TWO DIMENSIONAL J-MATRIX APPROACH TO QUANTUM SCATTERING

BY

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All dedication is to Allah, the Almighty, for making this work a success.

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ABSTRACT

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We present an extension of the J-matrix method of scattering to two dimensions in cylindrical coordinates. In the J-matrix approach we select a zeroth order Hamiltonian, H_0, which is exactly solvable in the sense that we select a square integrable basis set that enable us to have an infinite tridiagonal representation for H_0. Expanding the wavefunction in this basis makes the wave equation equivalent to a three-term recursion relation for the expansion coefficients. Consequently, finding solutions of the recursion relation is equivalent to solving the original H_0 problem (i.e., determining the expansion coefficients of the system's wavefunction).

The part of the original potential interaction which cannot be brought to an exact tridiagonal form is cut in an NxN basis space and its matrix elements are computed numerically using Gauss quadrature approach. Hence, this approach embodies powerful tools in the analysis of solutions of the wave equation by exploiting the intimate connection and interplay between tridiagonal matrices and the theory of orthogonal polynomials. In such analysis, one is at liberty to employ a wide range of well established

methods and numerical techniques associated with these settings such as quadrature approximation and continued fractions.

To demonstrate the utility, usefulness, and accuracy of the extended method we use it to obtain the bound states for an illustrative short range potential problem.

ملخص الرسالة

الاسم الكامل: إسماعيل أديوال أولومقيبون

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نقدم في هذه الدراسة امتدادا لنهج مصفوفة J ثنائية البعد للتشتت الكمي في الإحداثيات الاسطوانية . في نهج المصفوفة J نختار هاميلتون من الدرجة الصفرية ، H_0 ، وهي قابلة للحل تماماً، بمعنى أن نختار أساساً مربعاً قابلاً للتكامل يمكننا أن يكون هناك تمثيل لا نهائي للهاميلتون H_0 . إن توسيع دالة الموجة على هذا الأساس يجعل معادلة الموجة تكافيء علاقة الإعادة ثلاثية الحدود لمعاملات التوسع. وبالتالي، فإن إيجاد حلول لعلاقة الإعادة هذه يكافيء حل مشكلة H_0 الأصلية (أي تحديد معاملات توسيع دالة الموجة للنظام).

وبالنسبة للأجزاء الأصلية من التفاعل التي لا يمكن جلبها إلى الشكل المحدد فإنه يتم قطعها في الفضاء على الأساس أساس N x N ويتم احتساب عناصر المصفوفة لها عددياً باستخدام نهج غاوس التربيعي. وبالتالي، فإن هذا النهج يجسد أدوات قوية في تحليل الحلول للمعادلة الموجية من خلال استغلال العلاقة

الوثيقة والتفاعل بين المصفوفات والنظرية متعددة الحدود المتعامدة. في مثل هذا التحليل، يستطيع الفرد توظيف مجموعة واسعة من أساليب راسخة، وتقنيات رقمية مرتبطة بهذه الإعدادات، مثل التقريب التربيعي والكسور المتصلة.

للتدليل على فائدة ، ودقة الأسلوب الذي نتبعه للطريقة الموسعة، فإننا نستخدمه للحصول على الحالات المحدودة لمسألة توضيحية ذات مدى قصير.

CHAPTER 1

INTRODUCTION

Theoretically, steady state solution of scattering problem can be obtained by solving the time-independent energy eigenvalue equation $(H-E)|\chi\rangle=0$, where H represents the Hamiltonian operator and E the positive continuous energy. It is a difficult challenge to solve the eigenvalue equation analytically for dynamic system in general. Only matrix diagonalization gives all possible eigenvalues, but fails to produce scattering states solution. This anomaly led to the emergence of the tri-diagonalization approach upon which the J-matrix method is built.

J-matrix is an algebraic technique suitable for solving eigenvalue problems and obtaining scattering information by employing the square integrability of the orthogonal polynomials. It deals with the reference Hamiltonian analytically, and solves the potential matrix element approximately using numerical approach. Also, the square integrable bases chosen must support a tridiagonal matrix representation. This idea gives strength to the J-matrix approach as a good computational tool. It is this basis that provides the parameters needed to ensure stability, convergence, and accuracy of the computational procedure.

The J-matrix method in three dimensional form was originally introduced in 1974 [1-2], and has since undergone several developments over the years. Some of the notable developments include:

1. Relativistic generalization of the J – matrix method by Horodecki [3] and its refinement by Alhaidari et al. [4]
2. Yamani et al. generalized the J-matrix method to any convenient L^2 – basis [5]
3. The case of long range potential was done by Vanroose et al. [6] with the introduction of additional term in the three term recursion relation which takes into account the asymptotic behavior of the potential.
4. Alhaidari et al. [7] presented the integration approach as an alternative to the classical differential approach for regularization of the reference problem. They also made notable developments and applications in [8], [9], [10].

In 2009, Alhaidari et al. developed the J-matrix formalism in one dimension [11]. Owing to the achievement in one and three dimensions, it sets the stage and motivates us to proceed in evolving the J-matrix formalism in two dimensions. This way, we would complete the J-matrix formalism in all physical dimensions.

There has been tremendous interest in two dimensional systems in recent years especially with the experimental realization of Graphene in 2004 [12]. Theoretical treatment of such two dimensional systems which include potential scattering theory, has greatly increased. Recently, Schneider et al. discussed the resonant scattering in Graphene based on the matrix green function formalism [13]. An important question of topological concern in two dimensional systems is the effect of the number of spacial dimensions. The advantage of a two dimensional space can be seen in the case of Poisson's equation for a point charge, which is solved for $(\ln r)$ in two dimensions with a stronger singularity at the origin rather than the r^{-1} in three dimensions.

1.1 Objectives of the study

We extend the J-matrix method of scattering to two dimensions with cylindrical symmetry, determine its tridiagonal representation, and obtain the bound states, resonances, and scattering phase shift for an illustrative problem. The main objectives to be achieved in this study are listed below.

Objective 1: To determine the regular solution of the J-matrix reference problem in Laguerre and oscillator basis. This is termed the Sine-like solution

Objective 2: J-matrix regularization of the irregular reference solution in Laguerre and oscillator basis. This is termed the Cosine-like solution.

Objective 3: Calculating the matrix element of the scattering potential using gauss quadrature.

Objective 4: Numerical computation of bound state and resonances for a short range potential.

Objective 5: Study of scattering through a short range potential and evaluation of the associated phase shift

CHAPTER 2

LITERATURE REVIEW

To comprehend the nature and dynamics of subatomic systems, there is need to carry out scattering experiments. A scattering experiments, where flux of particles is uniformly directed towards the target we seek to understand. The flux of radiation scattered off an obstacle, with the scattered radiation containing the relevant information about the system under study. A theory of potential scattering formulation is needed to study and analyze scattering experiments.

