

The overall matrix which connects the coefficients in region 1 and 4 will be denoted by \( M_{32} \), and given by:

\[
\begin{bmatrix}
M_{32}
\end{bmatrix}
= \begin{bmatrix}
M_1
\end{bmatrix}
\begin{bmatrix}
M_2
\end{bmatrix}
\begin{bmatrix}
M_4
\end{bmatrix}
\]

(IV.35)

In order to evaluate \( M_{32} \), one can use the relations given in (IV.34), we get first:

\[
\begin{bmatrix}
M_2
\end{bmatrix}\begin{bmatrix}
M_1
\end{bmatrix}
= \gamma_{12}
\begin{bmatrix}
R_{21}
\end{bmatrix}
+ \begin{bmatrix}
R_{12}
\end{bmatrix}
+ \begin{bmatrix}
R_{11}
\end{bmatrix}
+ 1
\quad \text{(IV.36)}
\]

and then:

\[
\begin{bmatrix}
M_{32}
\end{bmatrix}
= (\gamma_{12}\gamma_{21} + C_1 + 1)
\begin{bmatrix}
R_{11}
\end{bmatrix}
+ \begin{bmatrix}
R_{12}
\end{bmatrix}
+ \gamma_{21}\begin{bmatrix}
R_{21}
\end{bmatrix}
+ \gamma_{12}\begin{bmatrix}
R_{22}
\end{bmatrix}
+ 1
\quad \text{(IV.37)}
\]

The eigenvalue conditions are given by:

\[
\begin{bmatrix}
R
\end{bmatrix}
= \begin{bmatrix}
M_{32}
\end{bmatrix}
\begin{bmatrix}
1
\end{bmatrix}
\]

This leads to:

a) \(-A_1\alpha_1(\gamma_{12}\gamma_{21} + C_1 + 1) - A_2\alpha_2\alpha_1\gamma_{21} - A_2\alpha_2\gamma_{12} = 0\) (IV.38)

b) \(B_1\alpha_1(\gamma_{12}\gamma_{21} + C_1 + 1) + B_2\alpha_2 + B_1\alpha_2\gamma_{21} + B_2\alpha_1\gamma_{12} + 1 = R\) (IV.39)
The method applied to a double potential well (four turning points).

Fig. (IV.2)
The condition for eigenvalues is given by solving (a). This leads to a polynomial equation in \( \xi \) of degree two:

\[
p \xi^2 - \xi(t + C_1 + C_2) - mc_1 = 0 \tag{IV.40}
\]

with:

\[
\xi = A_1 \alpha_1
\]
\[
m = A_2 \alpha_2
\]
\[
p = B_2 \beta_2
\]
\[
t = A_1 A_2 \beta_1 \beta_2 + B_2 \beta_2 \alpha_2 \alpha_2 - m B_1 \beta_1
\]

The solution of (IV.40) will give the eigenvalues. At this point, one can remark that, in the limiting case when the barrier is infinitely high which implies corresponding high values for \( B_2 \) and \( \beta_2 \), the equation (IV.40) converges to equation (III.36) which is the eigenvalue condition for a single potential well.

This result can be generalized to potentials with more than two wells:

In (IV.36), we have a polynomial in \( \xi \) of degree one, and in (IV.37), a polynomial of degree two in \( \xi \). Each time we have a potential with an additional well, the overall matrix has to be multiplied by (IV.36) which gives a polynomial in \( \xi \) of one degree higher. Thus, for example (see Fig. IV.3), \( [M_1 N23] \) which is the overall matrix for a potential with six turning points (three bowls), will give as eigenvalue condition a polynomial of degree three. \( [M_1 N23] \) is expressed as:

\[
[M_1 N23] = \left( Y_{12} Y_{21} + C_1 + 1 \right) \left( Y_{12} Y_{21} + C_1 \right) + C_2 \quad Y_{12} Y_{21} + 1 \right] [R_{11}]^T +
+ \left[ Y_{21} \left( Y_{12} Y_{21} + C_1 + C_2 + 1 \right) \right] [R_{12}] + \left[ Y_{12} \left( Y_{12} Y_{21} + C_1 + C_2 + 1 \right) \right] [R_{21}]^T +
+ \left[ Y_{12} Y_{21} + C_2 + 1 \right] [R_{22}] + I \tag{IV.42}
\]

And the polynomial equation in \( \xi \) which will give the eigenvalues as solutions can be expressed as:
The method applied to a potential with 6 turning points (three bowls): overall matrix.
\[ - \xi^3 p^2 + \xi^2 \left[ 2p \left( t + C_1 + C_2 \right) \right] - \xi \left[ t^2 + 2t \left( C_1 + C_2 \right) \right] + \left[ C_1^2 + C_1 C_2 + C_2^2 - mpC_1 \right] - mc_i \left[ t + C_1 + C_2 \right] = 0 \quad (IV.43) \]

We can say that for a potential with an even number of turning points 2n, the eigenvalues are given by the solution of a polynomial of degree n in \( \xi (= A_i \alpha_i) \).

The results above have been derived assuming \([M_1] = [M_3] = [M_5] = \ldots \) and \([M_2] = [M_4] = [M_6] = \ldots \) etc. ... The same general conclusions are reached if one considers a potential where all the connection matrices are totally different. This is given in Appendix C. It is obvious that the result will not be as simple as the above expressions.

IV - 4: Results For A Symmetric Double Potential Well

We now consider a double potential well where, for simplicity, each well is an harmonic oscillator. With this assumption we have \( C_1 = -1 \) and \( C_2 = -1 \). The equations (IV.38) and (IV.39) become in this case:

\[ - A_i \alpha_i \quad \gamma_{12} \quad \gamma_{21} \quad - A_i \alpha_i \quad \gamma_{21} \quad - A_i \alpha_i \quad \gamma_{12} = 0 \quad (IV.44) \]

\[ B_i \alpha_i \quad \gamma_{12} \quad \gamma_{21} \quad + B_i \alpha_i \quad \gamma_{21} \quad + B_i \alpha_i \quad \gamma_{12} + 1 = R \quad (IV.44) \]

The solutions of (IV.44) are:

a) \( \xi = \left( B_i \alpha_i + 1 \right) \frac{\alpha_i}{\beta_i} \)

b) \( \xi = \left( B_i \alpha_i + 1 \right) \frac{A_i}{B_i} \)

If we apply solution a) to equation (IV.44) one gets \( R = 1 \).

This means that the corresponding wave function is symmetric.

By applying solution b) to equation (IV.44), one gets \( R = -1 \).

The corresponding wave function is antisymmetric.

One can say that, due to the coupling of the two bowls, as provided by the possibility for tunneling, each energy level in the
single harmonic oscillator which corresponds to $\xi = 0$, splits in two
energy levels: one corresponding to a symmetric wave function and
another corresponding to an antisymmetric wave function.

Above the potential barrier, the energy levels are given by the
condition corresponding to a single potential well, i.e. an energy shift
occurs rather than a split.

The split between the two energy levels which we call $\delta E$ is
equal to:

$$\delta E = (B_2 \alpha_1 + 1) \left( \frac{B_2 \alpha_2 - A_2 \beta_2}{B_2 \beta_2} \right)$$

which gives:

$$\delta E = -2 \left( \frac{B_2 \alpha_1 + 1}{B_2 \beta_1} \right)$$

(KIV,46)

Knowing that near the bottom of the potential well, the value
of $Z$ at the cut (2) is large and so will be the values for $B_2 \beta_2$,
one can see that the split will be small. $Z$ at the cut (2) will de-
crease as the energy approaches the top of the potential barrier and so
$B_2$ and $\beta_2$ will decrease also; this implies that the split will become
larger.

All these results are shown in Fig. (IV.4) along with the fact
that the use of this method gives the exact position of the energy
levels. The positions of the energy levels obtained for three bowls are
also shown in Fig. (IV.5).

IV - 5: Ring Structure For Many Bowls

An identical method can be used to solve the problem of an $N$-
fold periodic potential and to find its energy levels. For a symmetric
rotor, the potential energy must be $N$-fold periodic as the internal
rotation angle $\alpha$ goes through $2\pi$, where $N$ represents the
Energy levels of a symmetric double potential well:

The energy levels of a symmetric double potential well are given in comparison to the single bowl harmonic oscillator levels.

Fig. (IV.4)
Energy levels of a symmetric potential with three bowls:

The energy levels of a symmetric potential with three bowls are given in comparison to the single bowl harmonic oscillator levels.

Fig. (IV.5)
number of bowls in the ring. (Fig. IV.6)

We can treat the general case of any integer $N$ right away. Each individual bowl $b (b = 1, 2, \ldots, N)$ is represented by two matrices $M_i^{(b)}$ and $M_2^{(b)}$ (see Fig. IV.6)

The overall matrix is then

$$M_{\text{tot}} = M_2^{(N)} M_2^{(1)} \cdots M_2^{(2)} M_2^{(1)} M_1^{(1)} M_1^{(2)}$$

where each product of two matrices of the same value $b$ is

$$M_i^{(b)} M_k^{(b)} = D_i D_k \left\{ \gamma_{k,l} \left[ R_{i,k} \right] + \left[ R_{i,l} \right] + \left[ R_{k,k} \right] + I \right\}$$

as apparent from equations (IV.34) and (IV.36)

The energy eigenvalue condition now takes the following form:

If $\vec{a} = (a_1, a_2)$ is the coefficient vector in a region, say region 1, then it has to reproduce itself after the total matrix $M_{\text{tot}}$ has been applied. Thus, at an energy eigenvalue,

$$M_{\text{tot}} \cdot \vec{a} = \vec{a}$$

must hold. It means that $\vec{a}$ must be an eigenvector of $M_{\text{tot}}$ with the eigenvalue 1.

