SOLUTION OF THE SCHRÖDINGER EQUATION FOR NON-CONVENTIONAL POTENTIALS USING THE ASYMPTOTIC ITERATION AND J-MATRIX METHODS

BY

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Dedication

First of all, I dedicate this project to God Almighty, my creator, my strong pillar, my source of inspiration, wisdom, knowledge and understanding. I also would be honored to dedicate this work to my beloved family for their unfailing support and continuous encouragement.

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LIST OF ABBREVIATIONS

AIM	:	Asymptotic Iteration Method
TRA	:	Tridiagonal Representation Approach
SCH	:	Schrodinger Equation
PC	:	Plateau of convergence

ABSTRACT

Full Name : Sadig Ali Mohammed Al-Buradah

Thesis Title : Solution of the Schrödinger Equation for Non-Conventional Potentials using the Asymptotic Iteration and J-Matrix Methods

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The objective of this work is to make a comparative study between the numerical and analytical results generated by the Asymptotic Iteration Method (AIM) and the Tridiagonal Representation Approach (TRA). In the AIM the calculation of the energy eigenvalues for a given potential is performed using the quantization condition that terminates the iterations asymptotically. While in the TRA the energy eigenvalues will be obtained using a suitable infinite L^2 basis which transforms the Schrödinger into a matrix eigenvalue problem. Usually, Jacobi and Laguerre basis are used, where the basis parameters are selected to ensure a tridiagonal and symmetric matrix representation of the Hamiltonian matrix. To test the accuracy and effectiveness of both methods we consider situations where the potential is either analytically or approximately solvable. In this case, one can give a more accurate assessment of the advantages and disadvantages of each method and, thus, can give a fair judgment on the superiority of one method over the other. Usually, in the AIM, the quantization condition that gives the energy spectrum depends also on the chosen configuration space point, say x_0. In this work, we observed that for a desired accuracy there exists an interval in configuration space (a *plateau* of convergence/stability) where

the calculated energy spectrum is independent of x_0 . This plateau of convergence grows up rapidly to an optimal iteration number and then shrinks slowly to a point. This constitutes one of our main contributions to the AIM in this Thesis.

ملخص الرسالة

الاسم الكامل: صـــــادق علي محمد البـــــرّده

عنوان الرسالة: حل معادلة شرود نجر لجهود غير تقليدية باستخدام طُرق مُقارب التكرار ومصفوفة J.

التخصص: فيـــزيـــاء

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يهدف هذا البحث الى دراسة مقارنة للنتائج التحليلية والعددية الناتجة من استخدام طريقة مُقارب التكرار وطريقة تمثيل المصفوفة ثلاثية القطر لمعادلة الموجة (شرود نجر). في طريقة مُقارب التكرار يتم حساب طيف الطاقة (القيم الذاتية للطاقة) بالنسبة للجهد المعطى باستخدام معادلة التكميم التي تعمل على إنهاء التكرار بشكل تقريبي. اما بالنسبة لطريقة تمثيل المصفوفة ثلاثية القطر فإنه يتم الحصول على القيم الذاتية للطاقة حيث يتم كتابة دالة الموجة على شكل متسلسلة لا نهائية بحيث تعتمد معاملات الحدود على الطاقة وثوابت المكونات التي يتم اختيارها لتحويل معادلة الموجة الى شكل معادلة القيم الذاتية . بالنسبة للحدود عباره عن اقتراحات مربعة التكامل تعتمد على مسار الجسم فقط. غالبا يتم استخدام متسلسلة جاكوبي ومتسلسلة لاقير حيث يتم اختيار معاملاتها للحصول على تمثيل المصفوفة ثلاثية القطر. لاختبار دقة وفعالية هاتين الطريقتين يؤخذ بعين الاعتبار الحالات التي يكون فيها الجهد إما قابل للحل بالتقريب أو بشكل مضبوط. في مثل هذه الحالات ، يمكننا تقديم تقييما اكثر دقة لمعرفة مزايا وعيوب كلتا الطريقتين عندئذ يمكن الحكم بأفضلية أو تفوق أي منهما. غالبا ، فإنه بالنسبة لمعادلة التكميم في طريقة مُقارب التكرار التي من خلالها يتم الحصول على الطاقة (القيم الذاتية) تعتمد على الموقع (لنفترض المتغير س) أو مسار لجسم. في هذا البحث عملنا على إيجاد ما يسمي (منحنى الاستقرار أو التقارب) حيث لدقة معينة فإنه يوجد مدى محدد في س (المسار) يكون فيه طيف الطاقة ثابت مهما تغيرت قيمة (س). لوحظ أيضا أن منحنى الاستقرار ينمو بشكل سريع إلى رقم تكرار مثالي ومن ثم يتناقص مع زيادة عدد التكرار إلى نقطة أو نقاط معينة. و هذه تشكل مساهمتنا الرئيسية في أدبيات البحث و التي تمثل إضافة جديدة لطريقة مُقارب التكرار.

CHAPTER 1

INTRODUCTION AND LITERATURE REVIEW

Almost all known methods of solution of the wave equation in quantum mechanics do very well (to a varying degree of accuracy) in problems with exactly solvable potentials. However, the real test of these methods is when the potential is not exactly solvable. There exist various methods to obtain approximate solutions. For instance, time-independent perturbation theory [1], WKB approximation [2], finite-element method [3, 4], and numerical method [5]. In atomic and molecular physics, numerical solution of the Schrödinger equation frequently employs self-consistent field approximation whereas in nuclear physics the Born-Oppenheimer approximation is used. Moreover, from the early days of quantum mechanics, numerical methods were already developed [6] in order to overcome the limitations of the number of exactly solvable problems. Therefore, in cases where analytical solutions are difficult to find or not possible, numerical methods are necessary [7]. In the past and in recent years, many developments in the numerical solution of the Schrödinger equation have appeared. Some of these methods include Matrix Diagonalization Method, Nikiforov-Uvarov method, Spectral Method, Discrete Variable Method and Runge-Kutta methods [8, 9]. In our work, we will compare the numerical advantages of two methods to obtain the energy eigenvalues: the Asymptotic Iteration Method (AIM) and Tridiagonal Representation Approach (TRA).

The AIM has been developed [10] to solve second order differential equations. For most Schrödinger equations with exactly solvable potentials, the AIM was found to reproduce very well the exact energy spectrum and wave functions [11-14]. Additionally, it gave very good results in the case of non-exactly solvable potentials [15-18]. Moreover, for analytically solvable potentials, the AIM formulation resulted in energy eigenvalues identical to those derived by other analytical means [19]. On the other hand, the TRA [20] has been successfully used to compute the wavefunction and energy eigenvalues for bound states and resonances associated with different short-range potentials. In particular, the approach was used for the Morse potential [21], the inverse Morse potential [22], the tamed Yukawa potential [23], the generalized Yukawa potential [24], the Hulthen potential [25], the Hellmann potential [26] and exponential-cosine-screened Coulomb potential [27]. However, there exist a class of non-conventional potentials with discrete spectra and in our work, we seek the solutions of such non-conventional potentials in the 1D Schrödinger equation. We plan to apply both AIM and TRA to this type of problems.

It is worthwhile to begin this work by a brief introducing of the famous equation in the physics that appears in most of the research work in the past and present. In quantum mechanics, the wave equation, Schrödinger equation (SCH.), is a partial differential equation which describes how a quantum system state (quantum state) changes with time was developed by the Austrian physicist Erwin Schrödinger, this equation was formulated in autumn 1925 and published in 1926 [28]. In quantum mechanics, the analog of Newton's law in classical mechanics, (F = ma), is the Schrödinger equation for a quantum system (molecules, atoms, and subatomic particles whether bound, free, or localized).

The wave function is also called the "state function" it describes the time-evolution of the system [1]. It has two forms; one is a time-dependent SCH in which time explicitly appears describing how the wave function of a particle will evolve in time [29]. The other is the time-independent SCH describing the allowed energies for the particle.

Time-dependent Schrödinger equation is defined by

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \mathrm{H}\Psi(r,t) \tag{1.1}$$

where $\hbar$ is the Planck constant divided by 2π, i is the imaginary unit, Ψ is the wave function of the quantum system, r and t are the position vector and time respectively, and H is the Hamiltonian operator (the total energy of the system).

Time-independent Schrödinger equation is

$$E\Psi = \mathrm{H}\Psi \tag{1.2}$$

In the case of a particle in one dimension, the Hamiltonian is:

$$\mathrm{H} = \frac{P^2}{2m} + V(x) \quad , \quad P = -i\hbar \frac{d}{dx} \tag{1.3}$$

Then, the general Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x), \tag{1.4}$$

In 1D the SCH Eq. is an ordinary differential equation, rather than a partial differential equation. However, the stationary solutions of the SCH Eq. take the form:

$$\psi(x,t) = \psi(x)e^{-iEt/\hbar}, \tag{1.5}$$

In this work, we concentrate on the one-dimensional time-independent linear Schrodinger

equation (in the atomic units $\hbar = m = 1$) that reads

$$\left[\frac{d^2}{dx^2} - 2V(x) + 2E\right]\psi(x) = 0, \tag{1.6}$$

Whereis the potential function (in higher dimensions with $V(x)$ is the energy and E central symmetry, this is an effective potential made up of the sum of the orbital term, which is proportional to x^{-2}, and the physical potential).

Generally, for problems with bound states we would like to obtain solutions of the time-independent wave equation $H|\psi_n\rangle = E_n|\psi_n\rangle$, which represents an eigenvalue problem, where $\{\psi_n\}$ are the eigen-functions, H is the Hamiltonian and $\{E_n\}$ are the corresponding eigen-energies [30]. In the AIM, we start by converting the Schrödinger equation into a standard form suitable for the method [10] and then use the quantization condition to terminate the iterations asymptotically and obtain the energy spectrum and eigenstates. On the other hand, in the TRA one expands the wavefunction in the space spanned by a suitable square integrable discrete basis set. The basis set is chosen to produce a tridiagonal matrix representation [31-34] for the wave operator. We start briefly by introducing both methods and then use them to calculate the energy spectra for some potentials in the two cases in situations where we have exactly and not exactly solvable potentials.

CHAPTER 2

ASYMPTOTIC ITERATION METHOD

2.1 Theoretical formulation

The AIM was established to obtain analytic solutions of second order ordinary differential equations [10] and was applied to a wide range of problems in quantum mechanics. The asymptotic iteration method was designed for solving second-order homogeneous linear differential equation considers the following standard form:

$$y''(x) = k_0(x)y'(x) + S_0(x)y(x) \tag{2.1}$$

Where $k_0(x)$ and $S_0(x)$ are $C_\infty[\Omega]$ functions (infinitely differentiable in a domain Ω of the complex plane) and not necessarily bounded but such that $k_0(x) \neq 0$. In practice, $k_0(x)$ and $S_0(x)$ have sufficiently many continuous derivatives.

In most applications, the functions $k_0(x)$ and $S_0(x)$ are polynomials or rational functions. The general solution of Eq. (2.1) can be obtained using the symmetric structure of the right-hand side of Eq. (2.1). We differentiate Eq. (2.1) and iterate up to $(n+1)^{th}$ and $(n+2)^{th}$ derivatives. Thus, due to the linearity of the right side of (2.1) in $y(x)$ and its first order derivative, we can easily obtain

$$y^{n+1}(x) = k_{n-1}y'(x) + S_{n-1}(x)y(x), \qquad y^{n+2}(x) = k_n y'(x) + S_n(x)y(x) \tag{2.2}$$

where $k_n(x)$ and $S_n(x)$ are defined recursively as follows

$$k_n(x) = k'_{n-1}(x) + S_{n-1}(x) + k_0(x)k_{n-1}(x), \qquad S_n(x) = S'_{n-1}(x) + S_0(x)k_{n-1}(x) \tag{2.3}$$

Once the functions $k_0(x)$ and $S_0(x)$ are determined, the sequences $k_n(x)$ and $S_n(x)$ can be computed using (2.3). However, it should be noted that one can start the iteration from $n=0$ with the initial condition $k_{-1}=1$ and $S_{-1}=0$.

The ratio of $(n+1)^{th}$ and $(n+2)^{th}$ derivatives of $y(x)$ gives

$$\frac{y^{n+2}}{y^{n+1}} = \frac{d}{dx}\ln\left[y^{n+1}(x)\right] = \frac{k_n\left[y' + (S_n/k_n)y\right]}{k_{n-1}\left[y' + (S_{n-1}/k_{n-1})y\right]} \tag{2.4}$$

Therefore, as per the asymptotic iteration technique and for adequately large *n,* we impose the termination condition:

$$\frac{S_n(x)}{k_n(x)} = \frac{S_{n-1}(x)}{k_{n-1}(x)} = \chi(x), \tag{2.5}$$

Asymptotically, the terminating function $\chi(x)$ is independent of *n.* Equation (2.4) reduce to:

$$\frac{d}{dx}\ln\left[y^{n+1}(x)\right] = \frac{k_n(x)}{k_{n-1}(x)} \tag{2.6}$$

Using Eq. (2.3) and substituting in Eq. (2.6) which yields:

$$y^{n+1}(x) = C_1 \exp\left[\int_x \frac{k_n(x)}{k_{n-1}(x)}dx\right] = C_1 k_{n-1}(x)\exp\left[\int_x \left[\alpha(\tilde{x}) + k_0(\tilde{x})\right]d\tilde{x}\right] \tag{2.7}$$

Where C_1 is the integral constant. Substituting Eq. (2.7) into Eq. (2.2) yields the general solution of the 2^{nd} order differential equation Eq. (2.1):

$$y(x) = \exp\left[-\int_x \chi_n\left(x'\right) dx' \right] \left\{ C_2 + C_1 \int_x \exp\left[\int_{x'} \left(k_0(x'') + 2\chi_n(x'') \right) dx'' \right] dx' \right\} \tag{2.8}$$

It should be noticed that although the general solution is given by Eq. (2.8), the first part of Eq. (2.8) is observed to give polynomial solutions which are convergent and physical, while, the second part gives non-physical solutions that are divergent. Therefore, $C_1 = 0$ in Eq. (2.8) and the wave functions are determined by the following

$$y(x) = C_2 \exp\left[-\int_x \chi_n\left(x'\right) dx' \right] = C_2 \exp\left[-\int_x \frac{S_n\left(x'\right)}{k_n\left(x'\right)} dx' \right] \tag{2.9}$$

The Energy spectrum (eigenvalues E_n) of the differential equation Eq. (1.6) such as Schrodinger equation are then obtained from the roots of the termination condition

$$\Delta_n\left(x, E\right) = k_n\left(x, E\right) S_{n-1}\left(x, E\right) - k_{n-1}\left(x, E\right) S_n\left(x, E\right) = 0, \qquad n = 1, 2, 3, ... \tag{2.10}$$

Where n is the number of iterations and this is called the quantization equation. Numerically, the eigenvalues of the n^{th} energy levels are obtained by the requirement that $\Delta_n\left(x, E\right)$ becomes vanishingly small for as large number of iterations as possible to achieve the desired accuracy.

2.2. Asymptotic Iteration Equation

In the application of this method to eigenvalue problems of Schrodinger-type, such as the time-independent one dimensional Schrodinger equation

$$-\frac{\hbar^2}{2m}\psi''(x)+\left[V(x)-E\right]\psi(x)=0$$

it is very clear that the direct application of the AIM is not possible. Thus, this equation (1.6) is not in the standard AIM form (2.1) and hence we need to make a transformation to bring it to (2.1). That is we need to introduce a first order derivative into the Schrodinger equation. Thus, the first step when applying AIM is the conversion of the eigenvalue problem to a standard form suitable to use in AIM.

2.2.1 Wave-Function Transformation

The general strategy is to rewrite the wave-function as $\psi(x)=g(x)f(x)$ together with a possible change of coordinate in order to transform Eq. (1.6) to the form (2.1). Thus, we select $g(x)$ so that the Schrödinger equation will be written as a function of $f(x)$ as follows:

$$f''(x)=k_0(x)f'(x)+S_0(x)f(x) \tag{2.11}$$

Where $k_0(x)=-2\frac{g'}{g}$, $S_0(x)=2V-\frac{g''}{g}-2E$ (2.12)

Where the prime denotes the derivative with respect to x, and equation (2.11) is now in the convenient form of the Asymptotic iteration equation. Usually, $g(x)$ is chosen so as to the factorize singularities in Eq. (2.11) or take care of the boundary condition requirements and/or the asymptotic behavior of the wavefunction.

2.2.2 Coordinate Transformation

Another technique to transform Eq. (1.6) into the AIM equation is to use a coordinate transformation $x \to y(x)$, which changes Eq. (1.6) into

$$\left[y'^2 \frac{d^2}{dy^2} + y'' \frac{d}{dy} - 2V(y) + 2E \right] \psi(y) = 0,$$

This again gives an AIM form that reads

$$\psi''(y) = k_0(y)\psi'(y) + S_0(y)\psi(y)$$

where the prime stands for the derivative with respect to y and

$$k_0(y) = -y''/y'^2 \equiv A_0(y)$$

$$S_0(y) = \frac{2}{y'^2}\left[V(y) - E\right] \equiv \alpha_0(y) + E\beta_0(y)$$

The functions $\alpha_0(y)$, $\beta_0(y)$ and $A_0(y)$ are defined for a given potential function and coordinate transformation.

2.3 Termination Condition Problem

In general, the AIM sequences $k_n(x)$ and $S_n(x)$, $n = 0,1,2,.....$ depends not only on x but also on the (unknown) energy E. Thus, the energy eigenvalue E_n that solves (2.10) depends generally on x. However, for analytically solvable potentials, the termination condition (2.10) gives an expression that depends just on E (independent of x). In such situations, the energy eigenvalues are simply the zeros of $\Delta_n(E) = 0, n = 1,2,.....$. Thus, the condition

$\Delta_n(E)=0$ gives the energy spectrum of the exact solutions. On the other hand for problems that are not exactly solvable the termination condition (2.10) produces for each iteration an expression that depends on both x and E. Nevertheless, physically the eigenvalues should not depend on the space variable. In such case, to find the eigenvalues by solving the termination condition equation we are usually faced with problems related to the convergence and sometimes instability of the numerical computation. Thus extra measures should be taken into consideration to overcome such problems and to improve the convergence.