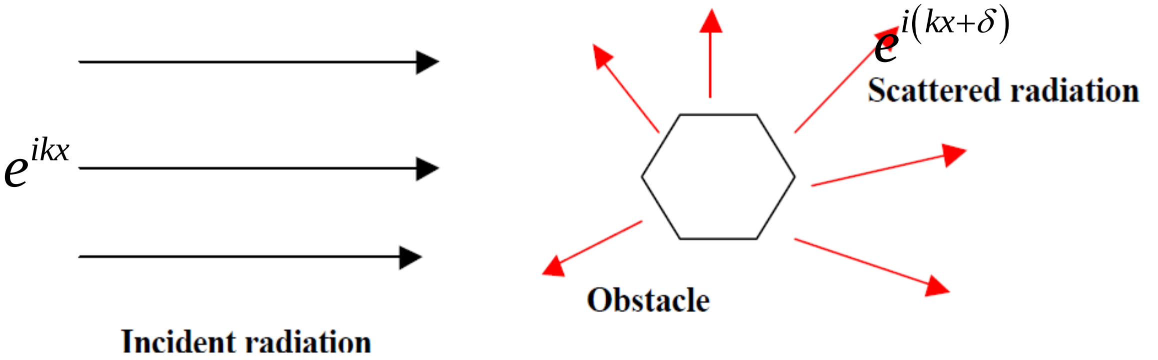

Figure 2.1: Schematic diagram of a typical scattering experiment

A potential function is configured in a manner that it models the scattering system (e.g target nuclei). The proposed model is then checked against the experimental results. The characteristic feature of such a potential function is that its range must be finite, so that it is zero in the asymptotic region. Owing to the freedom of the incident and scattered particles, it then only makes sense to represent them with sinusoidal wave functions, whose phase difference (phase shift) is the carrier of information for the scattering system. Mathematically, we can represent the solution of the free wave equation by two independent sinusoidal functions like sin(kx) and cos(kx + δ), with x representing the space of configuration. The phase shift δ dependents on angular momentum and the model potential parameter and energy.

For a large class of physical models, the Hamiltonian can be decomposed into the sum of two components, namely the reference Hamiltonian, H_0 and the potential V, such that $H = H_0 + V$. The reference Hamiltonian is simple; possess an infinite range and a high degree of symmetry, it can thus be solved analytically. For the potential, it can either be solved by perturbation methods if its contribution is infinitesimal or by algebraic methods if it is limited to a region confined in function or configuration space. For the class of scattering problems to be examined, it is assumed that the potential will vanish at the asymptotic region that is beyond the finite region. As a result, the solution to the problem can be obtained by solving the reference wave equation $(H_0 - E)|\psi\rangle = 0$. Using the algebraic scattering method, the kinematic solution of the reference Hamiltonian is obtained by calculating the matrix components of the operators in a complete set of square integrable bases. The two asymptotic solutions of the reference Hamiltonian are written as infinite series of square integrable basis functions that are in equivalence with the Hamiltonian's domain. The basis however, is required to support a tridiagonal matrix with infinite representation of the wave operator. This sort of Tridiagonalization creates a regular solution space. This special basis, when extended to infinite space, will produce continuous value of energy, which is an important requirement for quantum scattering. In addition, the solution of the reference Hamiltonian is obtained as an orthogonal polynomial which obeys three term recursion relations based on the infinite tridiagonal matrix representation.

2.1 Basis set technique and diagonalization

The Evolution of fast computing machines has made it possible to perform structural calculations in both nuclear and atomic systems. The Hamiltonian of such systems is represented by a matrix using a finite bound state like basis. The matrix so constructed is then diagonalized to yield discrete energy eigenvalues and eigenfunctions which approximated the energy spectrum of the system and the resulting discrete state's wave function. The problem with the use of diagonalization is that it only provides us with information on discrete states and not on the continuous spectrum of the Hamiltonian. This led theorist to believe that the basis set technique could not be used for the purpose of extracting scattering information.

However, the work of Hazi and Taylor [14] gave a glimpse of hope by expanding a set of discrete exponentially decaying function followed by diagonalization of the Hamiltonian to describe resonances. Their approach is called the "stabilization method", where they stabilize real discrete eigenvalues around the resonance energy by varying the computational parameters. The stabilization method produced good approximations around the resonant energies regions. Although the work of Hazi and Taylor was based on a one dimensional potential model, stabilization method has accurately obtained resonance energies of ideal systems like e^- and H_2 [15].

Building on the stabilization technique, the Reinhardt group at Harvard was able to obtain scattering information from discrete eigenvalues of both the reference and scattering Hamiltonian [16]. They were able to accurately obtain scattering results using the assumption that if the basis $\{\phi_n\}_{n=0}^{N-1}$ is a certain Laguerre function, then the abscissas fall as the transformed zeros of an orthogonal polynomial with known properties [17]. This ensures that the discrete eigenfunctions of the finite N X N Hamiltonian H_o, can be expressed as a finite sum of L^2 basis as

$$|\psi_N(E)\rangle = B_N(E)\sum_{n=0}^{N-1} P_n(E)|\phi_n\rangle \tag{2.1.1}$$

Where $P_n(E)$ is an orthogonal polynomial.

Heller and Yamani of the Harvard group proposed that the potential be represented by a finite subset of complete basis. This idea gave birth to the J–matrix method. The name arose from the fact that the operator J = H_o – E in either Laguerre or oscillator basis function is Tridiagonal.

2.2 Orthogonal polynomials and recursion relation

Let $\{P_n(x)\}_{n=0}^{\infty}$ be a complete set of orthogonal polynomials in the space with coordinate $x \in [a,b] \subset \Re$. Orthogonality can be defined in terms of the weight function $\rho(x)$ as

$$\int_a^b \rho(x) p_n(x) p_m(x) dx = \delta_{mn} \tag{2.2.1}$$

and $p_n(x)$ is a polynomial of degree n in x. These polynomials satisfy the following symmetric three-term recursion relation.

$$x p_n(x) = a_n p_n(x) + b_{n-1} p_{n-1}(x) + b_n p_{n+1}(x) \qquad ; \quad n \geq 0, \quad b_{-1} \equiv 0 \tag{2.2.2}$$

together with the initial condition $p_0(x) = 1$. The "recursion coefficient" $\{a_n, b_n\}$ are elements of $\Re$. Associated with these orthogonal polynomials is the following infinite dimensional real tridiagonal symmetric matrix.

$$H = \begin{pmatrix} a_0 & b_0 & & & & & \\ b_0 & a_1 & b_1 & & & & \\ & b_1 & a_2 & b_2 & & & \\ & & b_2 & a_3 & x & & \\ & & & x & x & x & \\ & & & & x & x & x \\ & & & & & x & x \end{pmatrix} \tag{2.2.3}$$

The recursion relation (2.2.2) could be written as the matrix eigenvalue equation, $x|p\rangle = H|p\rangle$. For numerical implementations, however, the space is reduced to a finite space in N dimension spanned by $\{P_n(x)\}_{n=0}^{N-1}$. The resulting tridiagonal matrix in (2.2.3) yields a finite NXN matrix. The set of real eigenvalues of this matrix, $\{\varepsilon_n\}_{n=0}^{N-1}$, are called the zeros of the polynomial $p_N(x)$, that is, $p_N(\varepsilon_n) = 0$. In this setting, Gauss quadrature integral approximation of a function f(x) that belongs to L^2 [a, b] states that

$$\int_a^b \rho(x) f(x) dx \cong \sum_{n=0}^{N-1} \omega_n f(\varepsilon_n) \qquad (2.2.4)$$

The “numerical weight”, ω_n, is the square of the zero component of the normalized eigenvector of H, $\{\Lambda_{mn}\}_{m=0}^{N-1}$, associated with the eigenvalue ε_n. That is $\omega_n = \Lambda_{0n}^2$, where $\mathrm{H}|\Lambda_n\rangle = \varepsilon_n |\Lambda_n\rangle$.