An interesting case is the one of $N$ bowls that are equal, so that

$$M_{\text{tot}} = M$$

where

$$M = M_2^{(1)} M_1^{(1)}$$

Instead of (IV.49) we can write for the matrix $M$

$$M \vec{a}_k = e^{i \frac{2 \pi k}{N}} \vec{a}_k$$

where $k$ is any natural sequence of $N$ integer numbers. Hence, the matrix $M$ must have the eigenvalues $\lambda_k = e^{i \frac{2 \pi k}{N}}$. Except for $\lambda_0 = 1$ (and possibly $\lambda_{N/2} = -1$, if $N$ is even), the eigenvalues occur in complex conjugate parts $\lambda_{-k} = e^{i \frac{2 \pi k}{N}}$

A matrix theorem states that

$$\text{Trace } (M) = \lambda_k + \lambda_{-k} \quad (\text{for } k = 0, \pm 1, \pm 2, \ldots),$$

(IV.52)
The method applied to the hindered rotation problem.

Fig. (IV.6)
so that
\[ m_{11} + m_{22} = 2 \cos \left( \frac{2\pi k}{N} \right) \]  
(IV.53)

now represents the energy eigenvalue condition.

It should be noted that equation (IV.50) or (IV.51) does not
determine the matrix \( M \) uniquely. In fact, any other matrix of the form
\[ M' = TM'T^{-1} \]  
(IV.54)
also satisfies equations (IV.50), (IV.52) and (IV.53), \( T \) being any non-singular matrix. However, different matrices \( M' \) will have different
coefficient-eigenvectors \( \tilde{a}_k \), in accordance with (IV.51). In fact, the
eigenvector coefficient then uniquely defines the eigenfunction \( Y(x) \).

Plotting out a wavefunction for a particular energy level is then a simple
matter of evaluating \( Z(x) \) and the Airy Functions, employing the coefficients
\( a_1 \) and \( a_2 \) as given by the components of the corresponding eigenvector \( \tilde{a}_k \).

As one goes from region to region, the coefficient eigenvector \( \tilde{a}_k \)
is subjected to the transformation matrices \( M_1 \) and \( M_2 \) to yield the coeffi-
cients in the various other regions.

Since \( \lambda_k = \lambda_k^* \), the two eigenvectors to the same energy level ('E' levels, doubly degenerate, corresponding to \( \lambda_k \) and \( \lambda_{-k} \)) can be written as
\[ \tilde{a}_k = \begin{pmatrix} 1 \\ a_1 \end{pmatrix} \quad \text{and} \quad \tilde{a}_{-k} = \begin{pmatrix} 1 \\ a_2^{*} \end{pmatrix} \]  
(IV.55)

where (under the assumption \( a_1 = 1 \))
\[ a_2 = \frac{\lambda_k - m_{11}}{m_{12}} = \frac{m_{21}}{\lambda_k - m_{12}} \]

Each one of them produces a complex wavefunction \( Y_k(x) \) corresponding to
a particle 'partially' circulating through the ring structure in one or
the other direction. We can rewrite any linear combination of \( Y_k \) and \( Y_{-k} \)
as a linear combination of real valued functions \( Y_{\text{real}} \) and \( Y_{\text{imag}} \), whose
coefficient vectors would be

\[ \begin{align*}
\vec{a}_{\text{real}} &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \vec{a}_{\text{imag}} &= \begin{pmatrix} 1 \end{pmatrix},
\end{align*} \]

so that

\[ \begin{align*}
\gamma(x) &= \eta_1 Y_{\text{real}} + \imath \eta_2 Y_{\text{imag}}
\end{align*} \]  

of course, the vectors \( \vec{a} \) can be normalized conveniently if so wanted.

Note that this matrix represents a rotation by an angle \( \varphi = 2\pi k/N \).

From equation (IV.48) we find the matrix elements of \( M \) as

\[ \begin{align*}
m_{11} &= D_1 D_2 \left[ (1 + \alpha_1 B_1)(1 + \alpha_1 B_2) - \alpha_1 A_1 \beta_2 B_2 \right] \\
m_{12} &= D_1 D_2 \left[ (1 + \alpha_1 B_1)(1 + \alpha_1 B_2) \beta_1 - (1 + \alpha_1 B_1) \beta_2 B_2 \right] \\
m_{21} &= D_1 D_2 \left[ (1 + \alpha_2 B_2)(1 + \alpha_1 B_1) - \alpha_2 A_1 \beta_1 B_2 \right] \\
m_{22} &= D_1 D_2 \left[ (1 + \alpha_2 B_2)(1 + \alpha_1 B_1) - \alpha_2 A_1 \beta_1 B_2 \right]
\end{align*} \]  

Thus, the energy eigenvalue condition (IV.53) becomes

\[ \begin{align*}
\varepsilon &= \alpha_1 A_1 = \beta_1 B_2 \left\{ 2(1 + \alpha_1 B_2)(1 + \alpha_2 B_2) - \alpha_1 A_1 \beta_1 B_2 - \frac{2}{\beta_2} \cos \left( \frac{2\pi k}{N} \right) \right\}
\end{align*} \]  

The coefficient vectors in region 1 are then

\[ \begin{align*}
\vec{a}_{\text{real}} &= \begin{pmatrix} \cos(2\pi k/N) - m_{11} \end{pmatrix}, \quad \vec{a}_{\text{imag}} &= \begin{pmatrix} \sin(2\pi k/N) \end{pmatrix}
\end{align*} \]  

With the other regional values given by repeated application of the matrices \( M_1 \) and \( Y_2 \), as needed.

Some remarks may be of interest.

a- For bowls which are separated by a high and wide barrier both \( \beta_1 \) and \( \beta_2 \) become very large compared to all other terms, thus leading to

\[ \varepsilon = \alpha_1 A_1 = 0 \] in the limit, as called for in equation (III.36).

b- Symmetry about the cuts involves \( D_1 = D_2 = 1 \).

c- According to equation (IV.53), each different value of \( \cos(2\pi k/N) \) leads to a different energy. One finds the following systematic behaviour. Each energy is associated with one of the points on the complex unit circle which represent the \( k \)-th root of 1 (see Fig. IV.7). As we
progress through the values of integer \( k \) (with \(-N/2 < k \leq N/2\)) we exhaust all the \( N \)-th roots of 1 on the unit circle. Since \( \cos(-\varphi) = \cos(\varphi) \), each pair of complex conjugate roots leads to a double degenerate energy level ("E level"), whereas roots that lie on the real axis lead to non-degenerate levels ("A levels"). In most cases (also in our example), the E levels would be bracketed by the A levels and one of the A levels is identical with the level A, for \( n = 1 \), the single bowl case. Due to the alternating sign of \( \mathcal{E}(E) \) at the energies in question, the pattern alternates as one goes from one fine structure pattern to the next higher one. Let \( n = 4 \) be an example: The lowest pattern is like \( A_{1}, E, A_{-1} \), the next highest like \( A_{-1}, E, A_{1} \), and so on. Here, \( A_{±1} \) denotes the fine structure level associated with the point \((±1, 0)\) on the unit circle. \( A \) represents the level for the single bowl case.

- Obviously, any deviation from the case of all identical bowls will result in a corresponding loss of E levels. Some or all of them would split up due to the fact that the real parts of the formerly conjugate complex pairs of roots would slightly differ.

As a test case for this method, the \( N \)-fold barrier potential given by

\[
W(\alpha) = 1 - \cos \alpha \quad 0 < \alpha < 2\pi
\]

(IV.56)

(for \( n = 1, 2, 3, 4 \)) was studied. The energy values obtained by this method are shown in Table (IV.1) along with the exact values obtained by Herschbach (10, 12) using a Mathieu function approach. Also shown are the values which one would obtain if one would use the unrefined \( W \) instead of \( U \), i.e. using Langer's method. Fig. IV.8 shows the resulting fine structure for the case \( n = 1 \) and \( n = 4 \).
Split up of the original single bowl energy levels:

The split up of the original single bowl energy levels for infinite range potentials and ring structure potentials as more bowls are added. Each additional bowl causes a new fine structure energy level. Note that in the ring structure, the lowest (or highest) level is the original single bowl level.

Fig. (IV.7)
Energy split-up pattern can be associated with \( n \)-th roots of 1 on the complex unit circle. A root on the real axis produces non-degenerate "A" level, whereas each pair of complex conjugate roots produces a doubly degenerate "E" level.

Fig. (IV.7)
<table>
<thead>
<tr>
<th>N</th>
<th>LANGER'S JWKB APPROXIMATION</th>
<th>THIS WORK</th>
<th>EXACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.7364</td>
<td>0.625</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>Not existent</td>
<td>1.922</td>
<td>1.91806</td>
</tr>
<tr>
<td>2</td>
<td>0.7364</td>
<td>0.625</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>0.7669</td>
<td>0.651</td>
<td>0.65233</td>
</tr>
<tr>
<td></td>
<td>1.725</td>
<td>1.601</td>
<td>1.59480</td>
</tr>
<tr>
<td></td>
<td>Not existent</td>
<td>1.922</td>
<td>1.91806</td>
</tr>
<tr>
<td>3</td>
<td>0.7364</td>
<td>0.625</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>0.7558</td>
<td>0.644</td>
<td>0.64413</td>
</tr>
<tr>
<td></td>
<td>1.785</td>
<td>1.648</td>
<td>1.64928</td>
</tr>
<tr>
<td></td>
<td>Not existent</td>
<td>1.922</td>
<td>1.91806</td>
</tr>
<tr>
<td>4</td>
<td>0.7364</td>
<td>0.625</td>
<td>0.62151</td>
</tr>
<tr>
<td></td>
<td>0.7509</td>
<td>0.638</td>
<td>0.63629</td>
</tr>
<tr>
<td></td>
<td>0.7669</td>
<td>0.651</td>
<td>0.65233</td>
</tr>
<tr>
<td></td>
<td>1.725</td>
<td>1.601</td>
<td>1.59480</td>
</tr>
<tr>
<td></td>
<td>1.859</td>
<td>1.708</td>
<td>1.71309</td>
</tr>
<tr>
<td></td>
<td>Not existent</td>
<td>1.922</td>
<td>1.91806</td>
</tr>
</tbody>
</table>

Energy levels for a N-fold barrier potential:

The energy levels for a N-fold barrier potential are given with the Langer's approximation and with the method proposed. A comparison with exact levels is also included.