2.3.1 Asymptotic Behavior of the Wave-Function

One of the methods that can help for stabilizing the process and improve the convergence is to rewrite the wave-function as $\psi(x)=g(x)f(x)$ and $g(x)$ is chosen to reflect the asymptotic form of the wavefunction and/or its behavior near the singularities of the Schrödinger wave operator. Thus, for the eigenvalue problem with $x\in\left[x^-,x^+\right]$ one should study the asymptotic behavior when $x\to x^+$ and $x\to x^-$ to obtain the suitable wave-function that yields the appropriate AIM standard form.

2.3.2 Boundary Condition

Much attention should be paid to the boundary condition of the eigenvalue problem when applying the AIM. In this case, the function $g(x)$ is chosen so as to include the effect of the boundary condition. Thus, the boundary condition is enforced into the wave-function in order to guarantee that the wavefunction vanishes at the endpoints. Thus, for $x\in\left[x^-,x^+\right]$ the wave-function can be rewritten as $\psi(x)=g(x)f(x)$ where

$\psi(x^+) = \psi(x^-) = 0$. This transforms Eq. (1.6) into an equation for $f(x)$ Eq. (2.11) where the characteristics functions $k_0(x)$ and $S_0(x)$ are given by:

$$k_0(x) = -2\frac{g'}{g} \quad , \quad S_0(x) = 2V - \frac{g''}{g} - 2E \, . \tag{2.12}$$

where the prime stands for the derivative with respect to x.

2.3.3 Plateau of Convergence

One of the most important procedures that strongly assist the stabilization of the process and improve the convergence is the appropriate choice of the initial value of the space variable. Traditionally, researchers who use the AIM choose x_0 as either the position of the minimum value of the potential under consideration or as the location of the maximum of the ground state wavefunction. Another option was used is by setting $S_0(x) = 0$. In this work, we present a more general and systematic method to choose a suitable value for x_0 to be within the plateau of stability, defined to be the range of x_0 values where the calculated energy eigenvalue is stable against variations in x_0. For this purpose, we solve the quantization equation Eq. (2.10) for certain value of x and then compute the eigenvalues $E_m^n(x)$ where n refers to the number of iterations and m refers to the order of the energy eigenvalues. This can be done by calculating the eigenvalues ($E_0^n, E_1^n, E_2^n, ...$) with different values of x in the given range, $x \in \left[x^-, x^+\right]$, and then we may plot them versus x to obtain the plateau of convergence for each eigenvalue.

As an example, the ground state energy E_0^n is calculated for different values of x then we

plot this eigenvalue versus x and observe that within a given range of x, called "*the plateau of stability*", the calculated energy eigenvalue does not change with x (within the chosen accuracy of calculation). Therefore, our mechanism that selects a natural or ideal point $x = x_0$ that gives stable and convergent results independent of this point for as large range of values of x_0 as possible. In principle, the solution should not depend on the choice of x_0 which means that the computation of the roots of $\Delta_n\left(x_0; E\right) = 0$ should be free of the choice of x_0. We refer to this range of values of x_0 as the "plateau of convergence" or "plateau of stability".

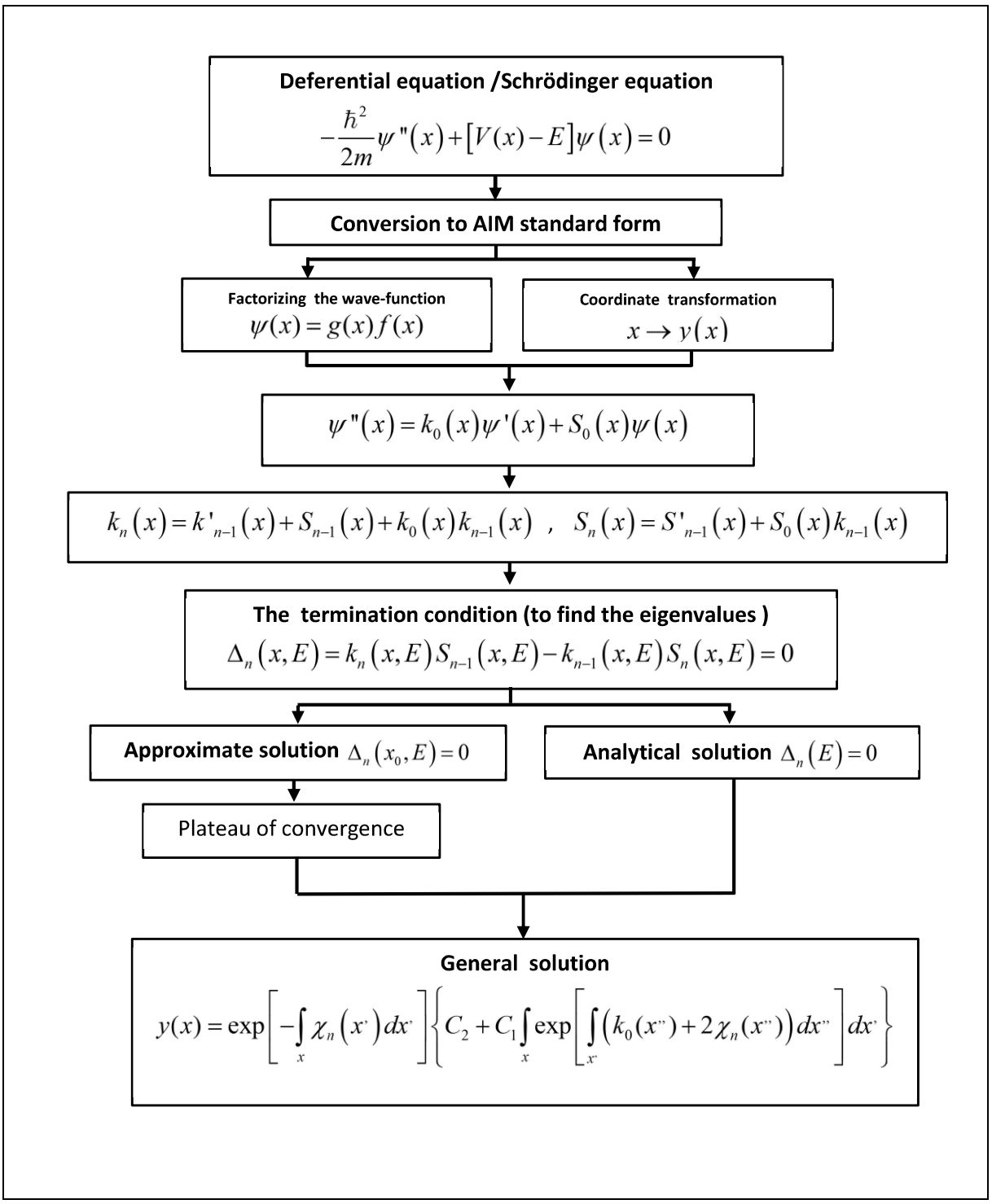

Figure 1 Flow chart for applying AIM

CHAPTER 3

TRIDIAGONAL REPRESENTATION APPROACH

This technique aims at solving the wave equation, $H|\psi\rangle = E|\psi\rangle$, where H is the Hamiltonian and E is the energy eigenvalue. The energy eigenvalue is either discrete (for bound states) or continuous (for scattering states). The eigenvalue equation can be solved algebraically without solving the differential equation. In this approach, the wave-function is written in terms of square-integrable basis set $\{\phi_m(x)\}_{n=0}^{\infty}$. Therefore, we start by expanding the wave function in a complete basis:

$$\psi_E(x) = \sum_m f_m(E)\phi_m(x) \tag{3.1}$$

$\{f_m(E)\}_{m=0}^{\infty}$ are the coefficients of expansion and the basis is chosen such that we get a tridiagonal symmetric matrix for the wave operator $J = H - E$. The following is the general form of the square-integrable basis:

$$\phi_m(x) = A_m w(y) P_m(y) \tag{3.2}$$

where $y = y(x)$, A_m is a normalization constant, $P_m(y)$ is a polynomial of a degree m in y and $w(y)$ is the associated weight function that vanishes on the boundaries of configuration space x. Consequently, the wave operator matrix elements are defined by

$$J_{n,m} = \langle \phi_n | H - E | \phi_m \rangle = \langle \phi_n | \left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x) - E \right] | \phi_m \rangle = 0 \qquad (3.3)$$

The transformation $x \to y(x)$ is chosen such that the space of the basis becomes compatible with the domain of the Hamiltonian x. With this coordinate transformation, the wave operator (3.3) becomes:

$$J_{n,m} = \frac{1}{2}\langle \phi_n | \left\{ -(y')^2 \frac{d^2}{dy^2} - y'' \frac{d}{dy} + 2U(y) \right\} | \phi_m \rangle = 0 \qquad (3.4)$$

where $U(y) = V(x(y)) - E$. The prime on y stands for the derivative with respect to x.

Requiring that this matrix be tridiagonal and symmetric (as shown in the next sections) transforms the wave equation into the following three-term recursion relation for the expansion coefficients of the wave-function:

$$J_{n,n} f_n(E) + J_{n,n-1} f_{n-1}(E) + J_{n,n+1} f_{n+1}(E) = 0 \qquad (3.5)$$

Where all the $J_{n,m}$'s are functions of energy and potential parameters. This equation can be solved either iteratively starting with a chosen $f_0(E)$ or using results from classical orthogonal polynomials, if any. Solving this recursion relation gives the energy spectrum and associated wave-functions.

3.1 Tridiagonal Representation Approach (TRA) to 1D Schrodinger Equation

In our present work we will be using the Jacobi basis where $P_m(y)$ are the Jacobi polynomials with $y \in [-1,+1]$ and the Laguerre basis where $P_m(y)$ are the Laguerre polynomials with $y \in [0,\infty[$.

3.1.1 TRA for the Jacobi Basis

The orthogonality relation of the Jacobi polynomial

$\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)dy = A_n\delta_{mn}$, suggest that we can consider $\phi_n(y) = A_n(1-y)^{\alpha}(1+y)^{\beta}P_n^{(\mu,\nu)}(y)$, as a complete basis set in $[-1,+1]$ and use the free parameters $\{\alpha,\beta,\mu,\nu\}$ to ensure a tridiagonal representation of the Hamiltonian. The Jacobi basis where $y \in [-1,+1]$ and $\{\phi_m(y)\}_{n=0}^{\infty}$ is written in the following form:

$$\phi_m(y) = A_m(1-y)^{\alpha}(1+y)^{\beta}P_m^{(\mu,\nu)}(y) \qquad (3.1.1)$$

where $A_m = \sqrt{\frac{2m+\mu+\nu+1}{2^{\mu+\nu+1}}\frac{\Gamma(m+1)\Gamma(m+\mu+\nu+1)}{\Gamma(m+\nu+1)\Gamma(m+\mu+1)}}$, $P_m^{(\mu,\nu)}(y)$ is the Jacobi polynomial of a degree m in y and the real dimensionless parameters $\{\alpha,\beta,\mu,\nu\}$ are such that $\alpha,\beta \geq 0$ and $\mu,\nu > -1$. These parameters will be chosen later to support the tridiagonal requirement of the wave operator matrix (3.4). The integration measure becomes $\int_{x_-}^{x_+}.....dx = \int_{-1}^{+1}...\frac{dy}{y'}$. Thus, compatibility with the weight functions of the Jacobi polynomial and dimensionality

requires that $y'=\lambda(1-y)^{a}(1+y)^{b}$ with a and b being real parameters and λ is a positive real parameter having a dimension of inverse length. In fact, the tridiagonal requirement of (3.4) also leads to the same form for y'. Using the differential equation of the Jacobi polynomial and its differential property, the wave operator matrix elements are obtained after some manipulation (shown in Appendix B1) as

$$J_{m,n}=A_mA_n\int_{-1}^{1}(1-y)^{2\alpha+a-1}(1+y)^{2\beta+b-1}P_m^{\mu,\nu}(y)\left\{-n(n+\mu+\nu+1)-(2\alpha\beta+\alpha b+\beta a)+\alpha(\alpha+a-1)\frac{(1+y)}{(1-y)}\right.$$
$$\left.+\beta(\beta+b-1)\frac{(1-y)}{(1+y)}-n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)\left(\frac{\mu+1-a-2\alpha}{(1-y)}-\frac{\nu+1-b-2\beta}{(1+y)}\right)-\frac{U(y)(1-y^2)}{(y')^2}\right\}P_n^{\mu,\nu}(y)dy$$
$$+A_mA_n\frac{2(n+\mu)(n+\nu)}{2n+\mu+\nu}\int_{-1}^{1}(1-y)^{2\alpha+a-1}(1+y)^{2\beta+b-1}P_m^{\mu,\nu}(y)\left(\frac{\mu+1-a-2\alpha}{(1-y)}-\frac{\nu+1-b-2\beta}{(1+y)}\right)P_{n-1}^{\mu,\nu}(y)dy=0 \tag{3.1.2}$$

3.1.2 TRA for the Laguerre Basis

In the spirit of the orthogonal property of the Laguerre polynomials $\int_0^{\infty}y^{\nu}e^{-y}L_n^{\nu}(y)L_m^{\nu}(y)dy=\frac{\Gamma(n+\nu+1)}{\Gamma(n+1)}\delta_{nm}$ which state that $\psi_n(y)=A_ne^{-y/2}y^{\nu/2}L_n^{\nu}(y)$, $A_n=\sqrt{n!/\Gamma(n+\nu+1)}$, form an orthonormal basis in $y\in[0,\infty[$. The following are general basis set and form a complete set in $[0,\infty[$. The Laguerre basis is defined as:

$$\phi_n(y)=A_ny^{\alpha}e^{-\beta y}L_n^{\nu}(y), \tag{3.1.3}$$

Where $y\in[0,\infty[$, $A_n=\sqrt{\Gamma(n+1)/\Gamma(n+\nu+1)}$, $L_n^{\nu}(y)$ is the polynomial of Laguerre of a degree n in y and real parameters $\{\alpha,\beta,\nu\}$ with $\nu>-1$ and $\alpha\geq 0$ to ensure convergence

of the Laguerre polynomial and compatibility with the boundary conditions. They will be determined later to support the tridiagonal requirements. In this basis, we use $y' = \lambda y^a e^{by}$ with a being real and positive so that y' vanishes only at the boundaries and no new singularity will be introduced in the differential wave operator. The integration measures are $\int_{x_-}^{x_+} .....dx = \int_0^\infty ... \frac{dy}{y'}$ and y' should be compatible with the weight function of the Laguerre polynomial. Using the differential equation of the Laguerre polynomial and its differential property, the wave operator matrix elements are obtained after some manipulation (shown in Appendix B2) as

$$J_{m,n} = A_m A_n \int_0^\infty y^{2\alpha+a-1} e^{-(2\beta-b)y} L_m^\nu(y) \left[n - b\alpha + a\beta + 2\alpha\beta - \beta(\beta-b)y - \frac{\alpha(\alpha+a-1)}{y} \right.$$
$$\left. - n\left(1 + b - 2\beta + \frac{2\alpha - \nu + a - 1}{y}\right) + U(y)\frac{y^{1-2a}e^{-2by}}{\lambda^2} \right] L_n^\nu(y)\, dy$$
$$+ A_m A_n (n+\nu) \int_0^\infty y^{2\alpha+a-1} e^{-(2\beta-b)y} L_m^\nu(y) \left(1 + b - 2\beta + \frac{2\alpha - \nu + a - 1}{y}\right) L_{n-1}^\nu(y)\, dy \tag{3.1.4}$$

3.2 1D Solvable Potentials using Tridiagonal Representation Approach

3.2.1 1D Solvable Potentials for Jacobi Basis

Generally, we are looking for the tridiagonal representation form of the $J_{m,n}$, thus, generally Eq. (3.1.2) has for the Jacobi polynomials the integral form

$\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)F(y)P_n^{\mu,\nu}(y)dy$. Therefore, the tridiagonal matrix requirement dictates that $F(y)$ be linear in y (e.g. $F(y)=py+q$) that is equivalent to the term

$(1\pm y)$. Thus, $F(y)$ should be selected in order to cancel terms that destroy the tridiagonal representation like $(1+y)/(1-y)$ and $(1-y)/(1+y)$.

Based on the fact that $\int_{-1}^{+1}(1-y)^{2\alpha}(1+y)^{2\beta}P_m^{\mu,\nu}(y)P_n^{\mu,\nu}(y)dy$ will be tridiagonal only for $(2\alpha,2\beta)=(\mu,\nu),(\mu+1,\nu),(\mu,\nu+1)$, which will be proven using three-term recursion relation for $P_n^{\mu,\nu}(y)$. So, the only tridiagonal terms in $J_{m,n}$ should have the following three forms:

$$\int_{-1}^{+1}(1-y)^{2\alpha+a-1}(1+y)^{2\beta+b-1}P_m^{\mu,\nu}(y)P_n^{\mu,\nu}(y)dy\sim\delta_{m,n}$$

$$\rightarrow \quad 2\alpha+a-1=\mu,\ 2\beta+b-1=\nu \tag{3.2.1a}$$

$$\int_{-1}^{+1}(1-y)^{2\alpha+a-1}(1+y)^{2\beta+b-2}P_m^{\mu,\nu}(y)P_{n-1}^{\mu,\nu}(y)dy\sim\delta_{m,n}+\delta_{m,n+1}+\delta_{m,n-1}$$

$$\rightarrow 2\alpha+a-1=\mu,2\beta+b-2=\nu \tag{3.2.1b}$$

$$\int_{-1}^{+1}(1-y)^{2\alpha+a-2}(1+y)^{2\beta+b-1}P_m^{\mu,\nu}(y)P_{n-1}^{\mu,\nu}(y)dy\sim\delta_{m,n}+\delta_{m,n+1}+\delta_{m,n-1}$$

$$\rightarrow 2\alpha+a-2=\mu,\ 2\beta+b-1=\nu \tag{3.2.1c}$$

Now, we can say that according to the recursion relation and orthogonality formula of the Jacobi polynomials that the matrix representation of the wave operator $J_{m,n}$ becomes tridiagonal only in three cases:

$$(1)\quad 2\alpha = \mu + 1 - a,\ 2\beta = \nu + 1 - b, \tag{3.2.2a}$$

$$(2)\quad 2\alpha = \mu + 1 - a,\ 2\beta = \nu + 2 - b, \tag{3.2.2b}$$

$$(3)\quad 2\alpha = \mu + 2 - a,\ 2\beta = \nu + 1 - b, \tag{3.2.2c}$$

For the previous three cases, we can find the tridiagonal matrix representation for the wave operator $J_{m,n}$ and the possible solvable potentials. The wave operator for the first case is given by:

$$\begin{aligned} J_{m,n} = A_m A_n \int_{-1}^{1} (1-y)^{\mu} (1+y)^{\nu} P_m^{\mu,\nu}(y) \Bigg[\left(n + \frac{\mu+\nu+1}{2} \right)^2 - \frac{1}{4}\left(\mu^2 + \nu^2 + 2ab - 1\right) \\ - A\frac{(1+y)}{(1-y)} - B\frac{(1-y)}{(1+y)} + \frac{U(y)(1-y)^{1-2a}(1+y)^{1-2b}}{\lambda^2} \Bigg] P_n^{\mu,\nu}(y)\, dy = 0 \end{aligned} \tag{3.2.3}$$

Since only $\int_{-1}^{+1} (1-y)^{\mu} (1+y)^{\nu} P_m^{\mu,\nu}(y) P_n^{\mu,\nu}(y)\, dy \sim \delta_{m,n}$, $\int_{-1}^{+1} (1-y)^{\mu+1} (1+y)^{\nu} P_m^{\mu,\nu}(y) P_n^{\mu,\nu}(y)\, dy \sim tridiag.$

$\int_{-1}^{+1} (1-y)^{\mu} (1+y)^{\nu+1} P_m^{\mu,\nu}(y) P_n^{\mu,\nu}(y)\, dy \sim tridiag.$ Then, we need to include in $U(y)$ all the possible tridiagonal terms, $py+q$ in addition, to counterterms that eliminate the non-tridiagonal terms in (3.2.3). Therefore, the solvable potential should have the following form:

$$\frac{U(y)(1-y)^{1-2a}(1+y)^{1-2b}}{\lambda^2} = A\frac{1+y}{1-y} + B\frac{1-y}{1+y} + py + q \tag{3.2.4}$$

Where we set $A = \frac{1}{4}\left[\mu^2 - (a-1)^2\right]$, and $B = \frac{1}{4}\left[\nu^2 - (b-1)^2\right]$.