2.3 Tridiagonal Physics: J-matrix method

The J-matrix method is a process of tridiagonalization where a linear operator, which can be a differential or difference operator acts on a function space given by a set of linearly independent function $\{f_n\}_{n=0}^{\infty}$ with the operator L acting tridiagonally on these functions $\{f_n\}_{n=0}^{\infty}$. That is

$$\begin{aligned} Lf_n &= A_n f_{n+1} + B_n f_n + C_n f_{n-1}, \qquad n \geq 1 \\ Lf_0 &= A_0 f_1 + B_0 f_0 \end{aligned} \qquad (2.3.1)$$

where A_n, B_n, C_n are constants for all $(n \in \mathrm{N})$

The two above equations can be combined with the assumption that $C_0 = 0$. It can then be said that $\sum_{n=0}^{\infty} p_n(z) y_n$ is a formal eigenfunctions of L for the eigenvalue z if p_n obeys

$$zp_n(z) = C_{n+1} p_{n+1}(z) + B_n p_n(z) + A_{n-1} p_{n-1}(z) \qquad (2.3.2)$$

for n ϵ N and $A_{-1} = 0$. In case $C_n \neq 0$ for $n \geq 1$, the recursion relation can be used to find $P_n(z)$ as a polynomial of degree n in z by defining $P_0(z) = 1$. This measure can provide relevant information on L if $\{y_n\}^{\infty}_{n=0}$ gives a basis for the function space on which L acts.

Tridiagonalization also provides information on eigenvalue, bound states etc. The Tridioagonal relation is a three term recursion relation, and the works of [18], [19], [20], [21], [22] has established the relationship between three term recursion relation and orthogonal polynomials. This background forms the basis of J-matrix approach. The work of Al-Salam and Chihara [23] also explained that if $\left\{ f_n \right\}_{n=0}^{\infty}$ is a class of orthogonal polynomial with differential relation

$$G(x)\frac{df_n(x)}{dx} = A_n f_{n+1}(x) + B_n f_n(x) + C_n f_{n-1}(x) \tag{2.3.3}$$

where $G(x)$ is a polynomial of degree ≤ 2, then the function f_n is either Jacobi, Laguerre or Hermite polynomials:

$$\begin{aligned}
&\left(1-x^2\right)\frac{d}{dx}P_n^{(\alpha,\beta)}(x) = A_n^{(\alpha,\beta)}P_{n+1}^{(\alpha,\beta)}(x) + B_n^{(\alpha,\beta)}P_n^{(\alpha,\beta)}(x) + C_n^{(\alpha,\beta)}P_{n-1}^{(\alpha,\beta)}(x) \\
&x\frac{d}{dx}L_n^{(\alpha)}(x) = nL_n^{(\alpha)}(x) - (n+\alpha)L_{n-1}^{(\alpha)}(x) \\
&\frac{d}{dx}H_n(x) = 2nH_{n-1}(x)
\end{aligned} \tag{2.3.4}$$

Where $P_n^{(\alpha,\beta)}(x)$, $L_n^{(\alpha)}(x)$, $H_n(x)$ denote Jacobi, Laguerre, and Hermite polynomials respectively.

2.4 The computational tools of the J-matrix method

If we consider a scattering system of incident particles and structureless targets with a total Hamiltonian H can be represented by a time-independent Schrodinger wave equation $(H-E)|\chi\rangle=0$, where $|\chi\rangle$ is the wavefunction. If the total Hamiltonian is broken into two components, such that

$$H=H_\infty+V \tag{2.4.1}$$

where H_∞ is the free Hamiltonian and V, the potential. The free Hamiltonian is considered to be the Hamiltonian of the system describing infinite separation of the incident particle from the target where V = 0.

If we assume that V is composed of two parts, such that

$$V=V_0+\tilde{V} \tag{2.4.2}$$

Where V_0 is the analytical part and $\tilde{V}$ the short range potential, which when added to the free Hamiltonian gives the reference Hamiltonian

$$H_0=V_0+H_\infty \tag{2.4.3}$$

which can be represented by a tridiagonal matrix using a proper L^2 basis, $\{|\varphi_n\rangle\}_{n=0}^{\infty}$.

Expanding the wavefunction $|\chi\rangle$ in terms of this complete basis, especially for the case of bound state determination,

$|\chi\rangle = \sum_n a_n |\varphi_n\rangle$, with the wavefunction energy-normalized as

$$\langle \chi(E) | \chi(E') \rangle = \delta(E - E') \tag{2.4.4}$$

However, in scattering phenomena, this approach does not necessarily give a solution to the Schrodinger equation. Nonetheless, by taking the short range potential to be zero ($H=H_0$), we can find in the basis, a state $|\psi\rangle$ so that

$$\langle \varphi_n | (H_0 - E) | \psi \rangle = 0 \quad \text{For all n.} \tag{2.4.5}$$

is satisfied outside a dense region of space, Ω^V, around $\tilde{V}$. An important condition for the selection of a suitable basis, is the fact that the operator $J = H_0 - E$ must be Tridiagonal or Jacobian. Tridiagonal, in this sense, means that $\langle \varphi_n | (H_0 - E) | \varphi_m \rangle = 0$ where $|n - m| > 1$. By expanding the basis $|\psi\rangle$ in the basis set $\{\varphi_n\}$, such that $|\psi\rangle = a_m |\varphi_m\rangle$ we can rewrite 2.4.5 as

$$\sum_m \langle \varphi_n | (H_0 - E) | \varphi_m \rangle a_m = 0 \text{ or } \sum_m J_{nm} a_m = 0 \text{ for all n.} \tag{2.4.6}$$

where J_{nm} represents the tridiagonal matrix of H_0-E in the basis set $\{\varphi_n\}$. J_{nm} can be used to express a recursion relation for a specific H_0 and $\{\varphi_n\}$ in terms of a_n and $a_{n\pm 1}$, such that we have

$$J_{n,n-1} a_{n-1} + J_{n,n} a_n + J_{n,n+1} a_{n+1} = 0 \text{ for n>1} \tag{2.4.7}$$

$$J_{00} a_0 + J_{01} a_1 = 0$$

The nature of Solution to the tridiagonal recursion equations is arrived at by considering H_0 as characteristically second order operator, and as such there exists two independent solutions to the tridiagonal equation. In the asymptotic region, these two solutions behave like free particles i.e. sin(kr) and cos(kr), where $k = \sqrt{2E}$. If we consider the two solutions as

$$\left|S\right\rangle = \sum_n s_n \left|\varphi_n\right\rangle \qquad \left|C\right\rangle = \sum_n c_n \left|\varphi_n\right\rangle \tag{2.4.8}$$

where s_n and c_n are two sets of independent expansion coefficients. In the asymptotic region, $\lim_{r\to\infty}\left\langle r\middle|S\right\rangle = \sin(kr)$ $\qquad \lim_{r\to\infty}\left\langle r\middle|C\right\rangle = \cos(kr)$