In the JWKB approximation, using \( f(x) = (n + \frac{1}{2}) \pi \) one finds for \( N = 1 \) the levels: 0.674109 and 1.778413

Table (IV.1)
Energy levels for a ring structure potential of $N$-fold periodicity

$$w(\alpha) = 1 - \cos \alpha$$

Fig. (IV.8)
APPENDIX A

Taylor Expansion of U(x)

Expanding U(x) near the classical turning point (assumed to be at x = 0) as:

\[ U(x) = x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + a_6 x^6 + a_7 x^7 \]  \hspace{1cm} (A.1)

we arrive at the following results:

\[ U'(x) = x^{-2} \left[ 1 + f_1 x + f_2 x^2 + f_3 x^3 + f_4 x^4 + f_5 x^5 + f_6 x^6 \right] \]

with:

\[ f_1 = -2a_2 \]
\[ f_2 = 3a_2^2 - 2a_3 \]
\[ f_3 = -4a_4 + 6a_2 a_3 - 2a_4 \]
\[ f_4 = 5a_4 - 12a_2^2 a_3 + 6a_2 a_4 + 3a_3^2 - 2a_5 \]
\[ f_5 = -6a_4 + 20a_2^3 a_3 - 12a_2 a_4^2 - 12a_2 a_3 - 6a_2 a_5 + 6a_3 a_4 - 2a_6 \]
\[ f_6 = 7a_4^2 - 30a_2 a_3 + 20a_2^4 a_4 + 30a_2 a_2^2 a_3 - 12a_2 a_3 a_5 - 24a_2 a_3 a_4 + 6a_4 a_6 - 4a_3^2 + 
\hspace{2cm} + 6a_3 a_5 + 3a_4^2 - 2a_7 \]

\[ U''(x) = x^{-1} \left[ 1 + h_1 x + h_2 x^2 = h_3 x^3 + h_4 x^4 + h_5 x^5 + h_6 x^6 \right] \]

with:

\[ h_1 = -a_2 \]
\[ h_2 = a_2^2 - a_3 \]
\[ h_3 = -a_4 + 2a_2 a_3 - a_4 \]
\[ h_4 = a_4 - 3a_2^2 a_3 + 2a_2 a_4 + a_3^2 - a_5 \]
\[ h_5 = -a_4 + 4a_2^3 a_3 - 3a_2 a_4 - 3a_2 a_3 + 2a_2 a_5 + 2a_3 a_4 - a_6 \]
\[ h_6 = a_4^2 - 5a_2 a_3 + 6a_2^2 a_4 + 6a_2 a_2^2 a_3 - 3a_2 a_3 a_4 - 6a_2 a_3 a_5 + 2a_2 a_6 - a_3^2 + 2a_3 a_5 + 
\hspace{2cm} + a_4^2 - a_7 \]

\[ U'''(x) = \frac{3}{4} x^{-3} \left[ 1 + b_1 x + b_2 x^2 + b_3 x^3 + b_4 x^4 + b_5 x^5 + b_6 x^6 \right] \]

72
with: (the .) for product)

\[ b_1 = \frac{-2}{5} a_2 \]

\[ b_2 = \frac{2 \cdot 3 \cdot 11}{5^2 \cdot 7} a_2 \cdot a_2 - \frac{3}{7} a_3 \]

\[ b_3 = \frac{-2 \cdot 17 \cdot 19}{3 \cdot 3 \cdot 7} a_2 \cdot a_3 + \frac{2 \cdot 29}{3 \cdot 5 \cdot 7} a_2 a_3 - \frac{1}{3} a_4 \]

\[ b_4 = \frac{3 \cdot 17 \cdot 73}{5 \cdot 7 \cdot 11} a_2 \cdot a_2 \cdot a_3 + \frac{2 \cdot 3 \cdot 17 \cdot 73}{5 \cdot 3 \cdot 7 \cdot 11} a_2 a_3^2 + \frac{4 \cdot 37}{7 \cdot 11} a_3^2 - \frac{3}{11} a_5 \]

\[ b_5 = \frac{-3 \cdot 37 \cdot 839}{5 \cdot 7 \cdot 11} a_2 \cdot a_3 + \frac{2 \cdot 3 \cdot 1867}{5 \cdot 7 \cdot 11} a_2 a_3 - \frac{2 \cdot 6 \cdot 1867}{5 \cdot 7 \cdot 11} a_2 a_4 - \frac{3 \cdot 4909}{5 \cdot 7 \cdot 11} a_2 a_3 - \frac{2 \cdot 3 \cdot 43}{5 \cdot 7 \cdot 11} a_4 + \frac{2 \cdot 3 \cdot 5}{7 \cdot 11} a_5 a_7 - \frac{3}{13} a_6 \]

\[ b_6 = \frac{3 \cdot 23 \cdot 199 \cdot 10243}{3 \cdot 5 \cdot 7 \cdot 11} a_2 \cdot a_2 - \frac{8205209}{3 \cdot 5 \cdot 7 \cdot 11} a_2 a_3 + \frac{2 \cdot 7 \cdot 1543}{3 \cdot 5 \cdot 7 \cdot 11} a_2 a_4 + \frac{2 \cdot 3 \cdot 17 \cdot 29 \cdot 1097}{3 \cdot 5 \cdot 7 \cdot 11} a_2 a_3 - \frac{2 \cdot 3 \cdot 1543}{5 \cdot 7 \cdot 11} a_2 a_5 - \frac{2 \cdot 17 \cdot 29}{3 \cdot 7 \cdot 11} a_2 a_4 + \frac{2 \cdot 2 \cdot 53}{5 \cdot 7 \cdot 11} a_3 a_5 - \frac{13 \cdot 157}{5 \cdot 7 \cdot 11} a_3 - \frac{2 \cdot 2 \cdot 53}{3 \cdot 7 \cdot 11} a_4 - \frac{1}{5} a_7 \]

\[(u'(x))^2 = 1 + e_1 x + e_2 x^2 + e_3 x^3 + e_4 x^4 + e_5 x^5 + e_6 x^6\]

with:

\[ e_1 = 4 a_2 \]

\[ e_2 = 4 a_2^2 + 6 a_3 \]

\[ e_3 = 12 a_2 a_3 + 6 a_4 \]

\[ e_4 = 10 a_5 + 9 a_3^2 + 16 a_2 a_4 \]

\[ e_5 = 12 a_6 + 20 a_2 a_5 + 24 a_3 a_4 \]

\[ e_6 = 14 a_7 + 24 a_2 a_6 + 16 a_4^2 + 30 a_3 a_5 \]

By replacing each term in the expression of \( \Delta [u, x] \) given in (II.9) by its value, one gets the expansion of \( \Delta [u, x] \) in the form

\( \Delta [u, x] = d_0 + d_1 x + d_2 x^2 + ... \)

It is important to remark here that in the expression of \( \Delta [u, x] \),
even if each term separately is singular at the classical turning point, the full expression is well behaved and can be expressed analytically be a power series expansion.

The results obtained in this case are:

\[
\begin{align*}
    d_0 &= -\frac{9}{35} a_2^2 - \frac{3}{7} a_3 \\
    d_1 &= \frac{-286}{525} a_2^3 + \frac{32}{21} a_2 a_3^2 - \frac{4}{3} a_4 \\
    d_2 &= \frac{6772}{8085} a_2^4 - \frac{26218}{8085} a_2 a_3^3 + \frac{100}{33} a_2 a_4 + \frac{846}{539} a_3^2 - \frac{30}{11} a_5 \\
    d_3 &= \frac{4996512}{4379375} a_2^5 + \frac{2938436}{525525} a_2 a_3^4 - \frac{26856}{5005} a_2^2 a_4 + \frac{115208}{21021} a_2 a_3^2 + \frac{720}{143} a_2 a_5 + \\
    &\quad + \frac{1636}{273} a_3 a_4 - \frac{60}{13} a_6 \\
    d_4 &= \frac{665792656}{459834375} a_2^6 - \frac{2866208}{334425} a_2 a_3^5 + \frac{625888}{75075} a_3 a_4 + \frac{9331159}{735735} a_2^2 a_5 - \\
    &\quad - \frac{7998}{1001} a_2 a_3^2 + \frac{49396}{3003} a_3 a_4 + \frac{98}{13} a_2 a_6 + \frac{607}{77} a_3 a_5 - \frac{10491}{3773} a_3^2 + \\
    &\quad + \frac{4}{5} a_4 - 7 a_7.
\end{align*}
\]

It is obvious that for a linear potential, all those coefficients are equal to zero.

Since all those coefficients are expressed as functions of the coefficients of the potential \( U(x) \), one can find relations between the \( a \)'s which can make \( d_0, d_1, \ldots \) equal to zero simultaneously.