Similarly, for the second case, the wave operator $J_{m,n}$ is written as:

$$J_{m,n} = A_m A_n \int_{-1}^{+1} (1-y)^{\mu}(1+y)^{\nu} P_m^{\mu,\nu}(y)\left[Q + Ky - A\frac{(1+y)^2}{(1-y)} + \frac{U(y)}{\lambda^2}(1-y)^{1-2a}(1+y)^{2-2b}\right]\times$$
$$P_m^{\mu,\nu}(y)dy - A_m A_n \frac{2(n+\mu)(n+\nu)}{2n+\mu+\nu}\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu} P_m^{\mu,\nu}(y)P_{n-1}^{\mu,\nu}(y)dy$$

(3.2.5)

and the solvable potential has the form:

$$\frac{U(y)(1-y)^{1-2a}(1+y)^{1-2b}}{\lambda^2} = A\frac{1+y}{1-y} + p\frac{y}{(1+y)} + \frac{q}{(1+y)} \tag{3.2.6}$$

Where

$$Q = \left(n + \frac{\mu+\nu+1}{2}\right)^2 - \frac{1}{4}\left(\mu^2+\nu^2+2ab-1\right) + \frac{1}{2}(\mu+1) - n\frac{\nu-\mu}{2n+\mu+\nu} - \frac{1}{4}(\nu-b+2)(\nu+b)$$

$$K = \left(n + \frac{\mu+\nu+1}{2}\right)^2 - \frac{1}{4}\left(\mu^2+\nu^2+2ab-1\right) + \frac{1}{2}(\mu+1) - n + \frac{1}{4}(\nu-b+2)(\nu+b)$$

The wave operator $J_{m,n}$ for the third case as follow:

$$J_{m,n}=A_mA_n\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)\left[W-My-B\frac{(1-y)^2}{(1+y)}+\frac{U(y)}{\lambda^2}(1-y)^{2-2a}(1+y)^{1-2b}\right]\times$$
$$P_m^{\mu,\nu}(y)dy+A_mA_n\frac{2(n+\mu)(n+\nu)}{2n+\mu+\nu}\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)P_{n-1}^{\mu,\nu}(y)\Big\}dy=0$$

(3.2.7)

The solvable potential:

$$\frac{U(y)(1-y)^{1-2a}(1+y)^{1-2b}}{\lambda^2}=B\frac{1-y}{1+y}+p\frac{y}{1-y}+\frac{q}{1-y} \tag{3.2.8}$$

Where

$$W=\left(n+\frac{\mu+\nu+1}{2}\right)^2-\frac{1}{4}\left(\mu^2+\nu^2+2ab-1\right)+\frac{1}{2}(\nu+1)-n\frac{\nu-\mu}{2n+\mu+\nu}-\frac{1}{4}(\mu+2-a)(\mu+a)$$

$$M=\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-\frac{1}{4}\left(\mu^2+\nu^2+2ab-1\right)+\frac{1}{2}(\nu+1)+n+\frac{1}{4}(\mu+2-a)(\mu+a)\right]$$

Now, as an application of the above cases, we can produce many solvable potentials using a possible transformation to be compatible with the Jacobi polynomials.

As an example, using the possible transformation:

$$y(\lambda x)=\sin(\lambda x)\ ,\qquad -L/2\le x\le L/2 \tag{3.2.9}$$

Where $y'=\lambda(1-y)^{1/2}(1+y)^{1/2}$, comparing with the general form $y'=\lambda(1-y)^{a}(1+y)^{b}$, the relation between the parameters α,β,μ and ν is given as $2\alpha=\mu+1/2$, $2\beta=\nu+1/2$. The wave operator for this case is written as follows:

$$J_{m,n} = A_m A_n \int_{-1}^{1} (1-y)^{\mu} (1+y)^{\nu} P_m^{\mu,\nu}(y) \left[\left(n + \frac{\mu+\nu+1}{2} \right)^2 - \frac{2A}{(1-y)} - \frac{2B}{(1+y)} + \frac{2V(y)}{\lambda^2} - \frac{2E}{\lambda^2} \right] P_n^{\mu,\nu}(y) dy = 0 \tag{3.2.10}$$

Then, the solvable potential can be found by eliminating terms $(2A/(1-y), 2B/(1+y))$ that are not tridiagonal and adding $py+q$ to have a linear form as the following:

$$\frac{2V(y)}{\lambda^2} = \frac{2A}{(1-y)} + \frac{2B}{(1+y)} + py + q$$

Then $$V(y) = \lambda^2 \frac{(A+B)-(B-A)y}{(1-y^2)} + \frac{\lambda^2 p}{2} y + \frac{\lambda^2}{2} q$$

Thus the solvable potential should have the form:

$$\boxed{V(x) = V_0 + \frac{(V_+ + V_-) - (V_+ - V_-)\sin(\lambda x)}{\cos^2(\lambda x)} + V_1 \sin(\lambda x)} \tag{3.2.11}$$

Where we set $V_- = \lambda^2 A = \frac{\lambda^2}{4}(\mu^2 - 1/4) \rightarrow \mu^2 = \frac{1}{4} + \frac{4V_-}{\lambda^2}$, $V_+ = \lambda^2 B = \frac{\lambda^2}{4}(\nu^2 - 1/4)$ $\rightarrow \nu^2 = \frac{1}{4} + \frac{4V_+}{\lambda^2}$, $p = \frac{2V_1}{\lambda^2}$, and $q = \frac{2V_0}{\lambda^2}$. According to the original requirement that $\alpha, \beta \geq 0$ the potential parameters V_+ and V_- satisfy the condition $V_\pm \geq -(\pi/4L)^2$. Similar procedures can be done for any possible transformation. The following is the table of some possible solvable potential using the TRA for the Jacobi polynomials in 1D Schrodinger equation. More details on this approach can be found in the recent comprehensive review by Alhaidari [35].

$y(x)$	$V(x)$	μ^2	ν^2	2α	2β	Bound	Scattering
$\sin(\lambda x)$ $-L/2 \le x \le L/2$	$V_0 + \dfrac{(V_+ + V_-) - (V_+ - V_-)\sin(\lambda x)}{\cos^2(\lambda x)} + V_1 \sin(\lambda x)$ $V_\pm \ge -(\pi/4L)^2$, $\lambda = \pi/L$	$\dfrac{1}{4} + \dfrac{4V_-}{\lambda^2}$	$\dfrac{1}{4} + \dfrac{4V_+}{\lambda^2}$	$\mu + 1/2$	$\nu + 1/2$	Infinite	No
$2(x/L)^2 - 1$ $0 \le x \le L$	$\dfrac{1/4}{\left(1-(x/L)^2\right)}\left[2V_0 + \dfrac{V_+}{(x/L)^2} + \dfrac{V_-}{\left(1-(x/L)^2\right)}\right] - V_1 \dfrac{(x/L)^2 - 1/2}{(x/L)^2 - 1}$ $V_+ \ge -1/2L^2$, $V_- \ge -2/L^2$, $\lambda = 2\sqrt{2}/L$	$1 + \dfrac{4V_-}{\lambda^2}$	$\dfrac{1}{4} + \dfrac{4V_+}{\lambda^2}$	$\mu + 1$	$\nu + 1/2$	Infinite	No
$2\tanh^2(\lambda x) - 1$ $x \ge 0$	$\dfrac{V_+}{\sinh^2(\lambda x)} + 2\dfrac{V_0 + V_1(2\tanh^2(\lambda x) - 1)}{\cosh^2(\lambda x)}$ $V_+ \ge -\lambda^2/8$, $E \le 0$	$-\dfrac{2E}{\lambda^2}$	$\dfrac{1}{4} + \dfrac{2V_+}{\lambda^2}$	μ	$\nu + 1/2$	Finite	Yes
$\tanh(\lambda x)$ $-\infty > x > \infty$	$\dfrac{V_0 + V_1 \tanh(\lambda x)}{\cosh^2(\lambda x)}$ $E \le 0$	$-\dfrac{2E}{\lambda^2}$	$-\dfrac{2E}{\lambda^2}$	μ	ν	Finite	Yes

$y(x)$	$V(x)$	μ^2	ν^2	2α	2β	Bound	Scattering
$1-2e^{-\lambda x}$ $x \geq 0$	$\frac{1}{\left(e^{\lambda x}-1\right)}\left[V_0+\frac{V_+/2}{\left(e^{\lambda x}-1\right)}+V_1\left(1-2e^{-\lambda x}\right)\right]$ $V_+ \geq -(\lambda/2)^2,\ E \leq 0$	$-\frac{8E}{\lambda^2}$	$1+\frac{4V_+}{\lambda^2}$	μ	$\nu+1$	Finite	Yes
$2\sin^2(\lambda x)-1$ $0 \leq x \leq L$	$4V_0+\frac{2V_+}{\sin^2(\lambda x)}+\frac{2V_-}{\cos^2(\lambda x)}+4V_1\left(2\sin^2(\lambda x)-1\right)$ $V_\pm \geq -(\pi/8L)^2,\ \lambda=\pi/2L$	$\frac{1}{4}+\frac{4V_-}{\lambda^2}$	$\frac{1}{4}+\frac{4V_+}{\lambda^2}$	$\mu+1/2$	$\nu+1/2$	Infinite	No
$2\cos^2(\lambda x)-1$ $0 \leq x \leq L$	$4V_0+\frac{2V_+}{\cos^2(\lambda x)}+\frac{2V_-}{\sin^2(\lambda x)}+4V_1\left(2\cos^2(\lambda x)-1\right)$ $V_\pm \geq -(\pi/8L)^2,\ \lambda=\pi/2L$	$\frac{1}{4}+\frac{4V_-}{\lambda^2}$	$\frac{1}{4}+\frac{4V_+}{\lambda^2}$	$\mu+1/2$	$\nu+1/2$	Infinite	No

Table 1 Solvable potentials using TRA for the Jacobi basis

3.2.2 1D solvable potentials for Laguerre basis

Similarly, we are looking for the tridiagonal representation form of the $J_{m,n}$, thus, generally Eq. (3.1.4) has for the Laguerre polynomials the integral form $\int_0^\infty y^\nu e^{-y} L_m^\nu(y) F(y) L_n^\nu(y)\, dy$. Therefore, the tridiagonal matrix requirement dictates that $F(y) = py + q$. Thus, $F(y)$ should be selected in order to cancel terms that destroy the tridiagonal representation like $1/y$ and y^2. Again orthogonality of the Laguerre polynomials $\int_0^\infty y^\nu e^{-y} L_m^\nu(y) L_n^\nu(y)\, dy = A_n \delta_{nm}$, $A_n = \Gamma(n+\nu+1)/\Gamma(n+1)$ along with the three-term recursion relation for $L_n^\nu(y)$ suggest that $\int_0^\infty y^\alpha e^{-\beta y} L_m^\nu(y) L_n^\nu(y)\, dy$, will be tridiagonal only for $\beta = 1$ and $\alpha = \nu, \nu+1$. So, the only tridiagonal terms in $J_{m,n}$ should have of the following two forms:

$$\int_0^\infty y^{2\alpha+a-1} e^{-(2\beta-b)y} L_m^\nu(y) L_n^\nu(y)\, dy \sim \delta_{m,n} \quad \rightarrow \quad 2\alpha + a - 1 = \nu,\ 2\beta = 1 + b \qquad (3.2.12a)$$

$$\int_0^\infty y^{2\alpha+a} e^{-(2\beta-b)y} L_m^\nu(y) L_{n-1}^\nu(y)\, dy \sim \delta_{m,n} + \delta_{m,n+1} + \delta_{m,n-1}$$

$$\rightarrow 2\alpha + a - 2 = \nu,\ 2\beta = b + 1 \qquad (3.2.12b)$$

Now, we can say that according to the recursion relation and orthogonality formula of the Laguerre polynomials that the matrix representation of the wave operator $J_{m,n}$ becomes tridiagonal only in two cases:

(1) $2\alpha = \nu - a + 1,\ 2\beta = b + 1$ (3.2.13a)

(2) $2\alpha = \nu - a + 2,\ 2\beta = b + 1$ (3.2.13b)

Similarly, we can find the tridiagonal matrix representation for the wave operator $J_{m,n}$ and the possible solvable potentials. The wave operator and solvable potential for the first case are written as the following:

$$J_{m,n} = A_m A_n \int_0^\infty y^\nu e^{-y} L_m^\nu(y) L_n^\nu(y) \left[n + \frac{1}{2}(\nu + 1 + ab) + \frac{1}{4}(1 - b^2) y + \frac{1}{4}\left[\nu^2 - (a-1)^2 \right] \frac{1}{y} - U(y) \frac{y^{1-2a} e^{-2by}}{\lambda^2} \right] dy \quad (3.2.14)$$

$$U(y) \frac{y^{1-2a} e^{-2by}}{\lambda^2} = A \frac{1}{y} + py + q \qquad , \ A = \frac{1}{4}\left[\nu^2 - (a-1)^2 \right] \quad (3.2.15)$$

For the second case:

$$J_{m,n} = A_m A_n \int_0^\infty y^\nu e^{-y} L_m^\nu(y) \left[-\frac{1}{4}(\nu - a + 2)(\nu + a) - n + \left(n + \frac{1}{2}(\nu + 2 + ab) \right) y - \frac{1}{4}(1 - b^2) y^2 + U(y) \frac{y^{2-2a} e^{-2by}}{\lambda^2} \right] L_n^\nu(y) dy + A_m A_n (n + \nu) \int_0^\infty y^\nu e^{-y} L_m^\nu(y) L_{n-1}^\nu(y) dy = 0 \quad (3.2.16)$$

$$U(y) \frac{y^{2-2a} e^{-2by}}{\lambda^2} = By^2 + py + q \qquad , \ B = \frac{1}{4}(1 - b^2) \quad (3.2.17)$$

And similarly, we can find the possible solvable potential using the TRA for Laguerre polynomials. The following is a table of some possible transformations to obtain the solvable potentials.

$y(x)$	$V(x)$	ν^2	2α	2β
$(\lambda x)^{\sigma}$ $-\infty \le x \le \infty$	$\frac{\sigma^2}{(\lambda x)^2}\left[\frac{V_+}{2}+(\lambda x)^{\sigma}\left(V_0+V_1(\lambda x)^{\sigma}\right)\right]$ $V_+ \ge -(\lambda/2\sigma)^2$	$\frac{1}{\sigma^2}+\frac{4V_+}{\lambda^2}$	$\nu+\frac{1}{\sigma}$	1
$\mu e^{-\lambda x}$ $-\infty \le x \le \infty$	$\mu e^{-\lambda x}\left(V_0+V_1\mu e^{-\lambda x}\right)$ $E \le 0$	$-\frac{8E}{\lambda^2}$	ν	1

Table 2 Solvable potentials in the Laguerre basis.

CHAPTER 4

RESULTS AND DISCUSSION

In this work, our main concern is to solve 1D Schrödinger equation with potentials that are analytically and approximately solvable using both the Asymptotic Iteration Method and Tridiagonal Representation Approach. The objective being to make a comparative study between the two approaches. In the following, we present a solution of 1D SCH for two exactly solvable potentials. These potentials are (i) the simple Harmonic oscillator potential

$$V(x)=\frac{x^2}{2}, \tag{4.1}$$

, where $0\le x\le\infty$ and (ii) the confining potential

$$V(x)=V_0\tan^2(x/a)\ , \tag{4.2}$$

where $x\in\left(-\frac{\pi a}{2},\frac{\pi a}{2}\right)$ and $V_0\ge 0$. Furthermore, we solved ID SCH with (iii) the generalized version of the trigonometric Scarf potential that is introduced using the Tridiagonal Representation Approach. The potential is defined by

$$V(x)=\begin{cases} V_0+\dfrac{V_+-V_-\sin(\pi x/L)}{\cos^2(\pi x/L)}+V_1\sin(\pi x/L), & -\dfrac{L}{2}\le x\le\dfrac{L}{2}\ , \\ \infty\ , & \text{outside} \end{cases} \tag{4.3}$$

where $\lambda=(\pi/L)$. Without the V_1 term, this is just the trigonometric Scarf potential, which

belongs to the conventional class of exactly solvable problems with the following energy spectrum

$$E_n = \frac{\lambda^2}{2}\left[n + \frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{4} + \frac{2W_+}{\lambda^2}} + \frac{1}{2}\sqrt{\frac{1}{4} + \frac{2W_-}{\lambda^2}} \right]^2 + V_0 , \tag{4.4}$$

where $W_\pm = V_+ \pm V_-$. The special case where $V_0 = V_\pm = 0$, which leaves only the new component, is just the infinite square well with a sinusoidal bottom that does not have an exact solution in the conventional formulation of quantum mechanics. However, using the TRA, the Authors in [36] were able to obtain an exact solution for this problem. In addition, for convenience and better understanding we apply the technique of the 'the plateau of convergence' to different potentials. In the following sections, we will compute the energy spectrum (energy eigenvalues E_m^n) associated with the three potentials defined above Eq.'s (4.1,4.2,4.3) using both the AIM and the TRA. to enable us to make a reasonable comparison of both approaches.