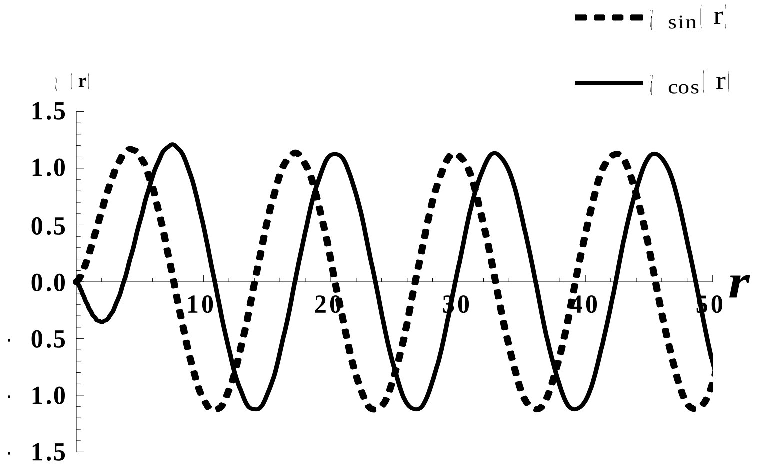

Fig. 2.2: Asymptotic plot of the sine-like and cosine-like solution for $\ell = 1$, $\lambda = 1$, $k = 0.5$ (atomic units)

However, at the origin, they behave differently. One solution $|S\rangle$ is regular everywhere, while the other solution $|C\rangle$ is irregular and blow up at the origin.

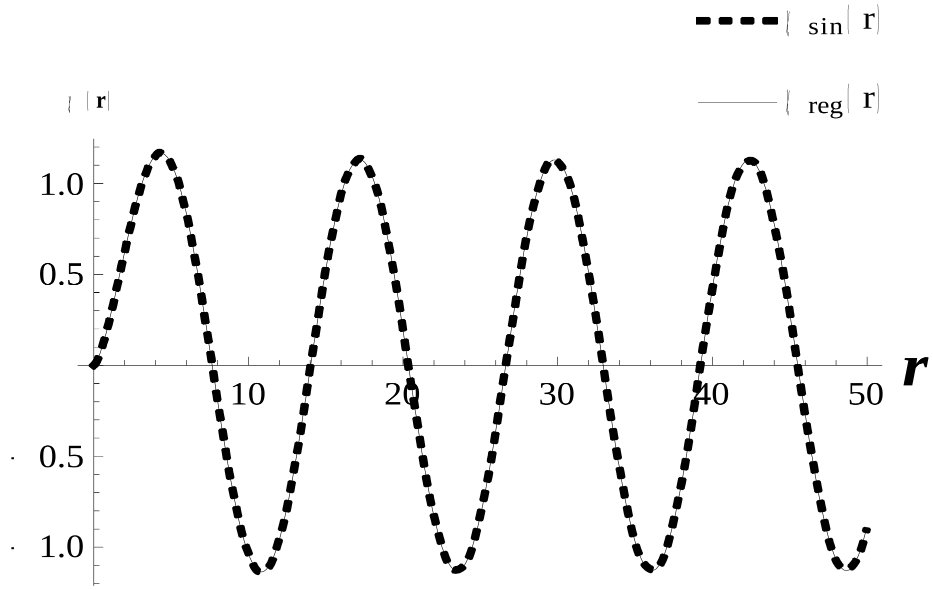

Fig. 2.3: Plot of the sine-like, and regular solutions for $\ell = 1$, $\lambda = 1$, $k = 0.5$ (atomic units)

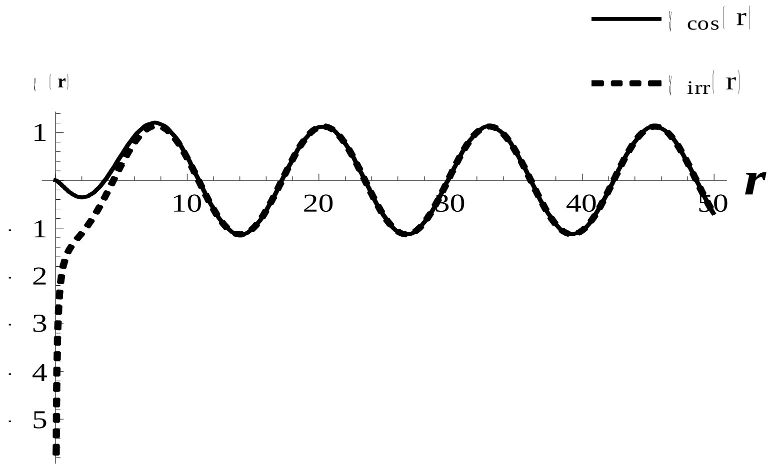

Fig. 2.4: Plot of the cosine-like and irregular solutions for $\ell = 1$, $\lambda = 1$, $k = 0.5$ (atomic units)

The regular solution is expanded in terms of the basis set $\{s_n\}$, and solved with the conditions that it satisfies the tridiagonal recursion relation and $\langle \varphi_n | (H_0 - E) | S \rangle = 0$, for all n. The irregular solution however, is expanded in the basis set $\{c_n\}$, and regularized with that conditions that the first tridiagonal relation is satisfied and $J_{00}c_0 + J_{01}c_1 = \frac{ks_0}{2}$.

2.5 Phase-shift and S-matrix

The matrix representation of $\tilde{V}$ can be approximated in the dense subspace Ω^V, owing to its short range nature. This is done using the first N elements of the basis set $\{|\varphi_n\rangle\}_{n=0}^{N-1}$ for some large integer N, so that the potential is confined to an "N-box" as

$$\tilde{V}_{nm} = \begin{cases} \langle \varphi_n | \tilde{V} | \varphi_m \rangle & \text{n,m} \leq \text{N-1} \\ 0 & \text{otherwise} \end{cases} \qquad (2.5.1)$$

This kind of approximation is similar to one employed in the R-matrix theory of scattering, where the effectiveness of $\tilde{V}$ is confined to a configuration space box of radius R.

$$\tilde{V} = \begin{cases} \tilde{V}(r) & \text{r} \leq \text{R} \\ 0 & \text{otherwise} \end{cases} \qquad (2.5.2)$$

Seeking the phase shift of scattering using the J-matrix approach:

$$\sum_{n=0}^{\infty} \langle \phi_m | \left(J + V^N \right) | \phi_n \rangle = 0 \qquad (2.5.3)$$

The m = 0 term gives:

$$\left(J+V^{N}\right)_{0n} d_{n}=0, \quad \text{for} \quad n=0,1,2,\ldots,N-1$$

$$\left(J+V^{N}\right)_{00} a_{0}+\left(J+V^{N}\right)_{01} a_{1}+\ldots+\left(J+V^{N}\right)_{0,N-1} a_{N-1}=0 \quad (2.5.4)$$

The m = 1 term gives:

$$\left(J+V^{N}\right)_{10} a_{0}+\left(J+V^{N}\right)_{11} a_{1}+\ldots+\left(J+V^{N}\right)_{1,N-1} a_{N-1}=0 \quad (2.5.5)$$

The m = N-1 term gives:

$$\begin{aligned}&\left(J+V^{N}\right)_{N-1,0} a_{0}+\left(J+V^{N}\right)_{N-1,1} a_{1}+\ldots\\&+\left(J+V^{N}\right)_{N-1,N-1} a_{N-1}+J_{N-1,N}\left(s_{N}+tc_{N}\right)=0\end{aligned} \quad (2.5.6)$$

The m = N gives:

$$J_{N,N}\left(s_{N}+tc_{N}\right)+J_{N,N+1}\left(s_{N+1}+tc_{N+1}\right)+J_{N-1,N}a_{N-1}=0 \quad (2.5.7)$$