Since we have

\[
\begin{align*}
    a_1 &= U'(0) \quad \text{assumed to be equal to 1.} \\
    a_2 &= \frac{U''(0)}{2} \\
    a_3 &= \frac{U'''(0)}{6} \\
    a_4 &= \frac{U^{(4)}(0)}{24} \\
    a_5 &= \frac{U^{(5)}(0)}{120} \\
    \ldots
\end{align*}
\]

where \( U^{(n)}(0) \) denotes the derivative of \( U(x) \) of
order \( n \) ( for \( x = 0 \)).

In the expression of \( \Delta[U_{(x)}] \):

\[
d_0 = 0 \iff a_3 = 0.6 a_2^2 \iff U_{(0)}^{(3)} = 0.9 \left( U_{(0)}^{(2)} \right)^2 \quad (A.2)
\]

with \( d_0 \) equal already to 0, we can obtain \( d_1 = 0 \iff a_7 = 0.28 a_2^3 \)
\[
\iff U_{(0)}^{(3)} = 0.84 \left( U_{(0)}^{(2)} \right)^3 \quad (A.3)
\]

with \( d_1 \) equal to zero we can also have:

\[
d_2 = 0 \iff a_5 = 0.112 a_2^5 \iff U_{(0)}^{(5)} = 0.84 \left( U_{(0)}^{(2)} \right)^5 \quad (A.4)
\]

\[
d_3 = 0 \iff a_6 = 0.04032 a_2^6 \iff U_{(0)}^{(6)} = 0.9072 \left( U_{(0)}^{(2)} \right)^6 \quad (A.5)
\]

\[
d_4 = 0 \iff a_7 = 0.01344 a_2^7 \iff U_{(0)}^{(7)} = 1.0584 \left( U_{(0)}^{(2)} \right)^7 \quad (A.6)
\]

If we take out the assumption that \( a = 1 \) one can obtain the following conditions:

\[
d_0 = 0 \iff a_3 = 0.6 a_2^2 \quad \iff U_{(0)}^{(3)} = 0.9 \left( U_{(0)}^{(2)} \right)^2 \quad (A.2)
\]

\[
d_1 = 0 \iff a_4 = 0.28 a_2^4 \quad \iff U_{(0)}^{(4)} = 0.84 \left( U_{(0)}^{(2)} \right)^4 \quad (A.4)
\]

\[
d_2 = 0 \iff a_5 = 0.112 a_2^5 \quad \iff U_{(0)}^{(5)} = 0.84 \left( U_{(0)}^{(2)} \right)^5 \quad (A.4)
\]

\[
d_3 = 0 \iff a_6 = 0.04032 a_2^6 \quad \iff U_{(0)}^{(6)} = 0.9072 \left( U_{(0)}^{(2)} \right)^6 \quad (A.5)
\]

\[
d_4 = 0 \iff a_7 = 0.01344 a_2^7 \quad \iff U_{(0)}^{(7)} = 1.0584 \left( U_{(0)}^{(2)} \right)^7 \quad (A.6)
\]

It has to be noted that with no assumption on \( a \), the expressions of \( d_0, d_1, d_2, d_3, d_4 \) will be modified in such a way that each term will be divided by \( (a_1)^n \) where \( n \) is the sum of the \( a \)'s powers in the numerator.
APPENDIX B

Gauss Integration

In order to evaluate \( \mathcal{M}(x) = \int_0^x \sqrt{|U(x)|} \, dx \), we use the Gaussian quadrature formula appropriate to the function:

\[
\int_0^1 x^{\lambda-1} f(x) \, dx = \sum_{j=1}^{\infty} H_j f(a_j) \tag{B.1}
\]

This formula is exact for all polynomials \( f(x) \) of degree not in excess of \( 2n - 1 \) : \( (3) \)

The abscissas \( a_j \) are roots of the polynomial

\[
\begin{vmatrix}
1 & x & x^2 & \cdots & x^n \\
\alpha_0 & \alpha_1 & \alpha_2 & \cdots & \alpha_n \\
\alpha_1 & \alpha_2 & \alpha_3 & \cdots & \alpha_{n+1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\alpha_n & \alpha_{n+1} & \alpha_{n+2} & \cdots & \alpha_{2n-1}
\end{vmatrix} = 0 \tag{B.2}
\]

where the \( \alpha_k \)'s stand for the moment coefficients defined by:

\[
\alpha_k = \int_0^1 x^{\lambda+k} \, dx = \frac{1}{\lambda+k} \tag{B.3}
\]

The corresponding weights \( H_j \) can eventually be obtained in a purely algebraic way by solving any one of the sets of equations:

\[
\alpha_{i+k} = \sum_{j=1}^{\infty} H_j a_j^{i+k} \tag{B.4}
\]

For our purpose, we have to solve:

\[
\int_0^x \sqrt{|U(x)|} \, dx
\]

This can be written as: \( \int_0^x \sqrt{|x|} \, f(x) \, dx \) where \( f(x) \) is a polynomial.

In our case, according to (A.1) we have: \( \lambda = \frac{3}{2} \)
1) We start with the case \( n = 1 \) (exact for \( f(x) \) polynomial of 1st degree:

solving (A.2) gives:

\[
\begin{vmatrix}
1 & x & x^2 \\
\alpha_0 & \alpha_1 & \alpha_2 \\
\alpha_3 & \alpha_4 & \alpha_5
\end{vmatrix} = 0 \Rightarrow \alpha_1 - \alpha_2 x = 0 \Rightarrow x = \frac{\alpha_1}{\alpha_0}
\]

with (A.3) \( \Rightarrow \alpha_0 = \frac{2}{3} \); \( \alpha_1 = \frac{2}{5} \) \( \Rightarrow x = 0.6 \)

This gives us: \( a_1 = 0.6 \)

solving (A.4) to get \( H_j \) we have:

\( \alpha_0 = H_j a_0 \Rightarrow H_j = \frac{2}{3} \)

In the expression of \( f \) we have:

\[
f = \int_0^Z \sqrt{|x|} \ f(x) \ dx
\]

Put: \( t = \frac{x}{Z} \Rightarrow \sqrt{x} = \sqrt{Z} \sqrt{t} \); \( Z dt = dx \)

\[
f = \int_0^1 \sqrt{Z} \sqrt{t} \ f(Z t) \ Z dt = Z^{3/2} \int_0^1 \sqrt{t} \ f(Z t) \ dt
\]

\[
= x^{3/2} \int_0^1 \sqrt{t} \ f(x t) \ dt = x^{3/2} \int_0^{\pi} \ f(x a_j)
\]

The result is given by:

\[
\int_0^x (A_0 + A_1 x) \ dx = \frac{2}{3} x^{3/2} f\left(0.6 \ x \right)
\]

(A.5)

2) Case: \( n = 2 \) (exact for \( f(x) \) polynomial up to 3rd degree)

\[
\begin{vmatrix}
1 & x & x^2 \\
\alpha_0 & \alpha_1 & \alpha_2 \\
\alpha_3 & \alpha_4 & \alpha_5
\end{vmatrix} = 0 \Rightarrow a_1 = 0.2899491979
\]

\[
\begin{vmatrix}
1 & x & x^2 \\
\alpha_0 & \alpha_1 & \alpha_2 \\
\alpha_3 & \alpha_4 & \alpha_5
\end{vmatrix} = 0 \Rightarrow a_2 = 0.8211619132
\]

with \( \alpha_0 = \frac{2}{3} \); \( \alpha_1 = \frac{2}{5} \); \( \alpha_2 = \frac{2}{7} \); \( \alpha_3 = \frac{2}{9} \)

\( H_1 = 0.2775559981 \)

\( H_2 = 0.3891106685 \)
This gives the result:
\[
\int_0^1 (A_0 + A_1 x + A_2 x^2 + A_3 x^3) \, dx = \\
x^{3/2} \left[ 0.2775559981 \, f(0.2899491979 \, x) + \\
+ 0.3891106685 \, f(0.8211619132 \, x) \right]
\] (B.6)

3) \textbf{Case } n = 3 \textbf{ (exact for } f(x) \textbf{ polynomial up to 5th degree)}

\[
\begin{vmatrix}
1 & x & x^2 & x^3 \\
\alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 \\
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\
\end{vmatrix} = 0
\]

with \( \alpha_4 = \frac{2}{11} \); \( \alpha_5 = \frac{2}{13} \)

This gives us:

\[
\begin{align*}
a_1 &= 0.1647102846 \\
a_2 &= 0.549868503 \\
a_3 &= 0.9008058294 \\
H_1 &= 0.1257826745 \\
H_2 &= 0.3076023698 \\
H_3 &= 0.2332816223
\end{align*}
\]

\[
\int_0^1 \sqrt{x} \left( A_0 + A_1 x + A_2 x^2 + A_3 x^3 + A_4 x^4 + A_5 x^5 \right) \, dx = \\
\begin{vmatrix}
H_1 \, f(a_1 \times x) + H_2 \, f(a_2 \times x) + H_3 \, f(a_3 \times x) \\
\end{vmatrix}
\] (B.7)

4) \textbf{Case } n = 4 \textbf{ (exact for } f(x) \textbf{ polynomial up to 7th degree)}

\[
\begin{vmatrix}
1 & x & x^2 & x^3 & x^4 \\
\alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\
\alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 \\
\alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 & \alpha_7 \\
\end{vmatrix} = 0
\]
with $\alpha' = \frac{2}{15}$; $\alpha = \frac{2}{17}$

we will get:

$$a_1 = 0.1051602826$$
$$a_2 = 0.3762245149$$
$$a_3 = 0.6989480098$$
$$a_4 = 0.9373342517$$

$$H_1 = 0.06568052077$$
$$H_2 = 0.1960962621$$
$$H_3 = 0.2525273495$$
$$H_4 = 0.4523625343$$

\[
\int_0^x (A_0 + A_1 x + A_2 x^2 + A_3 x^3 + A_4 x^4 + A_5 x^5 + A_6 x^6 + A_7 x^7) \, dx = \\
x^{3/2} \left[ H_1 f(a_1 - x) + H_2 f(a_2 - x) + H_3 f(a_3 - x) + H_4 f(a_4 - x) \right]
\]