4.1 Solving Schrodinger equation for Harmonic oscillator potential

4.1.1 Solution using AIM

Consider the simple example, the Harmonic oscillator potential:

$$V(x)=\frac{x^2}{2}, \qquad 0\le x\le\infty \tag{4.1.1}$$

The time-independent linear Schrodinger equation (in the atomic units ($\hbar=m=1$) reads

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}-E\right]\psi(x)=0, \tag{4.1.2}$$

According to the AIM solution procedures, the first step is to convert SCH Equation into the AIM form. Thus, to obtain the AIM form we rewrite the wave function as $\psi(x)=g(x)f(x)$. The wave function that satisfy the asymptotic behavior for large x of the Schrödinger wave operator can be written as:

$$\psi(x)=g(x)f(x)=e^{-\frac{x^2}{2}}f(x) \tag{4.1.3}$$

This transforms Eq. (4.1.2) into an equation for $f(x)$ as

$$f''(x)=2xf'(x)+(1-2E)f(x)\ , \tag{4.1.4}$$

Now, this equation is in the form of the AIM (2.4), thus, the characteristics functions $k_0(x)$ and $S_0(x)$ defined as:

$$k_0(x)=2x \quad , \qquad S_0(x)=1-2E\ . \tag{4.1.5}$$

Using the iteration formulas (2.3), the functions $k_n(x)$ and $S_n(x)$, $n=1,2,...$ will be calculated as it is shown below

$$k_1(x)=k_0'(x)+S_0(x)+k_0(x)k_0(x)=3+4x^2-2E$$

$$S_1(x) = S_0'(x) + S_0(x)k_0(x) = 2x - 4xE$$

$$k_2(x) = k_1'(x) + S_1(x) + k_1(x)k_0(x) = \left(16x + 8x^3\right) - 8xE$$

$$S_2(x) = S_1'(x) + S_0(x)k_1(x) = \left(5 + 4x^2\right) - \left(12 + 8x^2\right)E + 4E^2 .$$

$$k_3(x) = k_2'(x) + S_2(x) + k_2(x)k_0(x) = \left(21 + 60x^2 + 16x^4\right) - \left(20 + 24x^2\right)E + 4E^2$$

$$S_3(x) = S_2'(x) + S_0(x)k_2(x) = \left(24x + 8x^3\right) - \left(56x + 16x^3\right)E + 16xE^2$$

and so on …

The Energy spectrum (eigenvalues E_n) of the Schrodinger equation Eq. (4.1.2) will be found from the root quantized equation (2.10)

$$\Delta_n(x,E) = k_n(x,E)S_{n-1}(x,E) - k_{n-1}(x,E)S_n(x,E) = 0$$

As mentioned before, one can start the iteration from $n = 0$ with the initial condition $k_{-1} = 1$ and $S_{-1} = 0$.

For $n = 0$, $\Delta_0(E) = 2E - 1 = 0$, $\Rightarrow E_0 = 1/2$

For $n = 1$, $\Delta_1(E) = 3 - 8E + 4E^2 = 0$, $(2E-1)(2E-3) = 0$ $\Rightarrow E_0 = 1/2$, $E_1 = 3/2$

For $n = 2$, $\Delta_2(E) = 15 - 46E + 36E^2 - 8E^3 = 0$,

$(2E-1)(2E-3)(2E-5) = 0$ $\Rightarrow$ $E_0 = 1/2$, $E_1 = 3/2$, $E_2 = 5/2$

For $n = 3$, $\Delta_3(E) = 105 - 352E + 344E^2 - 128E^3 + 16E^4 = 0$,

$(2E-1)(2E-3)(2E-5)(2E-7) = 0$ $\Rightarrow E_0 = 1/2$, $E_1 = 3/2$, $E_2 = 5/2$, $E_3 = 7/2$

and so on …

The previous calculations yield the exact eigenvalues $E_n = n + 1/2$. From the above calculation, it is clear that we are dealing with an eigenvalue problem that is analytically solvable (a closed form of a solution). The termination condition (2.10) leads to an expression that is independent of x and depends only on the eigenvalues E. Therefore, we found out that the energy eigenvalues are simply the roots of $\Delta_n(E_n) = 0$. This leads to the exact solutions of the Schrodinger equation for the harmonic oscillator potential [$E_n = n + 1/2, n = 0,1,2,.....]$. Another interesting point is that by induction we conclude that $S_{2n}(x)$ and $S_{2n+1}(x)$ are polynomials in E of degree $n+1$. Whereas, $k_{2n}(x)$ and $k_{2n-1}(x)$ are polynomials of degree n in E. Thus, from the quantization equation (2.10) we conclude that $\Delta_n(x,E)$ is a polynomial in E of degree $n+1$, and $\Delta_n(E) = 0$ gives the energy spectrum $\{E_m\}_{m=0}^{m=n}$. In addition, we would like to show how to find the wave functions of the Schrodinger equation for this case, using Eq.(2.9) we deduce the wavefunctions for the first five iterations with $C_2 = 1$.

For $n = 0$ $\chi_0(x) = \dfrac{S_0(x)}{k_0(x)} = \dfrac{1-2E_0}{2x}$, $f_0(x) = \exp[0] = 1$

$\psi_0(x) = e^{-x^2/2} f_0(x) = e^{-x^2/2}$

For $n = 1$, $\chi_1(x) = \dfrac{S_1(x)}{k_1(x)} = \dfrac{2x - 4xE_1}{3 + 4x^2 - 2E_1}$, $f_1(x) = \exp\left[\int_x \dfrac{1}{x} dx\right] = x$

$\psi_1(x) = e^{-x^2/2} f_1(x) = xe^{-x^2/2}$

For $n = 2$, $\chi_2(x) = \dfrac{S_2(x)}{k_2(x)} = \dfrac{\left(5 + 4x^2\right) - \left(12 + 8x^2\right)E_2 + 4{E_2}^2}{\left(16x + 8x^3\right) - 8xE_2}$,

$$f_2(x)=\exp\left[\int_x \frac{4x}{2x^2-1}dx\right]=2x^2-1 \quad , \qquad \psi_2(x)=e^{-x^2/2}f_2(x)=\left(2x^2-1\right)e^{-x^2/2}$$

For $n=3$, $\chi_3(x)=\dfrac{S_3(x)}{k_3(x)}=\dfrac{\left(24x+8x^3\right)-\left(56x+16x^3\right)E_3+16xE_3{}^2}{\left(21+60x^2+16x^4\right)-\left(20+24x^2\right)E_3+4E_3{}^2}$,

$$f_3(x)=\exp\left[\int_x \frac{6x^2-3}{2x^3-3x}dx\right]=2x^3-3x \quad , \quad \psi_3(x)=e^{-x^2/2}f_3(x)=\left(2x^3-3x\right)e^{-x^2/2}$$

and so on …

The functions $f_n(x), n=0,1,2,...$ represent the Hermite polynomials. The wavefunctions of the Schrodinger equation can be represented by the special Hermite function in confluent hypergeometric functions form as the following:

$$\psi_n(x)=(-1)^n\frac{(2n)!}{n!}e^{-\frac{x^2}{2}}M\left(-n;1/2;x^2\right), \qquad \text{for} \qquad n=0,2,4,... \tag{4.1.6}$$

$$\psi_n(x)=(-1)^n\frac{2(2n+1)!}{n!}xe^{-\frac{x^2}{2}}M\left(-n;3/2;x^2\right), \quad \text{for} \qquad n=1,3,5,...$$

4.1.2 Solution using TRA

The transformation of this problem is defined by $y=x^2$. In this case, the variable space is in $[0,\infty[$, thus, we use the Laguerre basis. Using equation (3.2.14), where $[\,y'=2y^{1/2}\rightarrow a=1/2, b=0,\ 2\alpha=\nu+1/2\,]$. The J-Matrix for this case will be as the following (see [37])

$$J_{n,m}=\left[2n\pm\frac{1}{2}+1-E\right]\delta_{n,m} \tag{4.1.7}$$

Then, the three-term recursion relation will reduce to a single term:

$$E_n f_n(E) = \left[2n \pm \frac{1}{2} + 1 \right] f_n(E) \tag{4.1.8}$$

This represents the diagonal term of the three-term recursion relation. The energy spectrum E_n (the eigenvalues) of the Schrodinger equation with the harmonic oscillator potential is given by

$$E_n = \begin{cases} 2n + \frac{1}{2}, & \nu = -\frac{1}{2} \\ 2n + \frac{3}{2}, & \nu = +\frac{1}{2} \end{cases} \tag{4.1.9}$$

Table 3 The first five exact eigenvalues (Energy spectrum) for harmonic oscillator potential.

Methods	E_0	E_1	E_2	E_3	E_4
Exact $(n+1/2)$	$1/2$	$3/2$	$5/2$	$7/2$	$9/2$
AIM	$1/2$	$3/2$	$5/2$	$7/2$	$9/2$
TRA($\nu = \pm 1/2$)	$1/2$	$3/2$	$5/2$	$7/2$	$9/2$

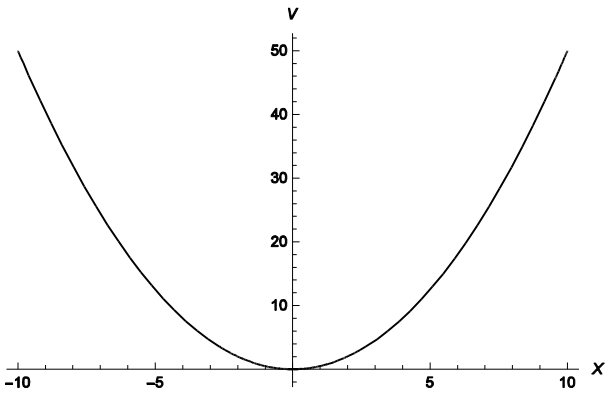

Figure 2 Plot of the harmonic oscillator potential.

4.2 Solving Schrodinger equation for the tangent square potential

The potential is defined as

$$V(x)=\begin{cases} V_0 \tan^2(x/a) & -\frac{\pi a}{2} \le x \le \frac{\pi a}{2} \\ \infty & \text{outside} \end{cases}, \qquad (4.2.1)$$

where $x \in \left(-\frac{\pi a}{2}, \frac{\pi a}{2}\right)$ and $V_0 \ge 0$. This potential contained within an infinite square well with sides at $x = \pm\frac{\pi a}{2}$, and V_0, gives an indication of how rapidly the potential increases within the well [38]. In this case, the time-independent Schrödinger equation reads

$$\left[-\frac{d^2}{dx^2} + 2V_0 \tan^2(x/a) - 2E\right]\psi(x) = 0 \qquad (4.2.2)$$

The boundary conditions are given by $\psi\left(-\frac{\pi a}{2}\right) = \psi\left(\frac{\pi a}{2}\right) = 0$.

4.2.1 Solution using AIM

To obtain the AIM standard form we take a different approach to reach the suitable form of AIM. we start by using the following transformation

$$y = \sin(x/a) \qquad (4.2.3)$$

where $y \in [-1, +1]$. Thus, Sch. Eq. reads

$$\psi''(y) = \frac{y}{\left(1-y^2\right)}\psi'(y) + \left[\frac{2a^2V_0y^2}{\left(1-y^2\right)^2} - \frac{2a^2E}{\left(1-y^2\right)}\right]\psi(y) \tag{4.2.4}$$

For convergence purposes, we use the substitution defined below which also takes into consideration the boundary conditions:

$$\psi\left(y\right) = \left(1-y^2\right)^{\alpha} g\left(y\right) \tag{4.2.5}$$

Then, Sch. Eq. can be written in a simple form for $g\left(y\right)$ as:

$$g''\left(y\right) = \frac{\left(4\alpha+1\right)y}{\left(1-y^2\right)}g'\left(y\right) + \frac{4\alpha^2 - 2a^2E - 2a^2V_0}{\left(1-y^2\right)}g(y) \tag{4.2.6}$$

Where $\alpha = \frac{1}{4}\left(1 \pm \sqrt{1+8a^2V_0}\right)$. Now, Equation (4.2.6) is a differential equation of an exactly solvable problem solved via AIM.

The Characteristics functions $k_0\left(y\right)$ and $S_0\left(y\right)$ are defined by the following:

$$k_0\left(y\right) = \frac{\left(4\alpha+1\right)y}{\left(1-y^2\right)} \quad , \qquad S_0\left(y\right) = \frac{4\alpha^2 - 2a^2E - 2a^2V_0}{\left(1-y^2\right)} \tag{4.2.7}$$

Similarly, like what we did for the previous problem, the iteration formula $k_n\left(y\right)$ and $S_n\left(y\right)$ will be computed using (2.3)

$$k_1\left(y\right) = \frac{\left(1+2\alpha\right)^2 + 2\left(1+6\alpha+6\alpha^2\right)y^2 + 2a^2\left(1-y^2\right)\left(V_0+E\right)}{\left(1-y^2\right)^2}$$

$$S_1(y)=\frac{2(3+4\alpha)\left(2\alpha^2-a^2(V_0+E)\right)y}{\left(1-y^2\right)^2}$$

$$k_2(y)=\frac{(3+4\alpha)\left[3+12\alpha+8\alpha^2+2y^2\left(1+6\alpha+4\alpha^2\right)+4a^2\left(1-y^2\right)(V_0+E)\right]y}{\left(1-y^2\right)^3}$$

$$S_2(y)=\frac{2\left(2\alpha^2-a^2(V_0+E)\right)\left[4(1+\alpha)^2+y^2(11+24\alpha+12\alpha^2)+2a^2\left(1-y^2\right)(V_0+E)\right]}{\left(1-y^2\right)^3}$$

And so on. Then, the termination condition (2.10)

$\Delta_n(y,E)=k_n(y,E)S_{n-1}(y,E)-k_{n-1}(y,E)S_n(y,E)=0$, yields the following results

$$\Delta_0=4\alpha^2-2a^2V_0-2a^2E=0 \quad\Rightarrow\quad E_0=\frac{1}{2a^2}\left[4\alpha^2-2a^2V_0\right]$$

$$\begin{aligned}\Delta_1&=2\alpha^2(1+2\alpha)^2-a^2\left(1+4\alpha+8\alpha^2\right)(V_0+E)+2a^4(V_0+E)^2\\&=\left(1-2a^2V_0+4\alpha+4\alpha^2-2a^2E\right)\left(4\alpha^2-2a^2V_0-2a^2E\right)=0\end{aligned}$$

$$\Rightarrow\quad E_0=\frac{1}{2a^2}\left[4\alpha^2-2a^2V_0\right],\qquad E_1=\frac{1}{2a^2}\left[4\alpha^2+4\alpha+1-2a^2V_0\right]$$

$$\begin{aligned}\Delta_2&=4\alpha^2\left(1+3\alpha+2\alpha^2\right)^2-2a^2\left(1+6\alpha+18\alpha^2+24\alpha^3+12\alpha^4\right)(V_0+E)\\&\quad+a^4\left(5+12\alpha+12\alpha^2\right)(V_0+E)^2-2a^6(V_0+E)^3\\&=\left(1-2a^2V_0+4\alpha+4\alpha^2-2a^2E\right)\left(4\alpha^2-2a^2V_0-2a^2E\right)\left(4-2a^2V_0+8\alpha+4\alpha^2-2a^2E\right)=0\end{aligned}$$

$$\Rightarrow\quad E_0=\frac{1}{2a^2}\left[4\alpha^2-2a^2V_0\right],\ E_1=\frac{1}{2a^2}\left[4\alpha^2+4\alpha+1-2a^2V_0\right],$$

$$E_2=\frac{1}{2a^2}\left[4\alpha^2+8\alpha+4-2a^2V_0\right]$$

And so on. It is obvious that the termination condition yields expression that is independent of the variable space y. In such case, the solution can be written in a closed form for the eigenvalues (Analytical solution). Thus, generalizing the results from the termination condition, we can write

$$\Delta_n = 0 \;\Rightarrow\; E_2 = \frac{1}{2a^2}\left[4\alpha^2 + 4n\alpha + n^2 - 2a^2V_0\right],$$

where $4\alpha^2 = 2\alpha + 2a^2V_0$, Therefore, the energy eigenvalues are given by

$$2a^2E_n = \left[n^2 + 2\alpha(2n+1)\right],$$

$$E_n = \frac{1}{2a^2}\left[n^2 + (2n+1)\left(\sqrt{2a^2V_0 + \frac{1}{4}} + \frac{1}{2}\right)\right], \qquad n = 0,1,2,... \tag{4.2.8}$$

4.2.2 Solution using TRA

Starting from the J-Matrix wave operator of the Schrodinger equation with the Jacobi polynomials Eq. (3.2.3), we use the transformation $y = \sin(x/a)$ where $y \in [-1,+1]$, $y' = \frac{1}{a}\cos(x/a) = \frac{1}{a}(1-y)^{1/2}(1+y)^{1/2}$, and compare with the general case $y' = \lambda(1-y)^a(1+y)^b$, [$a = b = 1/2, \lambda = 1/a$]. The potential function is given as $U(y) = 2V(y) - 2E = 2V_0\frac{y^2}{(1-y^2)} - 2E = 2V_0\frac{1}{(1-y^2)} - 2V_0 - 2E$. The wave operator matrix elements for this problem reads

$$J_{m,n}=A_mA_n\int_{-1}^{1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-2\frac{\left(A+B-V_0a^2\right)+\left(A-B\right)y}{\left(1-y^2\right)}\right.$$

$$\left.-2V_0a^2-2a^2E\right]P_n^{\mu,\nu}(y)dy=0 \qquad (4.2.10)$$

Where $A=\frac{1}{4}\left[\mu^2-1/4\right]$, $B=\frac{1}{4}\left[\nu^2-1/4\right]$

According to the tridiagonal representation requirement, terms inside the square bracket must be linear in y. Moreover, terms that destroy the tridiagonal representation must be eliminated. Therefore, tridiagonal representation requirement yields the following relation between the parameters $\mu^2=\nu^2=\frac{1}{4}+2a^2V_0$, and regarding the original requirement, $\alpha,\beta\geq 0$, the strength of the potential should have the condition $V_0\geq-\frac{1}{2}\left(\frac{1}{2a}\right)^2$. Then, the $J_{m,n}$ matrix elements are

$$J_{m,n}=A_mA_n\int_{-1}^{1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-2V_0a^2-2a^2E_n\right]P_n^{\mu,\nu}(y)dy=0 \qquad (4.2.11)$$

And the three-term recursion relation of the wave operator gives the diagonal term as bellow:

$$E_nf_n(E)=\frac{1}{2a^2}\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-2a^2V_0\right]f_n(E) \qquad (4.2.12)$$

The energy spectrum for Schrodinger equation (4.2.2) given as:

$$E_n = \frac{1}{2a^2}\left[\left(n + \frac{\sqrt{1+8a^2V_0}+1}{2}\right)^2 - 2a^2V_0\right]$$

$$E_n = \frac{1}{2a^2}\left[n^2 + (2n+1)\left(\sqrt{2a^2V_0 + \frac{1}{4}} + \frac{1}{2}\right)\right] \tag{4.2.13}$$

ε_n	AIM	TRA	Exact
ε_0	1	1	1
ε_1	3.5	3.5	3.5
ε_2	7	7	7
ε_3	11.5	11.5	11.5
ε_4	17	17	17

Table 4 The lowest five Eigen-energies of the SCH for the tangent square potential with the potential parameters defined as $V_0 = 1$ and $a = 1$, using AIM and TRA.