Thus,

$$\left(J_{N,N}s_{N}+J_{N,N+1}s_{N+1}\right)+t\left(J_{N,N}c_{N}+J_{N,N+1}c_{N+1}\right)+J_{N-1,N}a_{N-1}=0 \quad (2.5.8)$$

Let us write the three term recurrence relation for s_N and c_N:

$$J_{N,N-1}d_{N-1}+J_{N,N}d_{N}+J_{N,N+1}d_{N+1}=0; \quad \text{where } d_m = s_m \text{ or } c_m \quad (2.5.9)$$

Thus,

$$J_{N,N}c_{N}+J_{N,N+1}c_{N+1}=-J_{N,N-1}c_{N-1} \quad (2.5.10a)$$

$$J_{N,N}s_N + J_{N,N+1}s_{N+1} = -J_{N,N-1}s_{N-1} \tag{2.5.10b}$$

Using (2.5.10a), (2.5.10b) in (2.5.8) we get:

$$J_{N,N-1}a_{N-1} - J_{N,N-1}\left(s_{N-1} + tc_{N-1}\right) = 0 \tag{2.5.11}$$

Writing our (N+1) equations in matrix form:

$$\begin{pmatrix} (J+V)_{00} & (J+V)_{01} & \cdots & (J+V)_{0,N-1} & 0 \\ (J+V)_{10} & (J+V)_{11} & \cdots & (J+V)_{1,N-1} & 0 \\ \cdots & \cdots & \cdots\ \cdots & & \cdots \\ (J+V)_{N-2,0} & (J+V)_{N-2,1} & \cdots & (J+V)_{N-2,N-1} & 0 \\ (J+V)_{N-1,0} & (J+V)_{N-1,1} & \cdots & (J+V)_{N-1,N-1} & J_{N-1,N}c_N \\ 0 & 0 & \cdots & J_{N,N-1} & -J_{N,N-1}c_{N-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \cdots \\ a_{N-2} \\ a_{N-1} \\ t \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -J_{N-1,N}s_N \\ J_{N,N-1}s_{N-1} \end{pmatrix} \tag{2.5.12}$$

A system of (N+1) equations in (N+1) unknowns: $(a_0,a_1,\ldots,a_N;t)$.

We remark here that the first set of N-equations can be solved independently for $(a_0,a_1,\ldots,a_{N-1})$, then we use the value of a_{N-1} found in (2.5.11) to obtain the phase shift through $t = \tan\delta$

$$\left(H - E\Omega\right)\hat{a} = W;\ \Omega_{nm} = \langle \phi_m | \phi_n \rangle, \quad \hat{a} = \left(a_0, a_1, \ldots, a_{N-1}\right)^t \tag{2.5.13}$$

$$W = \begin{pmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ 0 \\ -J_{N-1,N}d_N \end{pmatrix}; \qquad d_N = s_N + tc_N \tag{2.5.14}$$

$$\hat{a} = \left(H - E\Omega\right)^{-1} W = GW\ ; \qquad G = \left(H - E\Omega\right)^{-1} \tag{2.5.15}$$

$$a_{N-1} = -G_{N-1,N-1} J_{N-1,N} d_N \qquad (2.5.16)$$

Using (2.5.16) in (2.5.11) and solving for t gives:

$$-J_{N,N-1}\left(G_{N-1,N-1} J_{N-1,N}\left(s_N + tc_N\right)\right) - J_{N,N-1}\left(s_{N-1} + tc_{N-1}\right) = 0 \qquad (2.5.17)$$

$$t = -\left(\frac{s_{N-1} + G_{N-1,N-1} J_{N-1,N} s_N}{c_{N-1} + G_{N-1,N-1} J_{N-1,N} c_N}\right) \qquad (2.5.18)$$

Since, $t = \tan\delta$, and $S = e^{2i\delta}$ then,

$$\tan\delta = \frac{\sin\delta}{\cos\delta} = \frac{1}{i}\frac{e^{i\delta} - e^{-i\delta}}{e^{i\delta} + e^{-i\delta}} = \frac{1}{i}\frac{e^{2i\delta} - 1}{e^{2i\delta} + 1} = \frac{1}{i}\frac{S-1}{S+1} \qquad (2.5.19)$$

$$\tan\delta = i\left(\frac{1-S}{1+S}\right) \qquad (2.5.20)$$

$$S = \frac{i - \tan\delta}{i + \tan\delta} \qquad (2.5.21)$$

But $\tan\delta = -\left(\frac{s_{N-1} + G_{N-1,N-1} J_{N-1,N} s_N}{c_{N-1} + G_{N-1,N-1} J_{N-1,N} c_N}\right)$

$$S = \frac{\left(c_{N-1} - is_{N-1}\right) + G_{N-1,N-1} J_{N-1,N}\left(c_N - is_N\right)}{\left(c_{N-1} + is_{N-1}\right) + G_{N-1,N-1} J_{N-1,N}\left(c_N + is_N\right)} \qquad (2.5.22)$$

Equation (2.5.22) is the same as equation (2.14) in the paper of Yamani & Abdelmonem [24]. Due to the fact that numerical computation and stability shows that $c_N + is_N$ blows up, we prefer to write (2.5.22) in terms of their ratios:

$$S=\frac{\left(c_{N-1}-is_{N-1}\right)}{\left(c_{N-1}+is_{N-1}\right)}\left(\frac{1+G_{N-1,N-1}J_{N-1,N}\,\dfrac{\left(c_{N}-is_{N}\right)}{\left(c_{N-1}-is_{N-1}\right)}}{1+G_{N-1,N-1}J_{N-1,N}\,\dfrac{\left(c_{N}+is_{N}\right)}{\left(c_{N-1}+is_{N-1}\right)}}\right) \tag{2.5.23}$$

Defining: $T_{N-1}\equiv\frac{\left(c_{N-1}-is_{N-1}\right)}{\left(c_{N-1}+is_{N-1}\right)}$ and $R_N^{\pm}\equiv\frac{\left(c_{N}\pm is_{N}\right)}{\left(c_{N-1}\pm is_{N-1}\right)}$

Thus,

$$S=T_{N-1}\left\{\frac{1+G_{N-1,N-1}J_{N-1,N}R_N^{-}}{1+G_{N-1,N-1}J_{N-1,N}R_N^{+}}\right\} \tag{2.5.24}$$

We recall that only G contains the scattering potential, so $G_{N-1,N-1}$ is the only dynamic factor. The factors T_{N-1}, $R_N^{\pm}$, and $J_{N-1,N}$ are kinematics related to the H_0-problem and are independent of V

2.6 The Numerical scheme

Solutions of Schrodinger equation for certain potentials have been studied in details over the years using several numerical and perturbative schemes since exact analytical solutions are non-existent. Several of these computational schemes for investigating electron scattering have focused on quantal methods [25]. In general, there are two class of numerical methods employed in electron scattering, namely the perturbation-series expansion and the non-perturbative close-coupling approach. The perturbation-series expansion is based on Born series variation, and has successfully been used for high energy collision. But, the close-coupling expansion is based on the basis set technique, and used to simulate low energy collision. Close-coupling has been achieved by various iterative, non-iterative, and algebraic numerical procedures [26], [27]. Over the years, calculation of energy spectrum has been achieved using numerical methods, with and without the Pekeris approximation [28-31]. Such as the variational method without the Pekeris approximation [32], hyper-virial perturbation method without the Perekis approximation [33], the modified shifted large 1/N approach [34], Supersymmetry [35, 36], and the shifted 1/N expansion [37]. Other semi-analytic numerical approach include asymptotic iteration methods (AIM) [38], the two-point quasi-rational approximation technique (TQA) [39], Nikiforov-Ufarov method [40, 41], and the exact quantization rule (EQR) [42]. Many of these numerical techniques suffer setbacks owing to their cumbersomeness, limited accuracy and too long computational time. Correction of these anomalies led to the emergence of the J-matrix approach.