Let us try now the General case:

if $\alpha_{k+1} = \frac{1}{\lambda + kq}$, we can write the general form of the determinant which we have to evaluate (B.2) in that manner:

$$D_m = \begin{vmatrix}
\frac{1}{\lambda_1} & \frac{1}{\lambda_2} & \frac{1}{\lambda_3} & \cdots & \frac{1}{\lambda_m} \\
\frac{1}{\lambda_1+q} & \frac{1}{\lambda_2+q} & \frac{1}{\lambda_3+q} & \cdots & \frac{1}{\lambda_m+q} \\
\frac{1}{\lambda_1+2q} & \frac{1}{\lambda_2+2q} & \frac{1}{\lambda_3+2q} & \cdots & \frac{1}{\lambda_m+2q} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1}{\lambda_1+kq} & \frac{1}{\lambda_2+kq} & \frac{1}{\lambda_3+kq} & \cdots & \frac{1}{\lambda_m+kq}
\end{vmatrix}

= \det \left( \frac{1}{\lambda + jq} \right) \quad (B.9)

with \( k = m - 1 \)
From this we get the recursion formula: \[
D_m = \prod_{j=0}^{m} \frac{\prod_{i=1}^{m} (\lambda_i + \eta_j)}{\prod_{i=1}^{m-1} (\lambda_i - \lambda_m)} \frac{\prod_{i=1}^{m-1} (\lambda_i + \eta_{j+1})}{\prod_{i=1}^{m-2} (\lambda_i - \lambda_{m-1})} 
\]
(E.11)
APPENDIX C

Matrix Formalism For TheTotally Non Symmetric Case

We assume a potential with \( m \) classical turning points for a given energy level. The connection matrix between two adjacent regions \((i)\) and \((i+1)\) is given by:

\[
\begin{bmatrix}
\frac{M_{i+1, i}}{D_{i+1}}
\end{bmatrix}
= D_{i+1}
\begin{pmatrix}
B_{i} \alpha_{i} & B_{i} \beta_{i} \\
-A_{i} \alpha_{i} & -B_{i} \beta_{i}
\end{pmatrix}
+ 
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\]

and:

\[
\begin{bmatrix}
\frac{M_{i+1, i}}{D_{i+1}}
\end{bmatrix}
= D_{i+1}
\begin{pmatrix}
B_{i} \alpha_{i+1} & B_{i} \beta_{i+1} \\
-A_{i} \alpha_{i+1} & -B_{i} \beta_{i+1}
\end{pmatrix}
+ 
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\]

The overall matrix will be given by the product of all the connections matrices. The number of connection matrices is given by:

\[n = m - 1\]

Let us call:

\[
T_{o} = 
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\]

\[
T_{i} = \sum_{i'=1}^{m} 
\begin{pmatrix}
B_{i} \alpha_{i'} & B_{i} \beta_{i'} \\
-A_{i} \alpha_{i'} & -A_{i} \beta_{i'}
\end{pmatrix}
\]

\[
T_{2} = \sum_{i < j} (B_{i} \alpha_{i} - A_{i} \beta_{i}) 
\begin{pmatrix}
B_{j} \alpha_{j} & B_{j} \beta_{j} \\
-A_{j} \alpha_{j} & -A_{j} \beta_{j}
\end{pmatrix}
\]

81
\[
T_3 = \sum_{i < j < k < l} \left( B_i \alpha_i - A_i \beta_i \right) \left( B_j \alpha_j - A_j \beta_j \right) \left( B_k \alpha_k - A_k \beta_k \right) \left( B_l \alpha_l - A_l \beta_l \right)
\]

\[
T_4 = \sum_{i < j < k < l} \left( B_i \alpha_i - A_i \beta_i \right) \left( B_j \alpha_j - A_j \beta_j \right) \left( B_k \alpha_k - A_k \beta_k \right) \left( B_l \alpha_l - A_l \beta_l \right)
\]

\[
\vdots
\]

\[
T_n = \sum_{i < j < \ldots < n} \left( B_i \alpha_i - A_i \beta_i \right) \left( B_j \alpha_j - A_j \beta_j \right) \left( B_k \alpha_k - A_k \beta_k \right) \left( B_l \alpha_l - A_l \beta_l \right) \ldots
\]

The overall matrix is then given by:

\[
\begin{bmatrix}
M_{i, m}
\end{bmatrix} = \begin{bmatrix}
M_{i, 2}
\end{bmatrix} \begin{bmatrix}
M_{2, 3}
\end{bmatrix} \ldots \begin{bmatrix}
M_{m, m}
\end{bmatrix} = D_1 D_2 \ldots D_n \sum_{j=0}^{n} T_j
\]

where

\[
D_i = \begin{vmatrix}
U_{i-i}
\end{vmatrix} \begin{vmatrix}
U_{i+1}
\end{vmatrix}
\]

For example, we have for a potential with four turning points (three connection matrices, \( n = 3 \))

\[
\begin{bmatrix}
M_{i, 4}
\end{bmatrix} = \begin{bmatrix}
M_{i, 2}
\end{bmatrix} \begin{bmatrix}
M_{2, 3}
\end{bmatrix} \begin{bmatrix}
M_{3, 4}
\end{bmatrix} = D_1 D_2 D_3 D_4 \left[ T_0 + T_1 + T_2 + T_3 \right]
\]

with:

\[
T_0 = I
\]

\[
T_1 = \begin{pmatrix}
B_1 \alpha_1 + B_2 \alpha_2 + B_3 \alpha_3
& B_1 \beta_1 + B_2 \beta_2 + B_3 \beta_3 \\
-A_1 \alpha_1 - A_2 \alpha_2 - A_3 \alpha_3
& -B_1 \beta_1 - B_2 \beta_2 - B_3 \beta_3
\end{pmatrix}
\]
\[ T_2 = (B_1 \alpha_2 - A_1 \beta_2) \begin{pmatrix} B_2 \alpha_1 & B_2 \beta_1 \\ -A_2 \alpha_1 & -A_2 \beta_1 \end{pmatrix} + (B_2 \alpha_3 - A_2 \beta_3) \begin{pmatrix} B_3 \alpha_2 & B_3 \beta_2 \\ -A_3 \alpha_2 & -A_3 \beta_2 \end{pmatrix} \]

and

\[ T_3 = (B_3 \alpha_3 - A_3 \beta_3) \begin{pmatrix} B_1 \alpha_2 & A_1 \beta_2 \\ -A_3 \alpha_2 & -A_3 \beta_2 \end{pmatrix} + \begin{pmatrix} B_3 \alpha_1 & B_3 \beta_1 \\ -A_3 \alpha_1 & -A_3 \beta_1 \end{pmatrix} \]

The eigenvalue conditions will then be given by:

1) \[-A_1 \alpha_1 - A_2 \alpha_2 - A_3 \alpha_3 - A_2 \alpha_1 (B_1 \alpha_2 - A_1 \beta_2) - A_3 \alpha_2 (B_2 \alpha_3 - A_2 \beta_3) - \\
\quad - A_3 \alpha_1 (B_2 \alpha_3 - A_2 \beta_3) (B_1 \alpha_2 - A_1 \beta_2) = 0 \]

2) \[B_1 \alpha_1 + B_2 \alpha_2 + B_3 \alpha_3 + B_2 \alpha_1 (B_1 \alpha_2 - A_1 \beta_2) + B_3 \alpha_2 (B_2 \alpha_3 - A_2 \beta_3) + \\
\quad + B_3 \alpha_1 (B_2 \alpha_3 - A_2 \beta_3) (B_1 \alpha_2 - A_1 \beta_2) + 1 = C \]

The eigenvalue conditions in the general case with n connection matrices will be given by:

1) \[- \sum_{i \neq j} A_i \alpha_i - \sum_{i \neq j} A_j \alpha_j (B_i \alpha_j - A_j \beta_j) - \sum_{i \neq j < k} \sum_{i \neq j < k} A_k \alpha_i (B_j \alpha_k - A_j \beta_k) - \\
\quad - (B_i \alpha_j - A_i \beta_j) - \ldots - \sum_{i < j \ldots < n} A_{m-1} \alpha_i (B_{m-1} \alpha_{m-1} - A_{m-1} \beta_{m-1}) \ldots (B_i \alpha_j - A_i \beta_j) = 0 \]

2) \[\sum_{i \neq j} B_i \alpha_i + \sum_{i \neq j} B_j \alpha_j (B_i \alpha_j - A_i \beta_j) + \sum_{i \neq j < k} B_k \alpha_i (B_j \alpha_k - A_j \beta_k) + \\
\quad + (B_i \alpha_j - A_i \beta_j) + \ldots + \sum_{i < j \ldots < n} B_{m-1} \alpha_i (B_{m-1} \alpha_{m-1} - A_{m-1} \beta_{m-1}) \ldots (B_i \alpha_j - A_i \beta_j) \]
APPENDIX D