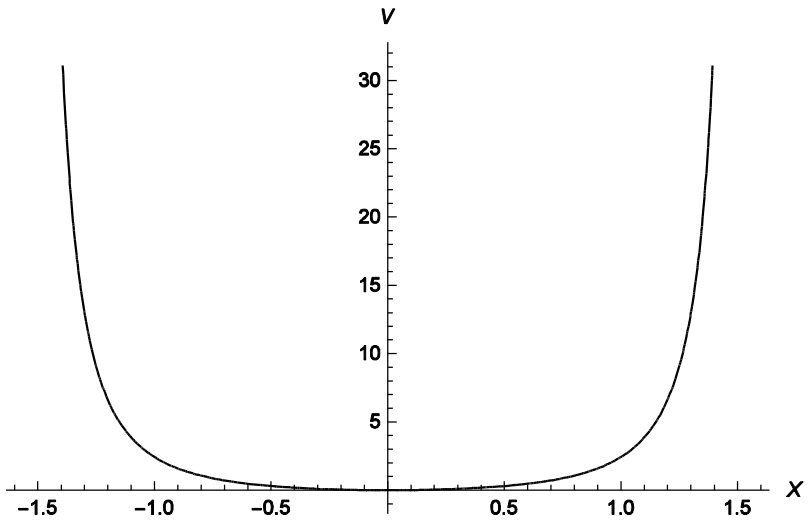

Figure 3 Plot of the tangent square potential for potential parameters $V_0 = a = 1$.

4.3 Solving Schrodinger equation for the Generalized Scarf Potential

4.3.1 Solution using TRA

Starting with the Tridiagonal Representation Approach, we consider the coordinate transformation $y=\sin(\lambda x)$ where $-L/2\le x\le +L/2$, $\lambda=\pi/L$ making $a=b=\frac{1}{2}$ and $y\in[-1,+1]$, we start by using equations (3.2.3) and (3.2.4), where we just consider the first case of (3.2.2). The tridiagonal matrix elements of the wave operator $J_{m,n}$ for this problem read as follows:

$$J_{m,n}=A_mA_n\int_{-1}^{1}(1-y)^{\mu}(1+y)^{\nu}P_m^{\mu,\nu}(y)\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-\frac{1}{4}\left(\mu^2+\nu^2-1/2\right)\right.$$

$$\left.-A\frac{(1+y)}{(1-y)}-B\frac{(1-y)}{(1+y)}+\frac{U(y)}{\lambda^2}\right]P_n^{\mu,\nu}(y)dy=0 \qquad (4.3.1)$$

Where we set $A=\frac{1}{4}\left[\mu^2-(a-1)^2\right]$, and $B=\frac{1}{4}\left[\nu^2-(b-1)^2\right]$. *A, B, p*, and *q* are real parameters with $A=\alpha(\alpha-1/2)$, $B=\beta(\beta-1/2)$. It results in the potential function defined bellow:

$$V(x)=V_0+\frac{V_+-V_-\sin(\lambda x)}{\cos^2(\lambda x)}+V_1\sin(\lambda x) \qquad (4.3.2)$$

where the basis parameters are obtained from the physical parameters $V_{\pm}$, V_0 and V_1 as $\mu^2=\frac{1}{4}+\frac{2}{\lambda^2}(V_+-V_-)$, $\nu^2=\frac{1}{4}+\frac{2}{\lambda^2}(V_++V_-)$, $p=2V_1/\lambda^2$ and $q=\frac{V_+}{\lambda^2}+\frac{2V_0}{\lambda^2}-\frac{2E}{\lambda^2}$. Thus, reality requires that $V_+\ge -2(\lambda/4)^2$ and $V_-\ge 0$. Figure 7, show this potential for a given

set of physical parameters. Using the orthogonality formula and the recursion relation of the Jacobi polynomials we obtain the matrix elements of the wave operator $J_{m,n}$ as follows:

$$J_{n,m}=\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2+\frac{2V_0}{\lambda^2}-\varepsilon\right]\delta_{n,m}+\frac{2V_1}{\lambda^2}\langle n|y|m\rangle \tag{4.3.3}$$

where $\varepsilon=2E/\lambda^2$. Using the form of $\langle n|y|m\rangle$ given in the Appendix, the wave operator matrix elements takes the following form:

$$J_{n,m}=\left[\frac{2V_1}{\lambda^2}\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}+\left(n+\frac{\mu+\nu+1}{2}\right)^2+\frac{2V_0}{\lambda^2}-\varepsilon\right]\delta_{n,m}$$

$$+\frac{2V_1}{\lambda^2}\left[\frac{2}{2n+\mu+\nu}\sqrt{\frac{n(n+\mu)(n+\nu)(n+\mu+\nu)}{(2n+\mu+\nu-1)(2n+\mu+\nu+1)}}\,\delta_{n,m+1}+\frac{2}{2n+\mu+\nu+2}\right.$$

$$\left.\times\sqrt{\frac{(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+3)}}\,\delta_{n,m-1}\right] \tag{4.3.4}$$

The diagonal representation requires $V_1=0$ giving $E_n=(1/2)\lambda^2\left[n+(\mu+\nu+1)/2\right]^2+V_0$, which is the well-known energy spectrum associated with the trigonometric Scarf potential. The three-term recursion relation associated with (4.3.4) reads as follows

$$\varepsilon_n f_n(\varepsilon)=\left[\frac{2V_1}{\lambda^2}\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}+\left(n+\frac{\mu+\nu+1}{2}\right)^2+\frac{2V_0}{\lambda^2}\right]f_n(\varepsilon)$$
$$+\frac{2V_1}{\lambda^2}\left[\frac{2}{2n+\mu+\nu}\sqrt{\frac{n(n+\mu)(n+\nu)(n+\mu+\nu)}{(2n+\mu+\nu-1)(2n+\mu+\nu+1)}}\,f_{n-1}(\varepsilon)\right.$$
$$\left.+\frac{2}{2n+\mu+\nu+2}\sqrt{\frac{(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+3)}}f_{n+1}(\varepsilon)\right] \qquad (4.3.5)$$

If we take the special case $V_+=V_-=0$ which leads to $\mu=\nu=\pm 1/2$ then this results in the infinite potential well in one-dimension with sine bottom $V_1\sin(\lambda x)$ which was treated in [31]. Under the restriction $\mu=\nu=1/2$, the three-term recursion relation equation reads as follows

$$\varepsilon_n f_n(\varepsilon)=\left[(n+1)^2+2V_0/\lambda^2\right]f_n(\varepsilon)+\left(V_1/\lambda^2\right)\left[f_{n-1}(\varepsilon)+f_{n+1}(\varepsilon)\right] \qquad (4.3.6)$$

Solving the three-term recursion relation (4.3.6) gives the energy spectrum ε_n for (eigenvalues of the Schrödinger equation with) the potential (4.3.5). The results are reported below and compared to the AIM.

4.3.2 Solution using AIM

For the AIM, the Schrödinger equation with the given potential reads:

$$\left\{-\frac{d^2}{dx^2}+2\left[V_0+\frac{V_+-V_-\sin(\lambda x)}{\cos^2(\lambda x)}+V_1\sin(\lambda x)\right]-2E\right\}\psi(x)=0 \qquad (4.3.7)$$

Now, to obtain the AIM form one should take into consideration of the boundary condition that requires the wavefunction to vanish at the boundaries $x=\pm L/2$. First, in order to

bring the independent variable domain to $[-1,+1]$, we use the following coordinate transformation

$$y=\sin(\pi x/L), \qquad -1\le y\le +1 \tag{4.3.8}$$

This transforms Schrödinger equation into the following form:

$$\psi''(y)=\frac{y}{(1-y^2)}\psi'(y)+\left[\frac{A_0+A_1y-\varepsilon}{(1-y^2)}+\frac{A_+-A_-y}{(1-y^2)^2}\right]\psi(y) \tag{4.3.9}$$

where $A_0=\frac{2V_0}{\lambda^2}, A_1=\frac{2V_1}{\lambda^2}, A_\pm=\frac{2V_\pm}{\lambda^2}$ and $\varepsilon=\frac{2E}{\lambda^2}$.

To enforce the boundary satisfaction we use the following substitution

$$\psi(y)=(1-y^2)^\alpha f(y) \tag{4.3.10}$$

Then equation (4-10) can be written in a compact form for $f(y)$ as follows:

$$f''(y)=\frac{(4\alpha+1)y}{(1-y^2)}f'(y)+\left[\frac{4\alpha^2+A_0+A_1y-\varepsilon}{(1-y^2)}+\frac{A_+-A_-y-2\alpha(2\alpha-1)}{(1-y^2)^2}\right]f(y) \tag{4.3.11}$$

From the mathematical point of view, the points $y=\pm 1$ are regular singular points of the differential equation (4.3.11). $k_n(y)$ and $S_n(y)$ with containing regular singular point and due to higher order derivative, the presence of the last term in $S_0(y)$ will play a very destructive role for the convergence of our termination condition. Thus to improve the convergence of the termination condition we need to perform a transformation that eliminates this spurious term. Equation (4.3.11) is now amenable to the AIM where the characteristic functions $k_0(y)$ and $S_0(y)$ are defined by

$$k_0(y)=\frac{(4\alpha+1)y}{(1-y^2)} \quad , \qquad S_0(y)=\frac{4\alpha^2+A_0+A_1y-\varepsilon}{(1-y^2)}+\frac{A_+-A_-y-2\alpha(2\alpha-1)}{(1-y^2)^2} \qquad (4.3.12)$$

By means of the iteration formulas (2.3), the functions $k_n(y)$ and $S_n(y)$ are computed for $n=1,2,...$ and then the energy spectrum (eigenvalues E_m^n) will be found using the roots of equation (2.10). In this work we consider two cases by just selecting the potential parameters:

CASE 1: $V_+, V_1 \neq 0,$, and $V_- = V_0 = 0$

The characteristic functions $k_0(y)$ and $S_0(y)$ written as follows:

$$k_0(y)=\frac{(4\alpha+1)y}{(1-y^2)} \quad , \qquad S_0(y)=\frac{4\alpha^2-\varepsilon+A_1y}{(1-y^2)}+\frac{A_+-2\alpha(2\alpha-1)}{(1-y^2)^2} \qquad (4.3.13)$$

For convergence purposes, we eliminate the spurious term in (4.3.13), so that $k_0(y)$ and $S_0(y)$ reads

$$k_0(y)=\frac{(4\alpha+1)y}{(1-y^2)} \quad , \qquad S_0(y)=\frac{\omega+A_1y}{(1-y^2)} \qquad (4.3.14)$$

where we set $\omega=4\alpha^2-\varepsilon$ and $\alpha=\frac{1}{4}\left(1+\sqrt{1+4A_+}\right)$. Using Eq. (2.3) and Eq. (2.10) the functions $k_n(y)$ and $S_n(y)$ are calculated as follows:

$$k_1(y)=\frac{1+4\alpha+y(1-y^2)A_1+y^2(2+12\alpha+16\alpha^2)+(1-y^2)\omega}{(1-y^2)^2}$$

$$S_1(y)=\frac{\left(1+y^2\left(2+4\alpha\right)\right)A_1+y\left(3+4\alpha\right)\omega}{\left(1-y^2\right)^2}$$

$$k_2(y)=\frac{2\left(1-y^2\right)\left(1+y^2(2+4\alpha)\right)A_1+y\left(3+4\alpha\right)\left(3+12\alpha+2y^2(1+6\alpha+8\alpha^2-\omega)+2\omega\right)}{\left(1-y^2\right)^3}$$

$$S_2(y)=\frac{1}{\left(1-y^2\right)^3}\Big[\omega\left(4+8\alpha+\omega+y^2\left(11+24\alpha+16\alpha^2-\omega\right)\right)$$
$$+y\left(9+12\alpha+2y^2\left(3+10\alpha+8\alpha^2-\omega\right)-2\omega\right)A_1-y^2\left(1-y^2\right)A_1^2\Big]$$

and so on. From the above calculations and by induction we conclude that $S_{2n}(y)$ and $S_{2n+1}(y)$ are polynomials in ε of degree $n+1$ while $k_{2n}(y)$ and $k_{2n-1}(y)$ are polynomials in ε of degree n in ε. The Energy spectrum (eigenvalues) will be calculated using the termination equation (2.10),

For $n=0$:

$$\Delta_0(y,\varepsilon)=a_1(\varepsilon)+y=0 \quad ; \quad a_1(\varepsilon)=\frac{1}{A_1}\left[4\alpha^2-\varepsilon\right]$$

With an appropriate choice of value, $y=y_0$ we will obtain the first eigenvalue ε_0.

For $n=1$:

$$\Delta_1(y,\varepsilon)=a_2(\varepsilon)+2a_1(\varepsilon)y+y^2=0 \quad ; \quad a_2(\varepsilon)=\frac{1}{A_1^2}\left[4\alpha^2+16\alpha^3+16\alpha^4-\varepsilon-4\alpha\varepsilon-8\alpha^2\varepsilon+\varepsilon^2\right]$$

Again, with the same appropriate value of $y=y_0$ we obtain $\varepsilon_0,\varepsilon_1$

For $n=2$

$$\Delta_2(y,\varepsilon)=a_3(\varepsilon)+3a_2(\varepsilon)y+3a_1(\varepsilon)y^2+y^3=0 \quad ;$$

$$a_3(\varepsilon)=\frac{1}{A_1^{\,3}}\begin{pmatrix}16\alpha^2+96\alpha^3+208\alpha^4+192\alpha^5+64\alpha^6-2A_1^2\\-\left(4+24\alpha+72\alpha^2+96\alpha^3+48\alpha^4\right)\varepsilon+\left(5+12\alpha+12\alpha^2\right)\varepsilon^2-\varepsilon^3\end{pmatrix}$$

giving $\varepsilon_0,\varepsilon_1,\varepsilon_3$.

and so on.

Where the relation between the termination condition equations for this problem obey

$$\frac{\partial\Delta_n(y,\varepsilon)}{\partial y}=(n+1)\Delta_{n-1}(y,\varepsilon) \tag{4.3.15}$$

Which implies that the termination condition takes the following from

$$\Delta_n(y,\varepsilon)=\sum_{k=0}^{n}a_k(\varepsilon)y^{k+1}+Q_{n+1}(\varepsilon) \tag{4.3.16}$$

and so on where $Q_n(\varepsilon)$ is a linear combination of $a_n(\varepsilon)$ with coefficients that can be drawn from Pascal triangle. It is worth mentioning that the general structure of $\Delta_n(y,\varepsilon)$ still holds independent of the specific potential and can be written as follows

$$\Delta_n(y,\varepsilon)=\sum_{k=0}^{n}a_k(\varepsilon)y^{k+p}+Q_{n+1}(\varepsilon) \tag{4.3.17}$$

Where p is an integer that is potential dependent. The coefficients $a_n(\varepsilon)$ are functions of energy and potential parameters, $Q_{n+1}(\varepsilon)$ are polynomials of degree $n+1$ in ε. Now, it is obvious that the function $\Delta_n(y,\varepsilon)$ is a polynomial of degree $n+1$ in ε. Thus, at the n^{th} iteration, there are $n+1$ eigenvalues that depend generally on the choice of y_0. Now, it is clear that this problem with the generalized Scarf potential given by Eq. (4.3.7) will not

have an analytic solution in the conventional formulation. In other words, the termination condition (2.10) gives an expression that depends on both y and ε. Therefore, one has to find the best possible starting value $y = y_0$ that stabilizes the process of computation of the energy spectrum. As mentioned before, the computation of the eigenvalues using (2.10) should be independent of the choice of y_0. Researchers traditionally choose this as either the minimum value of the potential or the maximum of the ground state wavefunction. However, the best choice of the starting value is observed to be critical only for the stability of the process, as well as to the speed of convergence. By means of the iteration formula (2-3) and the termination condition (2.10), the eigenvalues are then computed. Our calculation shows the effect of (i) different choice of initial values $y = y_0$ and (ii) the number of iterations on the accuracy and convergence of the eigenvalues. In Table 5, we have considered only the lowest two Eigen-energies while varying y_0 in the range $-1 \le y_0 \le +1$. It is obvious that by increasing the iterations the process stabilizes and the values of y_0 that are very close to the singular points lead to strong oscillations and divergence. It is very clear in this table that for the ground state (for a given accuracy) for 4 iterations the Eigen-energies are stable for any initial value within the range $-0.1 \le y_0 \le +0.1$ (plateau of convergence). Increasing the number of iterations to 5 iterations makes the plateau increase and the Eigen-energies are stable for any value in the given range (away from the singular points). Continuing, for 6 and further iterations, the plateau shrinks slowly to a point, in this problem it is zero. Similarly, for the first excited states, the plateau of convergence has the same behavior that it grows up to an optimal

number of iteration and then shrinks to a point (or points). For a better display of precision and convergence, the eigenvalues of the ground state are computed within the range $-0.1 \le y_0 \le +0.1$ and for iterations ranging from 1 to 100. It is obvious for AIM that the accuracy increases by increasing the number of iterations. The results are shown in Table 6 by comparing the ground state obtained via TRA (Table 7) with that obtained using AIM for different iterations. From the above two Tables, we observe that by choosing a certain accuracy the termination condition can be solved for any starting value at a certain number of iterations. For this number of iterations, the eigenvalues are stable against variation in y within a given range. After that optimal number of iterations, the plateau starts to shrink to a point which can be considered as the ideal starting value of the space variable to ensure a good accuracy and convergence of the process. Therefore, we predict that for this problem, the best choice of y_0 is $y_0 = 0$. Many published researches used to set the initial value of space variable to be zero without explanation. In this work, we tried to have a closer look at the termination condition and its behavior (Eq. (4.3.16) and studied its plateau of convergence). The termination condition depends on the iteration formula (2.3) which rely on derivative terms. For higher number of iteration, the termination condition equation becomes more and more complex and more difficult to solve.