2.7 Model potential

To understand the scattering of subatomic structures, there is need for a configuration potential function that will model the system. Such potentials provide an effective model for physical systems, and a test model for numerical procedure constructed for solving complicated systems. Some of these potentials have been studied over the years, such as the Hellman potential, Hulthen potential, Yukawa potential, tamed Yukawa potential, Morse potential, Inverse Morse potential, to mention but a few. These potentials have been used to model singular but short-range interactions in different areas of Physics, especially high energy physics, and atomic-molecular physics.

Table 2.1: Different potentials and their parameters

Potential	Function	Parameters
Yukawa	$V_Y = -\frac{A}{r} e^{-\mu r}$	A, μ
Hulthen	$V_{Hu} = -A \frac{\mu}{e^{\mu r} - 1}$	A, μ
Hellman	$V_{He} = -\frac{A}{r} + B \frac{e^{-\mu r}}{r}$	A,B, μ
Morse	$V_M = D_e [e^{-2\alpha(r-r_e)/r_e} - 2e^{-\alpha(r-r_e)/r_e}]$	D_e , r_e ,α
Kratzer	$V_K(r) = -D_e \left(\frac{2r_e}{r} - \frac{r_e^2}{r^2} \right)$	D_e , r_e
Inverted Kratzer	$V_I(r) = \frac{1}{r} - \frac{\tau}{2r^2}$	τ

An important property of these potentials is that they are singular short range potentials (except Morse potential is regular). Short range potentials are characterized by two important parameters; the strength, and range of the potential. They can be generally described as

$$V(r) = -\frac{\alpha}{r} g(\mu r) \tag{2.7.1}$$

where α and 1/ μ are respectively the strength and range of the potentials. Short range potentials are exponentially small in the asymptotic domain, $V(r) = O(e^{-\mu r})$, $\mu > 0$, for $r \to \infty$. Also, these potentials have the behavior $V(r) \to -\frac{1}{r}$, for $r \to 0$, that is they show a coulomb-like behavior at small distances. The short range feature of the potentials is enhanced by the fact that $g(\mu r)$ decays sharply at large distances. Computation of resonances has suffered a setback owing to the singularity of these potentials at the origin. Hence, the need for an approach that will take care of this singularity while giving an accurate and stable solution. In fact, this is a major benefit of the J-matrix approach. The J-matrix absorbs the singularity in the reference Hamiltonian while leaving the non-singular part to numerical computation. The Hamiltonian is decomposed into two parts; the reference Hamiltonian H_0, and the effective potential U(r). $H = H_0 + U(r)$

The reference Hamiltonian (H_0) absorbed the isolated singularity, while the effective potential which is bounded everywhere and non-singular is treated numerically.

2.8 Bound and Resonance states

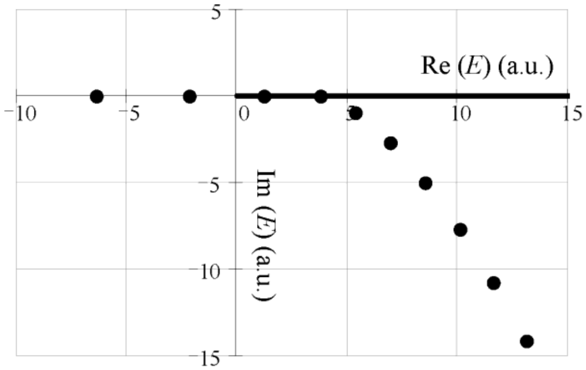

Fig. 2.5: typical distribution of bound and resonances states (Ref: [44])

If we consider a particle of mass m moving on the real line $x \in (-\infty, \infty)$ subject to a constant potential energy V(x) at both ends, such that

$$V_L \xleftarrow[-\infty \leftarrow x]{} V(x) \xrightarrow[x \to \infty]{} V_R$$

$$\lim_{x \to \pm\infty} x[V(x) - V_{R,L}] = 0 \qquad (2.8.1)$$

Then, we have a bound potential V(x) when $V_L \neq V_R$, assuming that smaller of V_L or V_R is zero. If we consider a quantum mechanical system described by a wave function $\psi(x, E)$ which obeys Schrodinger's equation

$$[\partial_x^2 + k^2 - V(x)]\psi(x, E) = 0. \qquad (2.8.2)$$

There exist three possible quantum states: bound state, resonant state, and scattering state. Bound states are characterized by real negative energy with square integrable wave function. Bound state solutions decay exponentially at the asymptotes. Resonant states are characterized by wave functions with only outgoing waves at large distance, and its solution exist at complex energy $E = E_{res} - i\frac{\Gamma}{2}$ $(E_{res} > 0, \Gamma > 0)$. While, scattering state has real positive energy whose wave function is a superposition of the incident and scattered waves. Alternatively, Bound states have negative energy states which are stationary, while resonance or quasi-bound states are states with positive energy which are initially bounded, but eventually tunnel through the potential barrier as shown below.

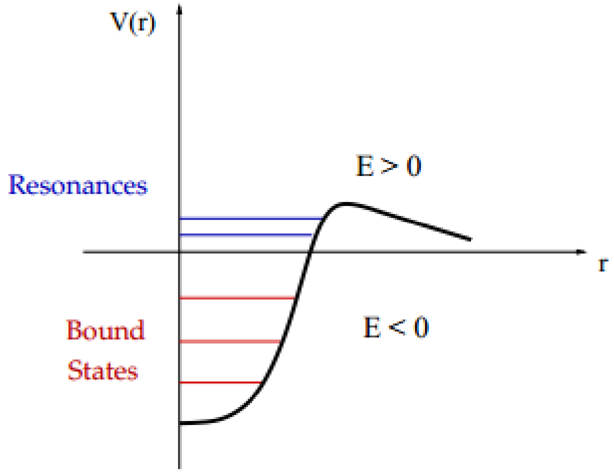

Fig. 2.6: potential supporting bound states and resonances.

Generally speaking, energy spectrum of the Hamiltonian as defined by the poles of the Green function $G_{L,Z}(E)$ in the complex energy plane can be grouped into three parts: (1) bound states which are characterized by a discrete set of points on the real negative energy axis. (2) Scattering states which are characterized by a continuum on the real positive energy line. (3) Resonant states which are composed of discrete set of points in the lower half of the complex energy plane.