//EXEC  FORLOAD
C****S:AD(1), DR2
C*****COMPUTE DELTA (F-VERSION), FIND THE NEW POTENTIAL USING THE ITERATION PROCEDURE AND FIND THE ENERGY EIGENVALUES.
DIMENSION XW(20,10), MDP(3), ALBP(2), ANOVA(13), B(10,12), 2PRE(20,6), NK(80), P(20,1), VA(20,1), XA(20,1), PA(20,1), 2FFA(20,1), FSA(20,1), ZA(20,1), XMUA(20,1), EX(10), VNE(20,1), 2, CO(10,10), W00(20,1)
REAL MO, MAXIM
COMMON B1, B2, B3, B4, B5, B6, B7, B0, J
COMMON F10, F11, F12, F13, F14, F15, F16
COMMON F20, F21, F22, F23, F24, F25
COMMON OMK, OM2, OM3, OM4, OM5, OH6
COMMON PHOM, PHOM, PHOM, PHOM, PHOM, PHOM
COMMON FF, FS, F2S, OMEG, OMEG, VZ, VSN, FXOM, XMUA, Z
COMMON AI, BI, ALI, BI, SUMA
COMMON AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER
DOUBLE PRECISION WK
CALL ERRSET (208, 256, -1, 1)

1003 CONTINUE
1000 READ(5, 20) XO, DX, XLMADA, VSN, DIM, ACCUR, DEG, XMIM
20 FORMAT(8F10.6)
   ACCUR=0.05
   DEG=4.
WRITE(6, 15) XO, DX, XLMADA, VSN, DIM, ACCUR, DEG, XMIM
15 FORMAT(1XO, DX, XLMADA, VSN, DIM, ACCUR, DEG, XMIM=78F10.6)
IF (XO.EQ.0.0.) GO TO 250
NDIM=INT(DIM+.2)
IF(XMIM.EQ.0.0.) MM=0

1001 CONTINUE-
   PG=3.141592654
   X1=-X0
17 CONTINUE
   XLMADA=XLMADA
   I=IFIX(DEG)
   X=X1
   DO 999 I=1,20
       DX=PG/19.
       XA(I,1)=X
       W=1.
       VO=-COS(X+X0)+COS(X0)
       V00(I,1)=VO
       Y=SQRT(ABS(VO/X))
       GO TO 819
819 XYW(I,1)=X
   XYW(I,2)=Y
   XYW(I,3)=W
   WRITE(6, 1200) X, V0, Y
1200 FORMAT(7.3, 2E15.8)
   X=X+DX
999 CONTINUE
C*****ITERATION PROCEDURE,
642 IX=20
N=20
RS0=100
MDP(1)=J
MDP(2)=0
MDP(3)=0
ALBP(1)=0.05
ALBP(2)=0.05
IB=10
IP=20
CALL RLFOR(X,W,IX,N,R,AL,EP,ANOVA,ND,IF,W,IIP)
C WRITE(6,32)(B(I,2),I=1,3)
C 32 FORMAT(10X,'B(1,?)) TO B(6,2) = ',SE15.7)
AT1=B(1,2)
AT2=B(2,2)
AT3=B(3,2)
AT4=B(4,2)
AT5=B(5,2)
AT6=B(6,2)
AT7=B(7,2)
AT8=0.
CALL Restau
25 WRITE (6,30) B0,B1,B2,B3,B4,B5,B6,B7,X1,DX,X2
30 FORMAT(' ',B0 TO B7,X1,DX,X2= ',
2/1X,SE13.6,3E7.3/4X,'X',6X,'U(X)',10X,'DELTA',11X, 
2,'EFFPOT',9X,'VNEW',15X,'VO',11X,'XMU',10X,'Z',11X,'FX')
B10=B0
B11=B1
B12=B2
B13=B3
B14=B4
B15=B5
B16=B6
B17=B7
SUMM=1.
WRITE (6,1234) J
1234 FORMAT(20X,'POLYNOMIAL F OF DEGREE = ',I2)
XLAMDA=XLAMDO
9999 B0=B10
B1=B11
B2=B12
B3=B13
B4=B14
B5=B15
B6=B16
B7=B17
SUMA=0.
2500 SUM=0.
SUMA=SUMA+1.
IF(SUMA.GT.40) GO TO 65
C****************************************
C COMPUTATION OF DELTA.
CALL PREPAR
WGJ=0.
DO 90 I=1,20
X=XA(I,1)
W=1.
VO=VV0(I,1)
DELTA0=DELTX0
VA(I,1)=VZ
FFA(I,1)=FF
FSA(I,1)=FS
XMUA(I,1)=XMU
ZA(I,1)=Z
EFFPOT=VZ+DELTA0
PX=VO-EFPOT
P(I,1)=ABS(PX)
PA(I,1)=PX
SUM=SUM+ABS(PX)
VNEW=VZ+XLAMDA*(VO-EFPOT)
VNEW(I,1)=VNEW
IF(WGJ.GT.0.) GO TO 92
IF(VNEW.GT.0.) GO TO 94
WJ1=VNEW
WJ1=X
GO TO 92
94  WGC=VNEW
WJ2=X
CHIFT=(WGC*WJ1-WJ1*WGC7(WGC-WJ1))
WJ1=1.
C  WRITE(6,98) CHIFT
C  FORMAT(10X,'CHIFT=',E20.10)
92  CONTINUE
IF(SUMM.GT.1.) GO TO 90
C
C
WRITE(6,40) X,V7,DELTAV,EFFPOT,VNEW,VO,XMU,Z,FX
40  FORMAT(6.40) X,V7,DELTAV,EFFPOT,VNEW,VO,XMU,Z,FX
C
C
C**** CONDITIONS FOR ENERGY EIGENVALUES USING THE ORIGINAL POTENTIAL.
C(I.EQ.1.) GO TO 1434
C(I.EQ.20.) GO TO 1435
GO TO 90

1434 CALL CONST
A10=A1
B10=BI
AI10=AI1
BI10=BI1
GAS01=0.5* (1./Z)
FII=3.141592654
ALSO1=FPI*(GAS01*A10+2.*AI10)
BES01=FPI*(GAS01*B10+2.*BI10)
HELO=A10*ALSO1
WRITE(6,1437) A10,B10,ALSO1,BES01,GAS01,U1,Z1,HELO
1437  FORMAT(8E15.6)
GO TO 1436
1435 CALL CONST
B20=BI
A20=AI
AI20=AI2
BI20=BI2
GASO2=0.5* (1./Z)
WRITE(6,1439) A20,B20,ALSO2,BES02,GASO2,U1,Z1
1439  FORMAT(7E17.8)
ALSO2=FPI*(GASO2*A20+2.*AI20)
BES02=FPI*(GASO2*B20+2.*BI20)
G012=B10*ALSO2-A10*BES02
G021=B20*ALSO2-A20*BES01
G03=G012+G021
FNO=2.* (1.+B10*ALSO1)* (1.+B20*ALSO2)-A20*ALSO2*B10*BES01
CODO=(FNO-2.)/(B20*BES02)
COND01=(FNO-2.)/(B20*BES02)
COND02=(FNO+1.0)/(B20*BES02)
COND03=FNO/(B20*BES02)
CODO=A10*ALSO1-COD0
COND01=A10*ALSO1-COND01
COND02=A10*ALSO1-COND02
COND03=A10*ALSO1-COND03
ENER=1.-COS(X0)
WRITE(6,1401) ENER,COD0,COND01,COND02,COND03
1401  FORMAT(2X,'ENERGO',2X,E20.10/7E16.8)
W01=1.+B10*ALSO1
W02=1.+B20*ALSO2
W03=B20*BF502
W04=1./W03
W05=0.5/W03
WRITE(6,1111) HELO,W01,W02,W03,W04,W05
1111 FORMAT (5X,'HELO,W01,W02,W03=',6E15.7)
1434 CONTINUE
C
C
90 CONTINUE
100 CONTINUE
DO 88 I=1,20
X=XA(I,1)+SHIFT
VNEW=VNE(I,1)
IF(ABS(X),LT.0.01) GO TO 199
Y=SQRT(ABS(VNEW/X))
GO TO 919
199 Y=ABS(B0+B1*SHIFT+B2*SHIFT*SHIFT)
919 CONTINUE
XYW(I,1)=X
XYW(I,2)=Y
XYW(I,3)=W
XA(I,1)=X
88 CONTINUE
C
C
SUMM=SUMM+1.
IX=20
N=20
RS0=100
MDF(1)=J
MDF(2)=0.
MDF(3)=0
ALBP(1)=0.05
ALBP(2)=0.05
IB=10
IF=20
AVPX=SUM/20.
MAXIN=0.
DO 666 I=1,20
M0=P(I,1)
666 IF (M0.GT.MAXIN) MAXIN=M0
C WRITE(6,500) AVPX,MAXIN
C500 FORMAT (2X,'AVPX=',6E15.8,10X,'MAXIN=',E15.8)
IF (AVPX.LT.20.0) GO TO 3000
GO TO 300
C****DEGREE OF ACCURACY WANTED.
3000 IF (M0.GT.LE.ACCUR) GO TO 333
CALL RLFOR(XYW,IX,N,RSQ,MDF,ALBP,ANOVA,B,IB,PRED,IF,HEK,IER)
C WRITE(6,34)(B(I,2),I=1,8)
C 34 FORMAT(10X,'B(1,2) TO B(8,2) ='/8E15.7)
AT1=B(1,2)
AT2=B(2,2)
AT3=B(3,2)
AT4=B(4,2)
AT5=B(5,2)
AT6=B(6,2)
AT7=B(7,2)
AT8=0.
CALL RESTAU
GO TO 2500
C
C
CONVERGENCE REACHED