At first look at (4.3.16), it seems that if we insist that the roots of $\Delta_n\left(y,\varepsilon\right)=0$ being independent of y then one obvious possibility is to set y = 0. In such case what is left are the roots of the energy polynomials $a_{n+1}\left(\varepsilon\right)$, hence the roots of these polynomials represent the eigenenergies of the problem. Therefore, the technique of plateau of stability described

above could be considered as one of the finest methods for choosing the best starting value of the space variable for the AIM.

Most of our computations in this work were done using the computation software Mathematica. In Tables 7, the lowest Eigen-energies using both AIM and TRA methods are reported for comparison purpose.

TABLE 5

	Iterations	-0.9	-0.7	-0.5	-0.3	-0.1	0	0.1	0.3	0.5	0.7	0.9
ε_0	1	1.11121596	1.10615724	1.10253753	1.10022861	1.09912022	1.09898585	1.09911675	1.10013464	1.10210036	1.10494881	1.10862200
	2	1.09528288	1.09546731	1.09559105	1.09567252	1.09572924	1.09575353	1.09577777	1.09583377	1.09591196	1.09602618	1.09618936
	3	1.09575954	1.09575561	1.09575330	1.09575206	1.09575153	1.09575148	1.09575155	1.09575212	1.09575338	1.09575565	1.09575938
	4	1.09575085	1.09575091	1.09575094	1.09575095	1.09575096	1.09575096	1.09575096	1.09575097	1.09575098	1.09575101	1.09575106
	5	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096
	6	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575098
	7	1.09575126	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575091
	8	1.09576026	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575136
	9	1.09589152	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09567190
	10	1.09669582	1.09575095	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09485162
	15	−48.402356	1.09575655	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575684	−50.91596
	20	−121.23852	1.15320760	1.09575021	1.09575096	1.09575096	1.09575096	1.09575096	1.09575096	1.09575147	17.129705	−760.34107
	30	−87475.723	−206.58849	1.11811404	1.09575097	1.09575096	1.09575096	1.09575096	1.09575097	1.09075267	−173.51422	−79170.112
	50	−29222.707	−18517.54	−503.87627	1.08537181	1.09575096	1.09575096	1.09575096	1.08153927	0..0000	−17002.7	−26036.89
	100	−1.896722	−25922.91	−86230.156	0.00000	1.09575096	1.09575096	1.09575103	0.0000	−86223.88	−26531.56	−1.89672
ε_1	1	3.818650	3.904766	3.989442	4.072808	4.154974	4.195636	4.236034	4.316073	4.395164	4.473372	4.550756
	2	4.223949	4.214475	4.207675	4.203303	4.201145	4.200837	4.201014	, 4.202745	4.206192	4.211224	4.217724
	3	4.196199	4.196484	4.196666	4.196777	4.196846	4.196873	4.196810	4.196964	4.197063	4.197220	4.197454
	4	4.196883	4.196879	4.196876	4.196874	4.196873	4.196873	4.196874	4.196874	4.196876	4.196878	4.196882
	5	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873
	6	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873
	7	4.196872	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196871
	8	4.196793	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196916
	9	4.197206	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.200175
	10	4.193668	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.208975
	15	−19.8271	4.196697	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196873	4.196795	0.000000
	20	−17.7743	2.039172	4.196878	4.196873	4.196873	4.196873	4.196873	4.196873	4.196862	99.3084	−361.064
	30	−10370.12	−21.6482	3.970720	4.196873	4.196873	4.196873	4.196873	4.196873	3.642828	25.3704	−20192.02
	50	−12256	−8848.12	−46.6361	4.272074	4.196873	4.196873	4.196873	4.166646	4.058064	−11492.6	−9821.21
	100	−3.2202	−2308.36	−56002.4	0.00000	4.196874	4.196873	4.196873	0.00000	−56004.09	−2178.59	−3.307368

Table 5: The effect of different initial value y_0 and number of iterations on the convergence and accuracy of the eigenvalues. We took the potential parameters as: $V_1 = 1, V_+ = 0.25, V_0 = V_- = 0$, and $L = 1$.

Iterations \ y_0	-0.1	0	0.1
1	1.0991202248315695	1.09898585279422	1.0991167526968348
2	1.0957292393803957	1.095753527922459	1.0957777701723037
3	1.0957515331417946	1.095751480043435	1.095751554739332
4	1.095750956836507	1.095750959070117	1.0957509613421887
5	1.0957509589138086	1.095750958910591	1.09575095891494
6	1.0957509588952719	1.095750958895319	1.09575095889537
7	1.095750958895318	1.095750958895318	1.0957509588953176
8	1.0957509588953167	1.095750958895317	1.095750958895317
9	1.095750958895314	1.095750958895318	1.0957509588953156
10	1.0957509588953172	1.095750958895317	1.095750958895318
15	1.0957509588953178	1.095750958895317	1.0957509588953191
20	1.0957509588953054	1.095750958895317	1.0957509588953052
30	1.0957509588953414	1.095750958895317	1.0957509588954089
50	1.0957509588941203	1.095750958895318	1.0957509588954446
100	1.0957509556475724	1.095750958895317	1.0957510397379888

Table 6: The effect of different initial values y_0 and number of iterations on the accuracy of the ground state energy for a different number of iterations with the potential parameter: $V_1 = 1, V_+ = 0.25, V_0 = V_- = 0$, and $L = 1$.

ε_n	AIM	TRA
0	1.095750958895317	1.095750958895317
1	4.196873325806087	4.196873325806094
2	9.292844177187838	9.29284417718781
3	16.389252331506132	16.38925233150634
4	25.485790081950977	25.48579008195058
5	36.58237913869347	36.58237913866615
6	49.678992506294904	49.67899250636078
7	64.77561899613518	64.77561887661372
8	81.87225251919959	81.8727900682211
9	100.97373751566363	100.9688405503092

Table 7: The lowest levels of the energy spectrum for CASE 1 with the potential parameters: $V_1 = 1, V_0 = V_- = 0, V_+ = 0.25$, and $L = 1$ for both methods AIM (40 iterations) and TRA (matrix size N=20). We took $y_0 = 0$.

CASE 2: $V_0, V_{\pm} = 0$ and $V_1 \neq 0$

We consider now the case of the infinite potential well with sine bottom $V(x) = V_1 \sin(\pi x/L)$. In the TRA this corresponds to $\mu = \nu = 1/2$. Equation (4.3.12) is then written as follows:

$$f''(y) = \frac{(4\alpha + 1)y}{(1 - y^2)} f'(y) + \frac{4\alpha^2 + A_1 y - \varepsilon}{(1 - y^2)} f(y) \tag{4.3.18}$$

Clearly, the same procedures for the calculation of the functions $k_n(y)$ and $S_n(y)$ as in the previous case will be used. Similarly, for this case, the stability of eigenvalues due to variation in y_0 has a similar behavior. The results of the AIM are reported in Table 8 with the TRA results for different parameters of the potential for comparison purpose. Due to the rapid convergence and stabilization of the process for this case, the results are displayed for 10 iteration with more than 10 decimals of accuracy. There is an excellent agreement regarding the accuracy of both methods.

In addition, we calculated the energy spectrum using the AIM in the case of Schrodinger equation with the potential $V(x) = V_1 \cos(\pi x/L)$, $0 \le x \le L$, that was treated in [36] by the TRA. Using the AIM described above, we rewrite the wavefunction that satisfies the boundary conditions as $\psi(x) = \sin(\pi x/L) f(x)$. Then, we use the transformation $y = \cos(\pi x/L)$, $-1 \le y \le +1$. The AIM basic equation for this case will be similar to that of equation (4.3.18) with $A_0 = A_{\pm} = 0$. The results shown in Table 9 are for $A_1 = 5$. The

computed eigenvalues ε_n using the AIM are in excellent agreement with the results obtained in [31] using the TRA. It should be obvious that the physical properties of the system with the potential $V(x) = V_1 \cos(\pi x/L)$ should be identical to that with $V(x) = V_1 \sin(\pi x/L)$ since one is obtained from the other by the artificial shift of configuration space $x \to x - \frac{1}{2}L$.

ε_n	AIM			TRA
	$y_0 = -0.1$	$y_0 = 0$	$y_0 = 0.1$	
ε_0	0.9965804414948887	0.9965804414948881	0.9965804414948877	0.9965804414948881
ε_1	4.001366326993638	4.0013663269936615	4.001366326993682	4.0013663269936615
ε_2	9.000586656216685	9.000586656216424	9.000586656216043	9.000586656216425
ε_3	16.00032590879089	16.000325908792934	16.000325908795052	16.000325908792927
ε_4	25.000207394742418	25.000207394728182	25.000207394715762	25.000207394728175
ε_5	36.00014358054208	36.00014358054704	36.00014358054918	36.0001435805457
ε_6	49.00010529186438	49.00010529226843	49.000105292787566	49.00010529227191
ε_7	64.00008070727844	64.00008065049936	64.00008070322694	64.00008052770214
ε_8	81.00003408297702	81.00006328059685	81.00009189292832	81.00060387125417
ε_9	100.00613182329307	100.00494124743338	100.0059053176835	100.000000000000

Table 8: The lowest levels of the energy spectrum for CASE 2 with the potential parameters $V_0 = V_\pm = 0, V_1 = 1$ and $L = 1$ for both methods AIM (10 iterations) and TRA (N=10).

	AIM	TRA
ε_0	-0.5955395581	-0.5955395590
ε_1	4.3453451807	4.3453451697
ε_2	9.3549646911	9.3549646942
ε_3	16.2001115697	16.2001100733
ε_4	25.1266893786	25.1266923657
ε_5	36.0878499905	36.0875520021
ε_6	49.0634094279	49.0641568654
ε_7	64.0974723518	64.0490437060
ε_8	80.9412278720	81.0387114885
ε_9	103.6280332706	100.0313345578

Table 9: The lowest levels of the energy spectrum for the potential with the parameters $A_0, A_{\pm} = 0$ and $A_1 = 5$, for both methods AIM (10 iterations, $y_0 = 0$) and TRA (N=20).

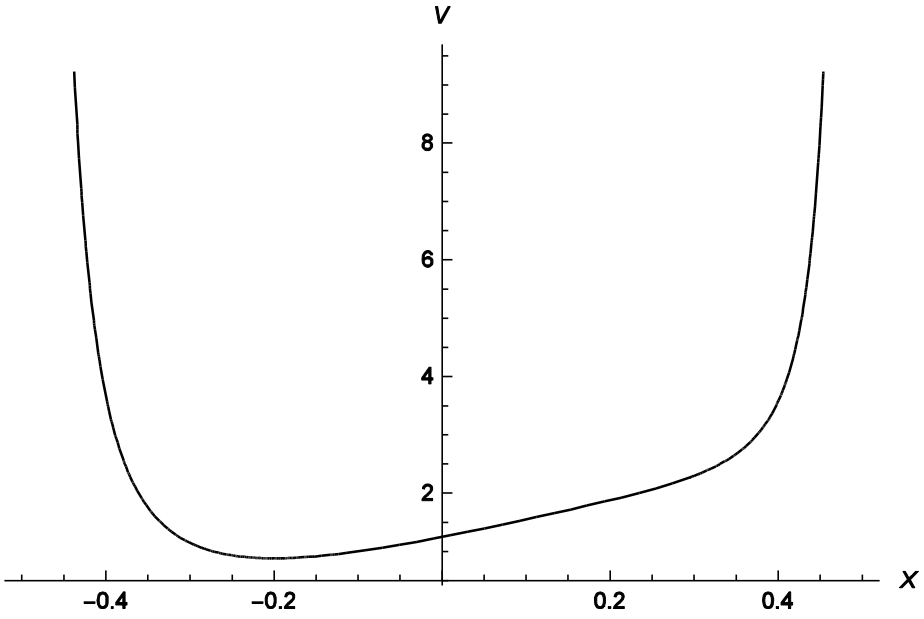

Figure 4: The generalized Scarf potential for the parameters $V_0, V_1 = 1, V_+ = 0.25, V_- = 0.1$, and $L = 1$.

4.4 Applying Plateau of Convergence (PC) technique to SCH type problems

Our objective in this section is to apply the plateau of convergence technique to different SCH equations with different potentials. This was done in order to feel its importance for our conclusions. For the AIM we have improved convergence of the quantization condition that terminates the iterations asymptotically. This is accomplished by looking for the range of initial values of the space variable in the terminating condition that produces stable results (plateau of convergence) for the SCH with the generalized scarf potential. We have shown that with a given accuracy the plateau of convergence shows up and broaden into an ideal number of iteration. Furthermore, the plateau of convergence shrinks with increasing the number of iterations to a single point that, in this problem (4.3) and is independent of the potential parameters. It is more convenient when applying this technique to see the behavior of the plateau of convergence for many problems in 1D (bound state). The following are the calculated eigenvalues for the ground state for different potentials. These tables show the effect of different initial values and number of iterations on the convergence and accuracy of the eigenvalues.

4.4.1 Sine square potential

$$V(x)=\begin{cases} V_0 \sin^2(x/a), & -\dfrac{\pi a}{2} \le x \le \dfrac{\pi a}{2} \\ \infty, & |x| \succ \dfrac{\pi a}{2} \end{cases}, \tag{4.4.1}$$

Where $a \neq 0$.

In this case, the time-independent Schrödinger equation reads:

$$\left[-\frac{d^2}{dx^2}+V_0 \sin^2(x/a)-E\right]\psi(x)=0 \tag{4.4.2}$$

The boundary condition $\psi\left(-\dfrac{\pi a}{2}\right)=\psi\left(\dfrac{\pi a}{2}\right)=0$.

However, to obtain the AIM standard form we take a different approach to reach the suitable form of AIM. We start by rewriting the wave-function that satisfies the boundary condition as the following

$$\psi(x)=\cos(x/a)f(x) \tag{4.4.3}$$

Then the Sch. Eq. is written as a function of $f(x)$ as follow:

$$f''(x)=\frac{2}{a}\tan(x/a)f'(x)+\frac{1}{a^2}\left[a^2V_0 \sin^2(x/a)-a^2E+1\right]f(x) \tag{4.4.4}$$

A further change of variable we use $y=\sin(x/a)$ where $y \in [-1,+1]$. Thus, Sch. Eq. reads

$$f''(y)=\frac{3y}{\left(1-y^2\right)}f'(y)+\left[\frac{\omega}{\left(1-y^2\right)}+\mu\right]f(y) \qquad (4.4.5)$$

Where we set that $\omega=1+\mu-a^2E$, $\mu=a^2V_0$ [38].

The Characteristics functions $k_0(y)$ and $S_0(y)$ are defined by the following:

$$k_0(y)=\frac{3y}{\left(1-y^2\right)} \quad , \qquad S_0(y)=\frac{\omega}{\left(1-y^2\right)}+\mu \qquad (4.4.6)$$

Similarly, like what we did for the previous problems, the iteration formula $k_n(y)$ and $S_n(y)$ will be computed using (2.3) Then, the termination condition (2.10)

$\Delta_n(y,E)=k_n(y,E)S_{n-1}(y,E)-k_{n-1}(y,E)S_n(y,E)=0$, yields the following

$$\Delta_0=1-a^2E+a^2V_0y^2$$

$$\Delta_1=15a^2E+a^4E^2-a^2V_0\left(1+2a^2E\right)y^2+a^4V_0^2y^4$$

$$\Delta_2=3a^2V_0\left(a^4E^2-1-2a^2V_0\right)y^2-3a^4V_0^2\left(2+a^2E\right)y^4+a^6V_0^3y^6+36+8a^2V_0 \\ -\left(2a^2V_0E+49\right)a^2E+14a^4E^2-a^6E^3$$

And so on. It is obvious that the termination yields expression that depends on the space variable y and the energy E. To obtain the eigenvalues we should find an appropriate initial value of y and this can be done by studying the plateau of convergence in the given range $[-1,+1]$.

TABLE 10

n	-0.9	-0.7	-0.5	-0.3	-0.1	0	0.1	0.3	0.5	0.7	0.9
1	0.92691415	0.95400784	0.97580666	0.99110672	0.99900133	0.99999910	0.99900133	0.99110672	0.97580666	0.95400784	0.92691415
2	1.02097524	1.02321323	1.02436189	1.02487677	1.02505930	1.02507862	1.02505930	1.02487677	1.02436189	1.02321323	1.02097523
3	1.02740435	1.02629859	1.02562845	1.02525894	1.02509767	1.02507862	1.02509767	1.02525894	1.02562845	1.02629859	1.02740435
4	1.02498177	1.02494362	1.02492823	1.02492309	1.02492182	1.02492171	1.02492182	1.02492309	1.02492823	1.02494362	1.02498177
5	1.02489881	1.02491177	1.02491710	1.02492068	1.02492161	1.02492171	1.02492161	1.02492068	1.02491710	1.02491177	1.02489881
6	1.02492170	1.02492199	1.02492209	1.02492211	1.02492212	1.02492212	1.02492212	1.02492211	1.02492209	1.02492199	1.02492170
7	1.02492168	1.02492216	1.02492213	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492213	1.02492216	1.02492168
8	1.02492635	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492635
9	1.02499440	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02499440
10	1.02251883	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02251883
15	1.24332085	1.02485600	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02485600	1.24332085
20	−97.146086	0.83771069	1.02492216	1.02492212	1.02492212	1.02492212	1.02492212	1.02492212	1.02492216	0.83771069	−97.146086
30	−979.8399	0.53452039	0.98928856	1.02492218	1.02492212	1.02492212	1.02492212	1.02492218	0.98928856	0.53452039	−979.8399
50	−2.0107590	−19063.84	−502.6964	1.02497698	1.02492212	1.02492212	1.02492212	1.02497698	−502.6964	−19063.84	−2.0107590
100	−967680.01	−273519.5	−113594.65	−1441.407	1.02492208	1.02492212	1.02492208	−1441.407	−113594.65	−273519.5	−967680.01

Table 10: The effect of different initial value y_0 and number of iterations on the convergence and accuracy of the eigenvalues. We took the potential parameters as: $V_0 = 0.1$, and $a = 1$.