The study of resonance is crucial to the understanding of scattering of particles. Over the years, different techniques have evolved to investigate and analyze resonances with a view to improving accuracy and enhance efficiency of computations with regard to locating resonance widths and positions. Resonance energies are subset or poles of the scattering S-matrix situated in the lower half of the complex energy plane. Resonance states are unstable bound like-state whose decay rate increases with the negative value of the imaginary part of the resonance energy. Resonance states can be classified as shallow or deep based on stability and decay rate. Shallow or sharp resonances are more stable resonances with slow decay rate located close to the real energy axis, while the deep or broad resonances are less stable resonances with fast decay rate located far from the real energy axis. An important sufficient condition for obtaining resonance position E_R and width $\Gamma = 2E_I$, is the singularity of the S-matrix elements at complex resonance energy E. $S^{-1}(E) = 0, \quad E = E_R \pm iE_I$. One way to expose hidden resonances is to use the complex rotation method.

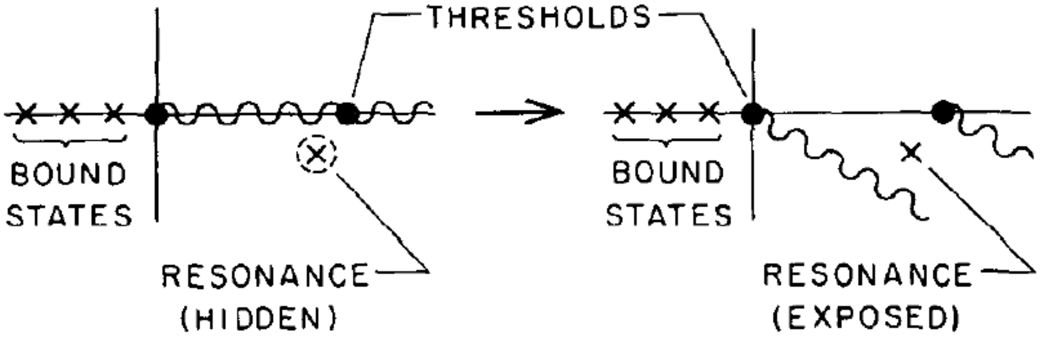

Fig. 2.7: Hidden resonance exposed by complex rotation (Ref: [45])

2.9 Complex scaling method

As stated earlier, resonance energies are subset of the Green's function poles $G_{l,Z}(E)$ (for real ℓ and Z), which are situated in the lower half of the complex energy plane. One way of exposing the "hidden resonances" which are situated below the real line of the complex energy plane is to employ the complex scaling (complex rotation) method. It exposes the resonance poles thereby ensuring their easier study and manipulation. This method transforms the radial component as $r \rightarrow re^{i\theta}$, where θ is the scaling angle. The pole structure is then transformed in the E-plane as:

$$G^{\theta}_{l,Z}(E) \equiv (H^{\theta} - E)^{-1} \qquad (2.9.1)$$

where H^{θ} is the complex-scaled full Hamiltonian, which is composed of : (1) the branch cut that lies on the real positive energy axis and undergoes a clockwise rotation by 2θ; (2) the discrete bound state energy on the negative energy axis; (3) isolated hidden resonances in the lower half of the complex E-plane get exposed. The complex E-plane is composed of two Riemann sheets. The first and second sheet represents the upper and lower half of the E-plane, respectively. The bound states are located on the upper half of the first energy sheet, while the conjugate anti-bound states are located on the lower half of the second energy sheet. Poles of the resonant and anti-resonant states are located on the lower half of the second energy sheet.

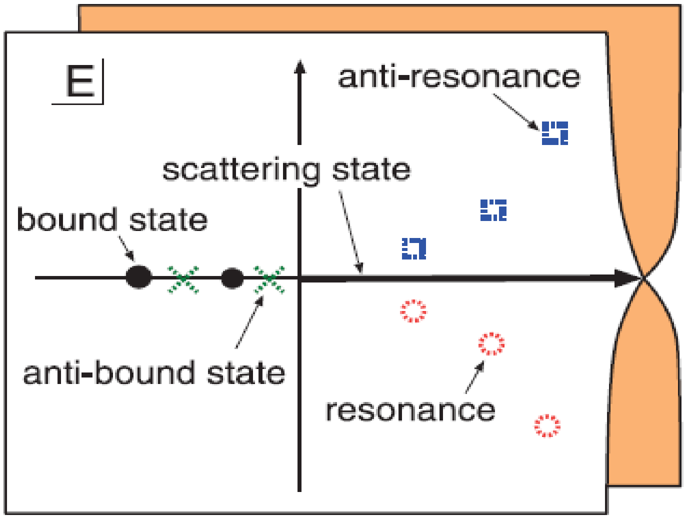

Fig. 2.8: Complex E-plane (Ref: [46]).

Complex scaling method (CSM) was laid down by Aguilar, Balslev, and Combes in 1971 [47, 48], and Simon proposed its direct application to resonance [49], where it was used to derive the resonance energy and width by solving the eigenvalue problem $H_\theta \psi_\theta = E\psi_\theta$, where E is a complex eigenvalue. The boundary condition for the outgoing wave for the complex scaled Schrodinger's equation should be such that $\left|\arg E\right| \leq 2\theta$. CSM has over the years been applied to the understanding of resonance in the field of nuclear, atomic and molecular physics to obtain resonance parameters and scattering cross-section [50]. In the work of Aguilar, Balslev, and Combes, CSM was formulated by using the transformation U(θ) for radial coordinate r and conjugate momentum k; $U(\theta)r = re^{i\theta},\ U(\theta)k = ke^{-i\theta}$. The complex scaled Schrodinger equation $H(\theta)\psi(\theta) = E(\theta)\psi(\theta)$ undergo transformation such that $H(\theta) = U(\theta)HU(\theta)^{-1}$, where $U(\theta)^{-1} = U(-\theta)$ and $\psi(\theta) = U(\theta)\psi = e^{3i\theta/2}\psi(\mathrm{re}^{i\theta})$. The factor $e^{3i\theta/2}$ resulted from the Jacobian transformation in three-dimensional space. The properties of the solution obtained are summarized as follows:

1. The bound and resonant state solutions are characterized by square integrable function.
2. The bound states energies are not affected by complex scaling
3. If the scaling angle θ is set to larger than θ_r $(\theta_r = \frac{1}{2}\tan^{-1}(\frac{\Gamma}{2E_r}))$, describing the resonance position. The resonance energy E_r and half width Γ/2 are real and imaginary parts of the complex eigenvalue E(θ) i.e. $E(\theta) = E_r$ -i$\frac{\Gamma}{2}$.

4. The continuum spectrum which is initially imparted to the beam is rotated clock wisely by 2θ from the positive real axis in the complex energy plane.