323 WRITE (6, 323) R0, R1, B7, D3, B4, R5, B6, B7, X1, DX, X2
323 FORMAT (' ', 'R0 TO B7, X1, DX, X2=', '2/1X, SE13.6, 3F7.3/4X, X', '6X, '(U(X), 15X, Z', '15X, PX)'), DO 75 I=1, 20
W=1,
X=XA(I, 1)
VZ=VA(I, 1)
FX=PA(I, 1)
FF=FFA(I, 1)
FS=FSA(I, 1)
XMU=XMUA(I, 1)
Z=ZA(I, 1)
WRITE(6, 44) X, VZ, Z, FX, FF, FS
44 FORMAT (F7.3, 5E20.10)
C**** CONDITIONS FOR ENERGY EIGENVALUES USING THE NEW POTENTIAL
C**** FOUND BY THE ITERATION PROCEDURE.
IF(I.EQ.1.) GO TO 2434
IF(I.EQ.20.) GO TO 2435
GO TO 66
2434 CALL CONST
U1=FF*FF+2. *X*FF*FS
Z1=Z*SQRT(ABS(VZ))/(1.5*XMU)
AII=AI
BII=BI
AII=AII
BII=BII
GAS1=0.5*(1./Z)-0.5*(U1/(Z1*VZ))
ALS1=PII*(GAS1*AII+2.*AII)
BES1=PII*(GAS1*BII+2.*BII)
HEL=AII*ALS1
WRITE(6, 2437) AII, BII, AII, BII, GAS1, U1, Z1, HEL
2437 FORMAT (8E15.6)
GO TO 2436
2435 CALL CONST
U1=FF*FF+2. *X*FF*FS
Z1=Z*SQRT(ABS(VZ))/(1.5*XMU)
B22=BI
A22=AI
BII=BII
MM=MH+1.
GAS2=0.5*(1./Z)-0.5*(U1/(Z1*VZ))
WRITE(6, 2439) A22, B22, AII, BII, GAS2, U1, Z1
2439 FORMAT (7E17.8)
ALS2=PII*(GAS2*A22+2.*AII)
BES2=PII*(GAS2*B22+2.*BII)
G12=BII*ALS2-AII*BES2
G21=B22*ALS1-A22*BES1
G13=G12*G21
FN=(B11*ALS1+1.)*(B22*ALS2+1.)*Z.-A22*ALS2*B11*BES1
COD=(FN-2.)/(B22*BES2)
COND1=(FN+2.)/(B22*BES2)
COND2=(FN+1.0)/(B22*BES2)
COND3=FN/(B22*BES2)
COD=AII*ALS1-COD
COND1=AII*ALS1-COND1
COND2=AII*ALS1-COND2
COND3=AII*ALS1-COND3
WRITE(6, 2401) COD, COND1, COND2, COND3
2401 FORMAT (7E16.8)
W1=1.+BII*ALS1
C**THE NEW POTENTIAL OBTAINED BY THE ITERATION PROCEDURE.
CALL RLFOR(XYW,IX,N,RSQ,MDP,ALBP,ANOVA,B,IB,PRED,IP,WK,IER)
AT1=B(1,2)
AT2=B(2,2)
AT3=B(3,2)
AT4=B(4,2)
AT5=B(5,2)
AT6=B(6,2)
AT7=B(7,2)
AT8=0.
CALL RESTAU

C WRITE (6,346) JJ,B0,B1,B2,B3,B4,B5
C346 FORMAT(20X,'NPOT OF DEGREE ',I3,5X,'COEFFICIENTS OF NPOT ='/
C 28E15.8)
C271 WRITE (6,146) (ANOVA(I),I=1,13)
C146 FORMAT (3F5.2,10E11.4)
C WRITE (6,246) (PRED(I,1),I=1,20)
C246 FORMAT (3E15.7)
IF(MM.LE.1.) GO TO 301
M=MM
DO 72 K=1,4
MT=M-1.
MN=MT
EXXi=EX(MN)
EXX2=EX(M)
CO01=CO(MN,K)
CO02=CO(M,K)
EE=(EXXi*CO02-CO01*EXX2)/(CO02-CO01)
WRITE(6,76) EE
76 FORMAT(20X,E20.8)
72 CONTINUE
GO TO 301
40 XLAMDA=XLAMDA*1.2
IF(XLAMDA.GE.0.75) GO TO 24
GO TO 232
300 CONTINUE
24 WRITE(6,51) XLAMDA
51 FORMAT(*NO CONVERGENCE YET: XLAMDA=*F10.6*)
301 CONTINUE
GO TO 1000
250 STOP
END

FUNCTION OMG(X)
COMMON B1,B2,B3,B4,B5,B6,B7,B0,J
COMMON F10,F11,F12,F13,F14,F15,F16
COMMON F20,F21,F22,F23,F24,F25
COMMON OMO,OM1,OM2,OM3,OM4,OM5,OM6
COMMON FOMV,FOM0,FOM1,FOM2,FOM3,FOM4,FOM5
COMMON FF,FS,F2S,OMEG,OMEG5,VZ,VSN,VXM,XMU,Z
COMMON AI,BI,ALI,BLI,SUMA
COMMON AT1,AT2,AT3,AT4,AT5,AT6,AT7,AT8,IER
OMG=OMO+X*(OM1+X*(OM2+X*(OM5+X*(OM5+X*OM6))))
RETURN
END

FUNCTION FOM(X)
COMMON B1,B2,B3,B4,B5,B6,B7,B0,J
COMMON F10,F11,F12,F13,F14,F15,F16
COMMON F20,F21,F22,F23,F24,F25
COMMON OMO,OM1,OM2,OM3,OM4,OM5,OM6
COMMON FOMV,FOM0,FOM1,FOM2,FOM3,FOM4,FOM5
COMMON FF,FS,F2S,OMEG,OMEG5,VZ,VSN,VXM,XMU,Z
COMMON AI,BI,ALI,BLI,SUMA
COMMON AT1,AT2,AT3,AT4,AT5,AT6,AT7,AT8,IER
IF(ABS(X)>.05) 40,40,50
40 FOM=FOM0+X*(FOM1+X*(FOM2+X*(FOM3+X*(FOM4+X*FOM5))))
FOM=2.*FOM
GO TO 60
50 FOM=(FS-OMEG5/2.)/X
60 FOMV=FOM
68 RETURN
END

FUNCTION F(X)
COMMON B1,B2,B3,B4,B5,B6,B7,B0,J
COMMON F10,F11,F12,F13,F14,F15,F16
COMMON F20,F21,F22,F23,F24,F25
COMMON OMO,OM1,OM2,OM3,OM4,OM5,OM6
COMMON FOMV,FOM0,FOM1,FOM2,FOM3,FOM4,FOM5
COMMON FF,FS,F2S,OMEG,OMEG5,VZ,VSN,VXM,XMU,Z
COMMON AI,BI,ALI,BLI,SUMA
COMMON AT1,AT2,AT3,AT4,AT5,AT6,AT7,AT8,IER
F=B0+X*(B1+X*(B2+X*(B3+X*(B4+X*(B5+X*(B6+X*B7))))))
RETURN
END

FUNCTION F1(X)
COMMON B1,B2,B3,B4,B5,B6,B7,B0,J
COMMON F10,F11,F12,F13,F14,F15,F16
COMMON F20,F21,F22,F23,F24,F25
COMMON OMO,OM1,OM2,OM3,OM4,OM5,OM6
COMMON FOMV,FOM0,FOM1,FOM2,FOM3,FOM4,FOM5
COMMON FF,FS,F2S,OMEG,OMEG5,VZ,VSN,VXM,XMU,Z
COMMON A1, B1, AII, BII, SUMA
COMMON A1, AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER
F1 = F10 * (F11 + X * (F12 + X * (F13 + X * (F14 + X * (F15 + X * F16))))))
RETURN
END

FUNCTION F2(X)
COMMON B1, B2, B3, B4, B5, B6, B7, B0, J
COMMON F10, F11, F12, F13, F14, F15, F16
COMMON F20, F21, F22, F23, F24, F25
COMMON OM0, OM1, OM2, OM3, OM4, OM5, OM6
COMMON FOM0, FOM1, FOM2, FOM3, FOM4, FOM5
COMMON FF, FS, F2S, OMEG, OMEG5, VZ, VSGN, FXOM, XMU, Z
COMMON AI, AII, BII, SUMA
COMMON AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER
F2 = F20 + X * (F21 + X * (F22 + X * (F23 + X * (F24 + X * F25))))
RETURN
END

***********************************************************************
SUBROUTINE PREPAR
COMMON B1, B2, B3, B4, B5, B6, B7, B0, J
COMMON F10, F11, F12, F13, F14, F15, F16
COMMON F20, F21, F22, F23, F24, F25
COMMON OM0, OM1, OM2, OM3, OM4, OM5, OM6
COMMON FOM0, FOM1, FOM2, FOM3, FOM4, FOM5
COMMON FF, FS, F2S, OMEG, OMEG5, VZ, VSGN, FXOM, XMU, Z
COMMON AI, AII, BII, SUMA
COMMON AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER

C**** FOR F1
F10 = B1
F11 = 2. * B2
F12 = 3. * B3
F13 = 4. * B4
F14 = 5. * B5
F15 = 6. * B6
F16 = 7. * B7

C**** FOR F2
F20 = F11
F21 = 2. * F12
F22 = 3. * F13
F23 = 4. * F14
F24 = 5. * F15
F25 = 6. * F16

C******* FOR OMEGA
OM0 = 4. * B1
OM2 = 2. * B3 / 3.