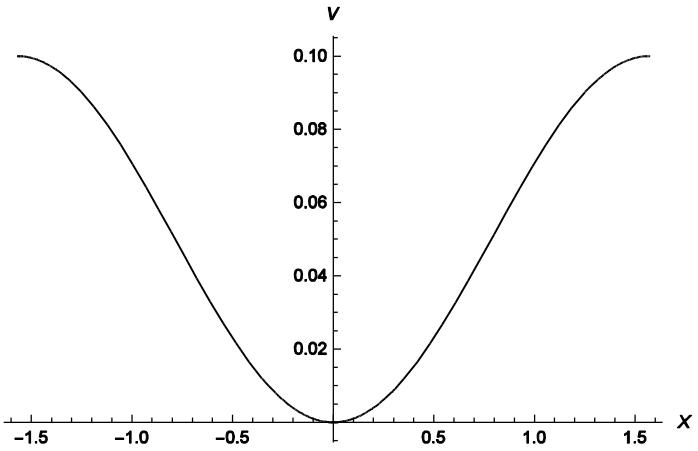

Figure 5 Plot of the sine square potential.

4.4.2 Deformed well potential

$$V(x) = A\cos(x) + B^2\sin^2(x) + \frac{\gamma(\gamma+1)}{\sin^2(x)}, \qquad 0 \le x \le \pi \qquad (4.4.7)$$

A, B, and γ are the potential parameters and $\gamma \in [0, \infty)$.

Schrodinger equation reads

$$\left[-\frac{d^2}{dx^2} + A\cos(x) + B^2\sin^2(x) + \frac{\gamma(\gamma+1)}{\sin^2(x)} - E \right] \psi(x) = 0 \qquad (4.4.8)$$

To obtain the AIM form we rewrite the wavefunction by taking care the boundary condition as:

$$\psi(x) = \sin^{\gamma+1}(x) e^{B\cos(x)} f(x), \qquad (4.4.9)$$

And using the transformation $y = \cos(x)$. $-1 \le y \le +1$ Then, Sch. Eq. written as the following:

$$f''(y) - 2\left(\frac{\sigma y}{1-y^2} - B \right) f'(y) - \frac{\xi y - \omega}{1-y^2} f(y) = 0 \qquad (4.4.10)$$

$$k_0(y) = 2\left(\frac{\sigma y}{1-y^2} - B \right) \quad , \; S_0(y) = \frac{\xi y - \omega}{1-y^2}$$

Where we set $\omega = E - (\gamma+1)^2$, $\xi = A + 2\sigma B$, and $2\sigma = 2\gamma + 3$ [39].

The termination condition (2.10)

$\Delta_n(y,E) = k_n(y,E)S_{n-1}(y,E) - k_{n-1}(y,E)S_n(y,E) = 0$, yields the following

$$\Delta_0 = 1 + 2\gamma + \gamma^2 - E + \xi y$$

$$\Delta_1 = 1 + \left(2 + 4\gamma + 2\gamma^2\right)\sigma + 2B\xi + \left(4 + 6\gamma^1 + 4\gamma^2 + \gamma^3\right)\gamma - \left(2 + 4\gamma + 2\gamma^2 + 2\sigma\right)E + E^2$$
$$+ \left(4B + 2\xi + 4\gamma\xi + 2\gamma^2\xi + 8B\gamma - 2E\xi - 4BE + 4B\gamma^2\right)y + \xi\left(2B + \xi\right)y^2$$

$$\Delta_2(y,E) = + \begin{pmatrix} 12B + 72B\gamma^2 + 48B\gamma^3 + 48B\gamma - 24BE + 12B\gamma^4 + 3\xi + 24B^2\xi + 12\gamma\xi + 18\gamma^2\xi \\ +12\gamma^3\xi + 3\gamma^4\xi + 24B\sigma + 48B\gamma\sigma + 24B\gamma^2\sigma + 6\xi\sigma + 12\gamma\xi\sigma + 6\gamma^2\xi\sigma + 6B\xi^2 \\ -6\left(\xi + 2\gamma\xi + 4B\gamma^2 + 8B\gamma + 4B\sigma + \xi\sigma + \gamma^2\xi\right)E + 3\left(\xi + 4B\right)E^2 \end{pmatrix} y$$
$$+ 3\begin{pmatrix} 12B^2 + 24B^2\gamma + 12B^2\gamma^2 + 9B\xi + 18B\gamma\xi + 9B\gamma^2\xi \\ +\xi^2 + 2\gamma\xi^2 + \gamma^2\xi^2 - \left(6B\xi + 12B^2 + \xi^2\right)E \end{pmatrix} y^2 + \xi\left(8B^2 + 6B\xi + \xi^2\right)y^3$$
$$+ \begin{pmatrix} 10\sigma + 32\gamma\sigma + 40\gamma^2\sigma + 24\gamma^3\sigma + 6\gamma^4\sigma + 8B\xi\sigma + 8\sigma^2 + 16\gamma\sigma^2 + 8\gamma^2\sigma^2 + 3 + 8B^2 + 14\gamma \\ +16B^2\gamma + 27\gamma^2 + 8B^2\gamma^2 + 28\gamma^3 + 17\gamma^4 + 6\gamma^5 + \gamma^6 + 6B\xi + 12B\gamma\xi + 6B\gamma^2\xi - 2\xi^2 \\ -\left(7 + 8B^2 + 20\gamma + 22\gamma^2 + 8\sigma^2 + 12\gamma^3 + 3\gamma^4 + 24\gamma\sigma + 12\gamma^2\sigma + 6B\xi + 16\sigma\right)E \\ +\left(5 + 6\sigma + 6\gamma + 3\gamma^2\right)E^2 - E^3 \end{pmatrix}$$

TABLE 11

n	-0.9	-0.7	-0.5	-0.3	-0.1	0	0.1	0.3	0.5	0.7	0.9
1	17.23224366	16.44348742	15.73791265	15.13271321	14.65562261	14.47920271	14.35653538	14.34454365	15.000000	–	–
2	14.71190187	14.44438197	14.23706271	14.08726749	13.98887339	13.95548302	13.92973771	13.88830436	13.8309316	13.71404795	13.49529364
3	13.98495318	13.94902167	13.92648466	13.91371529	13.90743182	13.90586576	13.90500554	13.90481805	13.90664097	13.91202382	13.92471711
4	13.90386321	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319
5	13.90386337	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386318
6	13.90386464	13.9038632	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386346
7	13.90388615	13.90386324	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.9038632	13.90386656
8	13.90400796}	13.90386322	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90440271
9	13.90835067	13.90386155	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386323	13.90608202
10	13.66990706	13.90386394	13.90386318	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386319	13.90386302	13.83149148
15	−12.469431	13.84427276	13.90385887	13.9038632	13.90386319	13.90386319	13.90386319	13.90386319	13.90386317	13.90490492	−97.73885
20	−682.67	510.526809	13.90578648	13.90386334	13.90386319	13.90386319	13.90386319	13.9038632	13.90386921	171.057157	−131.188
30	−4012.92	−515.43680	5.880679473	13.90367723	13.90386319	13.90386319	13.90386319	13.90386256	14.71717265	−308.74786	−404.13
50	−339615	−20145	−689.53	93.05225829	13.90386314	13.90386319	13.90386319	13.85895864	−660.27107	−6461.12	−45217
100	−6203.7943	-4×10^{6}	−125900	−508.11	13.90406298	13.90386319	13.90386331	−5.3369	−63360	−414577.62	−13131.948

Table 11 The effects of choosing different starting values of $y \equiv y_0$ on the desired accuracy of E_0^n for different iterations. We took the potential parameters as: $\xi = 4, \gamma = 3, B = 1,$, and $\sigma = 4.5$.

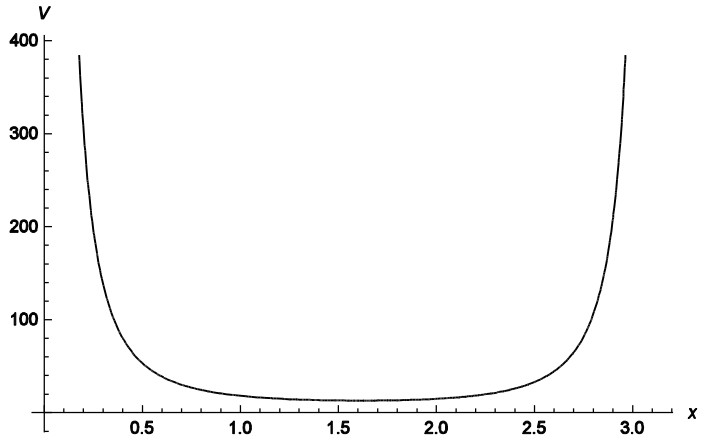

Figure 6 Plot of the deformed well potential

4.5 REMARKS ABOUT AIM

In this work, we have made some important remarks that should be taken into consideration especially for the main part of this work which is the implementation of the Asymptotic Iteration Method. The following is a summary of the most important remarks that should be stressed when applying the Asymptotic Iteration Method.

There are two main problems we can face when applying AIM

I. <u>The conversion of Schrodinger equation into the standard form of AIM</u>

$$y''(x) = k_0(x)\,y'(x) + S_0(x)\,y(x)$$

To obtain the standard form of AIM, much attention should be paid to the convergence of the solution.

- Check the given boundary condition of the problem, this will leads to a proper choice of the wave-function.
- Rewrite the wave-function so that it satisfies the given boundary condition.
- Keep track of the singular behavior of the wave operator.
- When obtaining AIM equation form use a convergence test which can be done as follows:

  Test the convergence of the ratio $\frac{y^{(n+2)}}{y^{(n+1)}} = \frac{d}{dx}\ln\left(y^{(n+1)}\right)$, or test the convergence

of the condition $\frac{S_n}{\lambda_n} = \frac{S_{n-1}}{\lambda_{n-1}}$, that gives the asymptotic aspect of the method and this condition leads to $\frac{y^{(n+2)}}{y^{(n+1)}} = \frac{\lambda_n}{\lambda_{n-1}}$.

Taking into consideration the previous steps before you start your calculation, will help to obtain the appropriate AIM form that has a rapid convergence and the desired solution without losing much time in the iterations.

II. The appropriate choice of the initial point of the space variable.

The best choice of the initial value plays a critical role that leads to a good convergence of the solution and saves your time in the iteration process. The following are some methods used to select the initial values.

- The maximum value of the wave-function and, some researcher suggest that $\frac{d}{dx} k_0(x) = 0$ can be used for this purpose, but it does not work for all problems.
- The minimum value of the potential that can be found using $\frac{d}{dx} V(x) = 0$, or from the potential plot .
- It can also be found by setting $S_0(x) = 0$.
- The systematic way is to find the plateau of convergence by plotting the eigenvalues versus the space variable which gives a certain space variable range over which the eigenvalues are stable against the variation in the space variable.

A remarkable point here should be noticed, that each problem has its properties so that the

first three ways sometimes do not work for some problems. Therefore the plateau of convergence is considered as one of the finest methods to be used for choosing the starting value.

In addition, from most solution adopted to the AIM, it is found that for problems that have $k_0(x) \sim 1/x, 1/x^2$ do not have a good convergence. Thus, to overcome this issue try to avoid this term by using another transformation. For convergence propose also, a term like $1/x^2$ should be eliminated in the Schrodinger equation by using an appropriate transformation. Usually, problems that have, $k_0(x) \sim x$, will not present a difficulty for the choice of the initial value of the variable space. It is also observed that when $k_0(x)$ and $S_0(x)$ do not have the same singularities (or order of the singularities) this play a destructive role on the convergence as well as the stabilization of the process.

Finally, we must also underline that there are some disadvantages of AIM which we hope to tackle in the future. Among the first to note is that an unappealing feature of the relation formula $k_n(x)$ and $S_n(x)$ in Eqs. (2.3). It is obvious that $k_n(x)$ and $S_n(x)$ depend on a derivative formula which means that at each iteration one must take the derivative of the k and S terms of the previous iteration. These cause problems for the computation and results in a slow convergence of the AIM. Some researchers worked on these issues by developing an improved version of the AIM which bypasses the need to take derivatives at each step [19]. Overcoming these types of problems will greatly improve both the accuracy and speed of the method.

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1 CONCLUSIONS

The Asymptotic Iteration and Tridiagonal Representation techniques were used to solve 1D Schrödinger equation and find the eigen-energies of some analytically and approximately solvable problem for the purpose of making a comparative study. In this work, we used some tested potentials such as the Harmonic oscillator and the tangent square potential for which both methods led to closed form (exact solution) of the energy spectrum. We also considered the generalized scarf potential which is non-exactly solvable in the AIM. This work brings up the importance of the asymptotic wave function and coordinates transformation used in introducing AIM. The aim of our approach is to improve the convergence and to eliminate the numerical instabilities that might be experienced in direct usage of the AIM. It was noticed that the existence of regular singularities will slow the convergence of the AIM. A remarkable observation, however, is that the use of plateau of stability in the implementation of the AIM plays an important role in the convergence, precision as well as the stability of the numerical algorithm. However, for a given accuracy the plateau widens rapidly with increased iterations up to an optimum number of iterations. After which the plateau shrinks slowly with increasing the number of iterations and converges to a single point. In the problem of generalized scarf potential, it seem to be independent of the potential parameters. In this work, we tried

to make a reasonable explanation to answer the question of why the zero initial value seems to be the convergence point of most published research. This was done by studying carefully the termination condition and its general structure and the plateau of convergence.

Generally, we have succeeded in making a conclusive comparative study between AIM and TRA approaches. For the AIM, we have investigated the most important factors that contribute to the improvement and rapid convergence of the quantization condition. Aside from analytically solvable potentials our investigations raise a real concern regarding the wide usage of the AIM for numerical computations of bound states. We also think that our assertion is well substantiated by our results but also due to the fact that AIM is really based on higher and higher order derivatives and hence it well known that successive numerical derivatives are not very reliable since the numerical accuracy reduces significantly with higher order derivatives which are the building blocks of the termination condition. We also expect that extensions of the AIM to deal with resonances, states with finite lifetime, will not converge rapidly for the above mentioned reasons.

However, we might want to underline that AIM is a viable technique to obtain exact solutions for second order differential equations, like Schrodinger equation. By using the technique we obtain the eigenvalues by transforming the second-order differential equation into a form of the asymptotic iteration method results in exact analytical solutions if it exists and provides closed forms for the energy eigenvalues. The energy eigenvalues are obtained using an iterative approach. As it is presented, AIM puts no constraint on the potential parameter values involved and it is easy to implement. This method also yields the corresponding eigen-functions which can be found via equations (2.9) and (2.10).

For the Tridiagonal Representation Approach, the wave-function is expanded in suitable discrete basis elements which must be compatible with a domain of the Hamiltonian and satisfying the boundary condition. The problems translated into three terms recursion relation for the expansion coefficients of the wave-function that solved either analytically or numerically to find the energy spectrum.

However, it is important to note that the implementation of the AIM is very sensitive to the evaluation of higher order derivatives which affect both the accuracy and stability of the approach. To sum up, the AIM and TRA are efficient and steady methods for obtaining the energy spectrum to many interesting physical problem. However, the TRA is much more robust due to the drawback of AIM caused by its strong dependence on higher order derivatives which are the main cause of numerical instabilities.

5.2 FUTURE WORK

The results of these investigations are sufficiently accurate for practical purposes. In this work we have succeeded in treating the 1D Schrödinger equation in the Asymptotic Iteration Method (AIM) and Tridiagonal Representation Approach (TRA). As explained in the literature the TRA can produce a wider class of solvable potentials. In this project, we have considered the general approach and then considered some cases in which were rich and led to solvable potentials. However, it is worth mentioning that we have restricted our work to Jacobi and Laguerre basis but one might try another square-integrable basis. It should be noticed here for future work that the problem is still open and other solvable potentials can be found using TRA, especially in higher dimensions. Moreover, we are interested in applying these methods to some real physical applications such as in graphene. It is worth also extending these methods to examine interacting systems.

Appendices

Appendix A: Classical polynomials

A.1 The Jacobi polynomials

The Jacobi polynomials $P_n^{(\mu,\nu)}(y)$ are a special class of classical orthogonal polynomials defined on $y \in [-1,+1]$ and $\mu > -1, \nu > -1$. These polynomials can be calculated using the Rodrigues' formula, given below[32, 34, 40, 41]:

$$P_n^{(\mu,\nu)}(y) = \frac{(-1)^n}{2^n n!}(1-y)^{-\mu}(1+y)^{-\nu}\frac{d^n}{dy^n}\left[(1-y)^{\mu}(1+y)^{\nu}(1-y^2)^n\right] \tag{A.1}$$

The Jacobi polynomials satisfy the following properties:

$$(1-y^2)\frac{d^2P_n^{(\mu,\nu)}(y)}{dy^2} - \left[(\mu+\nu+2)y+\mu-\nu\right]\frac{dP_n^{(\mu,\nu)}(y)}{dy} + n(n+\mu+\nu+1)P_n^{(\mu,\nu)}(y) = 0 \tag{A.2}$$

$$(1-y^2)\frac{dP_n^{(\mu,\nu)}(y)}{dy} = -n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)P_n^{(\mu,\nu)}(y) + 2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}P_{n-1}^{(\mu,\nu)}(y) \tag{A.3}$$

$$\left(\frac{1\pm y}{2}\right)P_n^{(\mu,\nu)}(y) = \frac{2n(n+\mu+\nu+1)+(\mu+\nu)\left(\frac{\mu+\nu}{2}\pm\frac{\nu-\mu}{2}+1\right)}{(2n+\mu+\nu)(2n+\mu+\nu+2)}P_n^{(\mu,\nu)}(y)$$
$$\pm\frac{(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}P_{n-1}^{(\mu,\nu)}(y) \pm \frac{(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}P_{n+1}^{(\mu,\nu)}(y) \tag{A.4}$$

$$\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)dy=\frac{2^{\mu+\nu+1}}{(2n+\mu+\nu+1)}\frac{\Gamma(n+\mu+1)\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}\delta_{nm} \tag{A.5}$$

$$yP_n^{(\mu,\nu)}(y)=\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}P_n^{(\mu,\nu)}(y)+\frac{2(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}P_{n-1}^{(\mu,\nu)}(y)$$
$$+\frac{2(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}P_{n+1}^{(\mu,\nu)}(y) \tag{A.6}$$

$$\begin{aligned}\langle n|y|m\rangle=&\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\delta_{n,m}\\&+\frac{2}{2n+\mu+\nu}\sqrt{\frac{n(n+\mu)(n+\nu)(n+\mu+\nu)}{(2n+\mu+\nu-1)(2n+\mu+\nu+1)}}\,\delta_{n,m+1}\\&+\frac{2}{2n+\mu+\nu+2}\sqrt{\frac{(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+3)}}\,\delta_{n,m-1}\end{aligned} \tag{A.7}$$

A.2 The Laguerre polynomials

The orthogonal Laguerre polynomials $L_n^{\nu}(x)$ are defined on $y\in[0,\infty[$ and $\nu>-1$. These polynomials can be calculated using the Rodrigues' formula, given below [32, 34, 40, 41]:

$$L_n^{\nu}(y)=\frac{y^{-\nu}}{n!}\left(\frac{d}{dy}-1\right)^n y^{n+\nu} \tag{A.8}$$

These polynomials satisfy the following properties:

$$yL_n^{\nu}=(2n+\nu+1)L_n^{\nu}-(n+\nu)L_{n-1}^{\nu}-(n+1)L_{n+1}^{\nu} \tag{A.9}$$

$$L_n^{\nu}(y)=\frac{\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(\nu+1)}\,{}_1F_1(-n;\nu+1;y) \tag{A.10}$$

$$\left[y\frac{d^2}{dy^2}+(\nu+1-y)\frac{d}{dy}+n\right]L_n^{\nu}(y)=0 \tag{A.11}$$

$$y\frac{d}{dy}L_n^\nu = nL_n^\nu - (n+\nu)L_{n-1}^\nu$$

(A.12)

$$\int_0^\infty y^\nu e^{-y} L_n^\nu(y) L_m^\nu(y) dy = \frac{\Gamma(n+\nu+1)}{\Gamma(n+1)}\delta_{nm} \tag{A.13}$$

$$\langle m|\, y\,|n\rangle = (2n+\nu+1)\delta_{m,n} - \sqrt{n(n+\nu)}\,\delta_{m,n-1} - \sqrt{(n+1)(n+\nu+1)}\,\delta_{m,n+1} \tag{A.14}$$

$$L_n(x) = M(-n,1,x) \tag{A.15}$$

Where

$${}_1F_1(a;b;x) = M(a,b,x) = 1 + \frac{a}{b}\frac{x}{1!} + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + \ldots, \quad b \neq 0,-1,-2,\ldots \tag{A.16}$$

In terms of the Pochhammer symbols

$$M(a,b,x) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n}\frac{x^n}{n!}, \tag{A.17}$$

A.3 Hermite functions:

$$H_{2n}(x) = (-1)^n \frac{(2n)!}{n!} M(-n,1/2,x^2) \tag{A.18}$$

$$H_{2n+1}(x) = (-1)^n \frac{2(2n+1)!}{n!} xM(-n,3/2,x^2) \tag{A.19}$$

Appendix B: Calculation details

B.1 The general form of wave operator matrix for Jacobi basis

The first derivatives of (3.1.1) is

$$\frac{d\phi_n}{dy} = A_n (1-y)^{\alpha} (1+y)^{\beta} \left\{ \frac{dP_n^{(\mu,\nu)}(y)}{dy} + \left(\frac{\beta}{1+y} - \frac{\alpha}{1-y} \right) P_n^{(\mu,\nu)}(y) \right\} \tag{B.1}$$

Using (A.3) and substitute in (B.1)

$$\frac{d\phi_n}{dy} = \left[\frac{\beta}{1+y} - \frac{\alpha}{1-y} - \frac{n}{\left(1-y^2\right)} \left(y + \frac{\nu-\mu}{2n+\mu+\nu} \right) \right] \phi_n(y) + \frac{2}{\left(1-y^2\right)} \frac{(n+\mu)(n+\nu)}{2n+\mu+\nu} \frac{A_n}{A_{n-1}} \phi_{n-1}(y) \tag{B.2}$$

The second derivative of (B.1):

$$\frac{d^2\phi_n}{dy^2} = A_n (1-y)^{\alpha} (1+y)^{\beta} \left\{ \frac{d^2}{dy^2} + \left(\frac{2\beta}{(1+y)} - \frac{2\alpha}{(1-y)} \right) \frac{d}{dy} + \frac{\alpha(\alpha-1)}{(1-y)^2} + \frac{\beta(\beta-1)}{(1+y)^2} \right.$$

$$\left. - \frac{2\alpha\beta}{(1-y)(1+y)} \right\} P_n^{(\mu,\nu)}(y) \tag{B.3}$$

Using (A.2), and $\frac{y}{\left(1-y^2\right)} = \frac{1}{2}\left(\frac{1}{(1-y)} - \frac{1}{(1+y)} \right)$, then

$$\frac{d^2\phi_n}{dy^2} = A_n (1-y)^{\alpha} (1+y)^{\beta} \frac{1}{(1-y^2)} \left\{ \left[\frac{(\mu+1-2\alpha)}{(1-y)} - \frac{(\nu+1-2\beta)}{(1+y)} \right] (1-y^2) \frac{d}{dy} \right.$$

$$\left. -n(n+\mu+\nu+1) + \alpha(\alpha-1)\frac{(1+y)}{(1-y)} + \beta(\beta-1)\frac{(1-y)}{(1+y)} - 2\alpha\beta \right\} P_n^{(\mu,\nu)}(y) \qquad \text{(B.4)}$$

Using (A.3)

$$(1-y^2)\frac{d^2\phi_n}{dy^2} = \left[-n(n+\mu+\nu+1) - 2\alpha\beta - n\left(y + \frac{\nu-\mu}{2n+\mu+\nu} \right) \left(\frac{(\mu+1-2\alpha)}{(1-y)} - \frac{(\nu+1-2\beta)}{(1+y)} \right) \right.$$
$$\left. + \alpha(\alpha-1)\frac{(1+y)}{(1-y)} + \beta(\beta-1)\frac{(1-y)}{(1+y)} \right] \phi_n(y) + 2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu} \times$$
$$\left(\frac{(\mu+1-2\alpha)}{(1-y)} - \frac{(\nu+1-2\beta)}{(1+y)} \right) \frac{A_n}{A_{n-1}} \phi_{n-1}(y) \qquad \text{(B.5)}$$

Using these derivatives (B.2) and (B.5) the action of the wave operator (3.1.4) on the basis element will be as follows:

$$\frac{-(1-y^2)}{(y')^2} J|\phi_n\rangle$$
$$= \left[-n(n+\mu+\nu+1) - 2\alpha\beta - n\left(y + \frac{\nu-\mu}{2n+\mu+\nu} \right) \left(\frac{(\mu+1-2\alpha)}{(1-y)} - \frac{(\nu+1-2\beta)}{(1+y)} \right) + \alpha(\alpha-1)\frac{(1+y)}{(1-y)} \right.$$
$$\left. + \beta(\beta-1)\frac{(1-y)}{(1+y)} + (1-y^2)\left[\frac{\beta}{1+y} - \frac{\alpha}{1-y} - \frac{n}{(1-y^2)}\left(y + \frac{\nu-\mu}{2n+\mu+\nu} \right) \right] \frac{y''}{(y')^2} - \frac{U(y)(1-y^2)}{(y')^2} \right] \phi_n(y)$$
$$+ 2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu} \left[\frac{y''}{(y')^2} + \left(\frac{(\mu+1-2\alpha)}{(1-y)} - \frac{(\nu+1-2\beta)}{(1+y)} \right) \right] \frac{A_n}{A_{n-1}} \phi_{n-1}(y) \qquad \text{(B.6)}$$

Now, for simple algebra, much attention should be paid to y', that must be compatible with the weight function $w(y)$ of the basis, where $\phi_n(y) = A_n w(y) P_n(y)$ and the integration measure is given as $\langle \phi_m | F(y) | \phi_n \rangle = A_m A_n \int_{-1}^{+1} w(y) P_m^{\mu,\nu}(y) F(y) P_n^{\mu,\nu}(y) \frac{dy}{y'}$.

Since the weight function of the Jacobi polynomials $w(y) = (1-y)^{\alpha}(1+y)^{\beta}$, then, compatibility with the solution of this function, we require that $y' = \lambda(1-y)^{a}(1+y)^{b}$, which puts a big constant and limitation on the transformations.

Thus, generally, where $y' = \lambda(1-y)^{a}(1+y)^{b}$, then we can use that $y'' = y'^{2}\left(\frac{b}{1+y} - \frac{a}{1-y}\right)$. Then, the J-matrix can be written as

$$
\begin{aligned}
&-J|\phi_n\rangle = \\
&\frac{(y')^2}{(1-y^2)}\left\{\left[-n(n+\mu+\nu+1) - 2\alpha\beta - \alpha b - \beta a - n\left(y + \frac{\nu-\mu}{2n+\mu+\nu}\right)\left(\frac{(\mu+1-a-2\alpha)}{(1-y)}\right.\right.\right. \\
&\left.\left.\left. - \frac{(\nu+1-b-2\beta)}{(1+y)}\right) + \alpha(\alpha+a-1)\frac{(1+y)}{(1-y)} + \beta(\beta+b-1)\frac{(1-y)}{(1+y)} - \frac{U(y)(1-y^2)}{(y')^2}\right]\phi_n(y)\right. \\
&\left. + 2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\left(\frac{(\mu+1-a-2\alpha)}{(1-y)} - \frac{(\nu+1-b-2\beta)}{(1+y)}\right)\frac{A_n}{A_{n-1}}\phi_{n-1}(y)\right\} \qquad \text{(B.7)}
\end{aligned}
$$

Where the integration measure is $\int_{x_-}^{x_+} .....dx = \int_{-1}^{+1} ... \frac{dy}{y'}$,

Then, $\langle \phi_m | \phi_n \rangle = \int_{-1}^{+1} \phi_m(y) \phi_n(y) \frac{dy}{y'} = A_m A_n \int_{-1}^{+1} (1-y)^{2\alpha}(1+y)^{2\beta} P_n^{(\mu,\nu)}(y) P_m^{(\mu,\nu)}(y) \frac{dy}{y'}$

The J-Matrix element reads as $J_{m,n}=\langle\phi_m|J|\phi_n\rangle=\int_{-1}^{+1}\phi_m(y)(J)\phi_n(y)\frac{dy}{y'}$

$$-J_{m,n}=\lambda\int_{-1}^{+1}(1-y)^{a-1}(1+y)^{b-1}\phi_m(y)\times$$
$$\left\{\left[-n(n+\mu+\nu+1)-2\alpha\beta-\alpha b-\beta a-n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)\left(\frac{(\mu+1-a-2\alpha)}{(1-y)}-\frac{(\nu+1-b-2\beta)}{(1+y)}\right)\right.\right.$$
$$\left.+\alpha(\alpha+a-1)\frac{(1+y)}{(1-y)}+\beta(\beta+b-1)\frac{(1-y)}{(1+y)}-\frac{U(y)}{\lambda^2}(1-y)^{1-2a}(1+y)^{1-2b}\right]\phi_n(y)$$
$$\left.+2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\left(\frac{(\mu+1-a-2\alpha)}{(1-y)}-\frac{(\nu+1-b-2\beta)}{(1+y)}\right)\frac{A_n}{A_{n-1}}\phi_{n-1}(y)\right\}dy \qquad \text{(B.8)}$$

In terms of $P_n^{(\mu,\nu)}(y)$ and $P_{n-1}^{(\mu,\nu)}(y)$ where $\phi_n(y)=A_n(1-y)^{\alpha}(1+y)^{\beta}P_n^{(\mu,\nu)}(y)$, $\phi_{n-1}(y)=A_{n-1}(1-y)^{\alpha}(1+y)^{\beta}P_{n-1}^{(\mu,\nu)}(y)$, then the J-Matrix has the following general form

$$J_{m,n}=\lambda A_m A_n\int_{-1}^{+1}(1-y)^{2\alpha+a-1}(1+y)^{2\beta+b-1}P_m^{\mu,\nu}(y)\left\{\left[n(n+\mu+\nu+1)+2\alpha\beta+\alpha b+\beta a\right.\right.$$
$$+n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)\left(\frac{\mu+1-a-2\alpha}{(1-y)}-\frac{\nu+1-b-2\beta}{(1+y)}\right)-\alpha(\alpha+a-1)\frac{(1+y)}{(1-y)}$$
$$\left.-\beta(\beta+b-1)\frac{(1-y)}{(1+y)}+\frac{U(y)}{\lambda^2}(1-y)^{1-2a}(1+y)^{1-2b}\right]P_n^{\mu,\nu}(y)-2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\times$$
$$\left.\left(\frac{\mu+1-a-2\alpha}{(1-y)}-\frac{\nu+1-b-2\beta}{(1+y)}\right)P_{n-1}^{\mu,\nu}(y)\right\}dy \qquad \text{(B.9)}$$

B.2 The general form of the wave operator matrix for Laguerre basis

The first derivatives of (3.1.3)

$$\frac{d\phi_n}{dy} = A_n y^{\alpha} e^{-\beta y} \left\{ \frac{d}{dy} + \frac{\alpha}{y} - \beta \right\} L_n^{\nu}(y) \tag{B.10}$$

Using (A.12):

$$y\frac{d\phi_n}{dy} = \left[n + \alpha - \beta y \right] \phi_n(y) - (n+\nu) \frac{A_n}{A_{n-1}} \phi_{n-1}(y) \tag{B.11}$$

For the second derivative of (B.10):

$$\frac{d^2\phi_n}{dy^2} = A_n y^{\alpha} e^{-\beta y} \left\{ \frac{d^2}{dy^2} + 2\left(\frac{\alpha}{y} - \beta \right) \frac{d}{dy} + \frac{\alpha(\alpha-1)}{y^2} - \frac{2\alpha\beta}{y} + \beta^2 \right\} L_n^{\nu}(y) \tag{B.12}$$

Using (A.11) and substitute in (B.12)

$$\frac{d^2\phi_n}{dy^2} = A_n y^{\alpha} e^{-\beta y} \left\{ \left(\frac{y - \nu - 1 + 2\alpha}{y} - 2\beta \right) \frac{d}{dy} - \frac{n}{y} + \frac{\alpha(\alpha-1)}{y^2} - \frac{2\alpha\beta}{y} + \beta^2 \right\} L_n^{\nu}(y)$$

Using (A.12), then

$$y\frac{d^2\phi_n}{dy^2} = \left[\beta^2 y - n - 2\alpha\beta + \frac{\alpha(\alpha-1)}{y} + n\left(1 - 2\beta + \frac{2\alpha - \nu - 1}{y} \right) \right] \phi_n(y)$$

$$-(n+\nu)\left(1 - 2\beta + \frac{2\alpha - \nu - 1}{y} \right) \frac{A_n}{A_{n-1}} \phi_{n-1}(y) \tag{B.13}$$

Using these derivatives (B.11) and (B.13) the action of the wave operator (3.1.4) on the basis element will be as follows:

$$-J\left|\phi_n\right\rangle=\frac{\left(y'\right)^2}{y}\times\left\{\left[\beta^2 y-n-2\alpha\beta+\frac{\alpha\left(\alpha-1\right)}{y}+n\left(1-2\beta+\frac{2\alpha-\nu-1}{y}\right)\right.\right.$$

$$\left.\left.+\left[n+\alpha-\beta y\right]\frac{y''}{\left(y'\right)^2}-\frac{U(y)y}{\left(y'\right)^2}\right]\phi_n\left(y\right)-(n+\nu)\frac{A_n}{A_{n-1}}\left[\frac{y''}{\left(y'\right)^2}+\left(1-2\beta+\frac{2\alpha-\nu-1}{y}\right)\right]\phi_{n-1}\left(y\right)\right\} \tag{B.14}$$

A similar explanation about the potential form of y' that are compatible with the Laguerre weight function that should be given as $y'=\lambda y^a e^{by}$, then we can use that $y''=y'^2\left(\frac{a}{y}+b\right)$, thus the J-matrix can be written as:

$$-J_{m,n}=\int_0^\infty \lambda y^{a-1}e^{by}\phi_m\left(y\right)\times$$

$$\left\{\left[n-b\alpha+a\beta+2\alpha\beta-\beta\left(\beta-b\right)y-\frac{\alpha\left(\alpha+a-1\right)}{y}-n\left(1+b-2\beta+\frac{2\alpha-\nu+a-1}{y}\right)\right.\right.$$

$$\left.\left.+U(y)\frac{y^{1-2a}e^{-2by}}{\lambda^2}\right]\phi_n\left(y\right)+(n+\nu)\frac{A_n}{A_{n-1}}\left(1+b-2\beta+\frac{2\alpha-\nu+a-1}{y}\right)\phi_{n-1}\left(y\right)\right\}dy \tag{B.15}$$

In terms of $L_n^\nu\left(y\right)$ and $L_{n-1}^\nu\left(y\right)$, where $\phi_n(y)=A_n y^\alpha e^{-\beta y}L_n^\nu(y)$, $\phi_{n-1}(y)=A_{n-1}y^\alpha e^{-\beta y}L_{n-1}^\nu(y)$, then the J-Matrix has the following general form

$$J_{m,n} = \lambda A_m A_n \int_0^\infty y^{2\alpha+a-1} e^{-(2\beta-b)y} L_m^\nu(y) \Bigg[n - b\alpha + a\beta + 2\alpha\beta - \beta(\beta-b)y - \frac{\alpha(\alpha+a-1)}{y}$$

$$-n\left(1+b-2\beta+\frac{2\alpha-\nu+a-1}{y}\right)+U(y)\frac{y^{1-2a}e^{-2by}}{\lambda^2}\Bigg] L_n^\nu(y)dy + A_m A_n(n+\nu)\times$$

$$\int_0^\infty y^{2\alpha+a-1} e^{-(2\beta-b)y} L_m^\nu(y)\left(1+b-2\beta+\frac{2\alpha-\nu+a-1}{y}\right) L_{n-1}^\nu(y)dy \qquad \text{(B.16)}$$

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