C******* FOR FOM
FOM0 = 2. * B2 / 7.
FOM4 = 2. * B6
FOM5 = 42. * B7 / 17.
RETURN
END

***********************************************************************
FUNCTION DELT(X)
COMMON B1, B2, B3, B4, B5, B6, B7, B0, J
COMMON F10, F11, F12, F13, F14, F15, F16,
    F20, F21, F22, F23, F24, F25
COMMON OHO, ON1, ON2, OM3, OM4, OM5, OM6
COMMON FOMV, FOM0, FOM1, FOM2, FOM3, FOM4, FOM5
COMMON FF, FS, F35, OMEG, OMEG5, VZ, VSGN, FXOM, XM1, Z
COMMON AI, BI, AII, BII, SUMA
COMMON AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER
FF = F(X)
VZ = VSGN * X * FF**2
OMEG = OMEG(X)
FS = F1(X)
F2S = F2(X)
OMEG5 = S * OMEG
FXOM = FF * X * OMEG
XMU = ABS((6666666666 X * FXOM * SORT(ABS(X)))
VZ = VSGN * X * FXOM * FIT(R)(ABS(X))*1.333333334
C = (FF * FOM(X) - S * OMEG*(FS-OMEG5/8.) + FS*X*OMEG**2/FF)
2/4.*(FXOM*FXOM)
508 DELT=3.*(FS/FF)**2/4.-F2S/(2.*FF)+C
RETURN
END

SUBROUTINE CONST
COMMON B1, B2, B3, B4, B5, B6, B7, B8, J
COMMON F10, F11, F12, F13, F14, F15, F16
COMMON F20, F21, F22, F23, F24, F25
COMMON OMO, OM1, OM2, OM3, OM4, OM5, OM6
COMMON FOMV, FOMO, FOM1, FOM2, FOM3, FOM4, FOM5
COMMON FF, FS, F35, OMEG, OMEG5, VZ, VSGN, FXOM, XM1, Z
COMMON AI, BI, AII, BII, SUMA
COMMON AT1, AT2, AT3, AT4, AT5, AT6, AT7, AT8, IER
IF(ABS(Z).GT.2.) GO TO 432
IF(ABS(Z).GT.3.) GO TO 432
C1 = 0.3550280538
C2 = 0.2588194037
C3 = C10*C10*FI-C20*GI
B1 = SORT(T,3.)*(C10*FI+C20*GI)
BII = 0.5*Z*Z+(1.140.)*Z*Z*Z*Z*Z*Z*Z*Z+(1.7076160.)*Z*Z*Z*Z*Z*Z*Z*Z+Z*Z*Z*Z*Z*Z*Z*Z
C10 = 1.333333334
C20 = 1.333333334
C30 = 1.333333334
C40 = 1.333333334
C50 = 1.333333334
C60 = 1.333333334
C70 = 1.333333334
C80 = 1.333333334
C90 = 1.333333334
D0 = 1.
DI = -(-7.35.)*C1
D2 = -(13.11.)*C2
D3 = -(19.17.)*C3
D4 = -(25.23.)*C4
D5 = -(31.29.)*C5
D6 = -(37.35.)*C6
GO TO 432
432 CO = 1.
C1 = 0.0694444444
C2 = 0.0371334877
C3 = 0.0379930591
C4 = 0.0576491904
C5 = 0.116019064
C6 = 0.2915913992
C7 = 0.8776669675
C8 = 1.847671818
C9 = 12.34157333
D0 = 1.
D1 = -(-7.35.)*C1
D2 = -(13.11.)*C2
D3 = -(19.17.)*C3
D4 = -(25.23.)*C4
D5 = -(31.29.)*C5
D6 = -(37.35.)*C6
GO TO 432
C7 = -(43./41.) C7
D6 = -(17./47.) C6
D7 = -(75./75.) C9
P1 = 1.772433851
P1 = 0.14159265
CUM1 = 1. + C1/XMU+C2/(XMU**2)-C3/(XMU**3)+C4/(XMU**4)-C5/(XMU**5)
2+C6/(XMU**6)-C7/(XMU**7)+C8/(XMU**8)-C9/(XMU**9)
CUM2 = 1. - C2/(XMU**2)+C4/(XMU**4)-C6/(XMU**6)+C8/(XMU**8)
CUM3 = C1/XMU-C3/(XMU**3)+C5/(XMU**5)-C7/(XMU**7)+C9/(XMU**9)
CUM4 = 1. + C1/XMU+C2/(XMU**2)+C3/(XMU**3)+C4/(XMU**4)+C5/(XMU**5)
2+C6/(XMU**6)+C7/(XMU**7)+C8/(XMU**8)+C9/(XMU**9)
DUM1 = 1. - D1/XMU+D2/(XMU**2)-D3/(XMU**3)+D4/(XMU**4)-D5/(XMU**5)
2+D6/(XMU**6)-D7/(XMU**7)+D8/(XMU**8)-D9/(XMU**9)
DUM2 = 1. - D2/(XMU**2)+D4/(XMU**4)-D6/(XMU**6)+D8/(XMU**8)
DUM3 = D1/XMU-D3/(XMU**3)+D5/(XMU**5)-D7/(XMU**7)+D9/(XMU**9)
DUM4 = 1. + D1/XMU+D2/(XMU**2)+D3/(XMU**3)+D4/(XMU**4)+D5/(XMU**5)
2+D6/(XMU**6)+D7/(XMU**7)+D8/(XMU**8)+D9/(XMU**9)
IF(Z.LT.0.) GO TO 433
AI = (0.5/(PI*ABS(XMU)))*CUM1
AII = (-0.5/(PI*EXP(ABS(XMU))))*DUM1
BI = (EXP(ABS(XMU)))/(PI*(Z**0.25)))*CUM4
BII = (EXP(ABS(XMU)))/(2.5)*DUM4
GO TO 438
433 AI = (1./PI*(ABS(Z)**0.25))*(SIN(XMU+PII/4.))*CUM2-COS(XMU+PII/4.)*CUM3
2*CUM5
AII = (ABS(Z)**0.25/PI)*(COS(XMU+PII/4.))*DUM2+sin(XMU+PII/4.)*DUM3
BT = (1./PI*(ABS(Z)**0.25))*(COS(XMU+PII/4.))*CUM2+sin(XMU+PII/4.)*CUM3
2*CUM5
BII = (ABS(Z)**0.25/PI)*(SIN(XMU+PII/4.))*DUM2-COS(XMU+PII/4.)*DUM3
438 RETURN
END
SUBROUTINE RESTAU
COMMON B1,B2,B3,B4,B5,B6,B7,B0,J
COMMON F10,F11,F12,F13,F14,F15,F16
COMMON F20,F21,F22,F23,F24,F25
COMMON QMC,QM1,QM2,QM3,QM4,QM5,QM6
COMMON FOMV,FOM0,FOM1,FOM2,FOM3,FOM4,FOM5
COMMON FF,FS,F28,QMEG,QMEO5,VZ,VG,FXQH,XMU,Z
COMMON AI,BI,AII,BII,SUMA
COMMON AT1,AT2,AT3,AT4,AT5,AT6,AT7,ATS,IER
B1=AT1
B2=AT2
IF(IER.EQ.33.) GO TO 10
IF(J.EQ.6) GO TO 7
IF(J.EQ.5) GO TO 6
IF(J.EQ.4) GO TO 5
IF(J.EQ.3) GO TO 4
IF(J.EQ.2) GO TO 3
B0=AT3
B3=AT3
B4=AT4
B5=AT5
B6=AT6
B7=AT7
GO TO 9
7 B0=AT7
B3=AT3
B4=AT4
B5=AT5
B6=AT6
B7=0.
GO TO 9
B0 = AT2
B1 = AT1
B2 = 0.
B3 = 0.
B4 = 0.
B5 = 0.
B6 = 0.
B7 = 0.
GO TO 9

B0 = AT3
B3 = AT3.
B4 = 0.
B5 = 0.
B6 = 0.
B7 = 0.
GO TO 9

B0 = AT4
B3 = AT4.
B4 = 0.
B5 = 0.
B6 = 0.
B7 = 0.
GO TO 9

IF (ABS(AT3) .GT. 100000.) GO TO 17
IF (ABS(AT3) .LT. 0.00000001) GO TO 17
GO TO 2

17 IF (ABS(AT7) .GT. 100000.) GO TO 16
IF (ABS(AT7) .LT. 0.00000001) GO TO 16
GO TO 7

16 IF (ABS(AT6) .GT. 100000.) GO TO 15
IF (ABS(AT6) .LT. 0.00000001) GO TO 15
GO TO 6

15 IF (ABS(AT5) .GT. 100000.) GO TO 14
IF (ABS(AT5) .LT. 0.00000001) GO TO 14
GO TO 5

14 IF (ABS(AT4) .GT. 100000.) GO TO 13
IF (ABS(AT4) .LT. 0.00000001) GO TO 13
GO TO 4

13 IF (ABS(AT3) .GT. 100000.) GO TO 1
IF (ABS(AT3) .LT. 0.00000001) GO TO 1
GO TO 3

1 B0 = AT2
B1 = AT1
B2 = 0.
B3 = 0.
B4 = 0.
B5 = 0.
B6 = 0.
B7 = 0.

RETURN
END
REFERENCES


8. Rapp, D., Quantum Mechanics (Holt, Rinehart and Winston, New York, 1971)


22. J. L. Dunham, Phys. Rev. 41, 721 (1932)
23. O. Klein, Z. Phys. 76, 226 (1932)
25. A. Jablonski, Phys. Rev. 68, 78 (1945)
31. F. J. Smith, Physica (Utrecht) 30, 497 (1964)
32. L. L. Barnes, N. J. Lane and C. C. Lin, Phys. Rev. 137, A388 (1965)
82. C. E. Hecht and J. E. Mayer, Phys. Rev. 106, 1156 (1957)
VITA AUCTORIS

I was born in Lebanon on December 24, 1942. In 1968, I obtained a "Licence" in Theology from the University of Saint Joseph in Beirut, in 1969 a "Licence" in Philosophy from the same University, in 1972 a "Licence d'enseignement" in Physics from the Lebanese University in Beirut and in 1973 an A.E.A. (Attestation d'Etudes Approfondies) in Physics from the "Centre d'Etudes Mathematiques et Physiques" of the University of Lyon in Beirut. In 1976, I began to work for my Ph.D. degree in Physics at the University of Windsor.