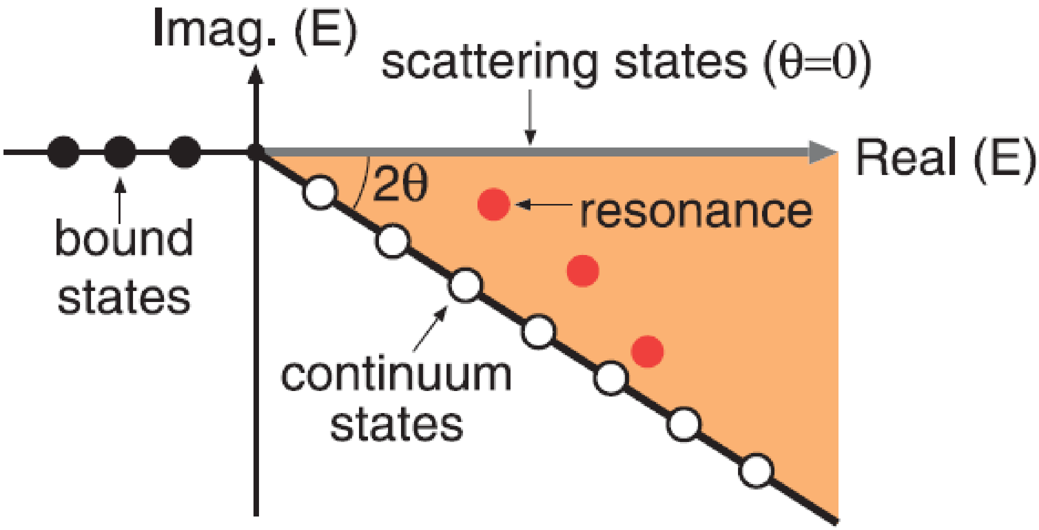

Fig. 2.9: A schematic distribution of the eigenvalue of H(θ) (Ref: [46])

2.10 Reference Hamiltonian in 3D J-matrix

The dynamical properties particle moving in a certain potential V(r) with spherically symmetry and under the influence of Coulomb field, can be illustrated by the Schrodinger equation,

$$(H-E)\chi=\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+\frac{Z}{r}+V(r)-E\right]\chi=0 \qquad (2.10.1)$$

where ℓ and E represents angular momentum quantum number and total energy respectively. In atomic units, $\hbar=m=e=1$. The wave function $\chi(r)$ which is parametized by ℓ, Z, and E, can be expanded in a complete basis set $\{\phi_n\}$. The choice of the basis is done to ensure that the reference Hamiltonian is represented in the form of a tridiagonal matrix. Hence, the basis must be compatible with the domain of the Hamiltonian, and satisfy the boundary conditions at $r = 0$ and $r \to \infty$. Also, the basis is parametized by a positive length scale parameter λ as $\{\phi_n(\lambda r)\}$.

$$\phi_n(\lambda r) = \sqrt{\lambda} A_n x^{\alpha} e^{-x/2} L_n^{v}(x); \quad \text{n=0,1,2,...} \tag{2.10.2}$$

where $x = \lambda r, \alpha > 0, v > -1, L_n^v(x)$ is a Laguerre polynomial, and A_n is a normalization constant $\sqrt{\Gamma(n+1)/\Gamma(n+v+1)}$. The reference Hamiltonian $H_0 (\equiv H - V)$ in the chosen basis, has a matrix representation

$$(H_0)_{nm} = \langle \phi_n(x) | -\frac{\lambda^2}{2}\frac{d^2}{dx^2} + \frac{\lambda^2}{2}\frac{l(l+1)}{x^2} + \frac{\lambda Z}{x} | \phi_m(x) \rangle \tag{2.10.3}$$

Following complex rotation and transformation on H_0 $(r \to re^{i\theta})$ or equivalently $\lambda \to \lambda e^{-i\theta}$, the reference Hamiltonian is then manipulated using differential equation, and properties of Laguerre polynomial to obtain a tridiagonal matrix representation for $2\alpha = v + 1$.

$$\begin{aligned}(H_0)_{nm} = {} & \frac{\lambda^2}{8}\left(2n + v + 1 + \frac{8Z}{\lambda}\right)\delta_{n,m} + \frac{\lambda^2}{8}\sqrt{n(n+v)}\,\delta_{n,m+1} \\ & + \frac{\lambda^2}{8}\sqrt{(n+1)(n+v+1)}\,\delta_{n,m-1} - \frac{\lambda^2}{2}\left[v^2 - (2l+1)^2\right]\left(x^{-1}\right)_{nm}\end{aligned} \tag{2.10.4}$$

$\left(x^{-1}\right)_{nm} = \frac{1}{v}\left(A_{n_>} \middle/ A_{n_<} \right)$ is a symmetric matrix, and $n_>(n_<)$ is the larger (smaller) of the integers m and n. Using $v = 2\ell + 1$ results in tridiagonal matrix representation of the reference Hamiltonian. The basis $\{\phi_n\}$, though not orthogonal, can be represented by an overlap matrix.

$$\langle\phi_n|\phi_m\rangle \equiv \Omega_{nm} = (2n+v+1)\delta_{n,m} - \sqrt{n(n+v)}\delta_{n,m+1} - \sqrt{(n+1)(n+v+1)}\delta_{n,m-1} \tag{2.10.5}$$

2.11 Potential matrix and Gauss quadrature in J-matrix

Gauss quadrature integral approximation of a function f(x) that belongs to L^2[a,b] states that

$$\int_a^b \rho(x)f(x)dx \cong \sum_{n=0}^{N-1}\omega_n f(\varepsilon_n) \tag{2.11.1}$$

The numerical weight, ω_n, is the square of the zero component of the normalized eigenvector of H, $\{\Lambda_{mn}\}_{m=0}^{N-1}$, associated with the eigenvalue ε_n. That is $\omega_n = \Lambda_{0n}^2$, where $H|\Lambda_n\rangle = \varepsilon_n|\Lambda_n\rangle$. One can show that $p_k(\varepsilon_n) = \Lambda_{kn}/\Lambda_{0n}$; $n,k = 0,1,\ldots,N-1$

Using the recursion relation, orthogonality of the Laguerre polynomial, together with $L_0^v(x) = 1$ suggest the definition of the density function $\rho(x) \equiv x^v e^{-x}/\Gamma(v+1)$ in the interval $[a=0, b\to\infty)$. Orthogonal polynomial p$_n$(x) can also be put into a standard form as $p_n(x) = \sqrt{\frac{\Gamma(v+1)\Gamma(n+1)}{\Gamma(n+v+1)}}L_n^v(x)$. Now, to calculate the matrix elements of the potential V(r), we evaluate

$$V_{nm}=\int_0^\infty \phi_n(\lambda r)V(r)\phi_m(\lambda r)dr\ =A_nA_m\int_0^\infty x^v e^{-x}L_n^v(x)L_m^v(x)V(x^\sigma/\lambda)dx \quad (2.11.2)$$

with some appropriate power σ. This integral can be put in the form

$$V_{nm}=A_nA_m\sqrt{\frac{\Gamma(n+v+1)\Gamma(m+v+1)}{\Gamma(n+1)\Gamma(m+1)}}\int_0^\infty \rho(x)p_n(x)p_m(x)V(x^\sigma/\lambda)dx \quad (2.11.3)$$

Using the definition of the Gauss quadrature approximation, we have

$$V_{nm}=A_nA_m\sqrt{\frac{\Gamma(n+v+1)\Gamma(m+v+1)}{\Gamma(n+1)\Gamma(m+1)}}\sum_{k=0}^{N-1}\Lambda_{nk}\Lambda_{mk}V(\varepsilon_k^\sigma/\lambda) \quad (2.11.4)$$

Using the normalization constant $A_n=\sqrt{\frac{\Gamma(n+1)}{\Gamma(n+v+1)}}$, the potential matrix elements become

$$V_{nm}=\sum_{k=0}^{N-1}\Lambda_{nk}\Lambda_{mk}V(\varepsilon_k^\sigma/\lambda)\,. \quad (2.11.5)$$

Based on the above formalism, the reference Hamiltonian is fully accounted for, while the potential V is approximated by its basis representation, such that

$$H_{nm}\cong\begin{cases}(H_0)_{nm}+V_{nm}, & 0\le \text{n,m}\le \text{N-1}\\ (H_0)_{nm}, & \text{N}\le n,m\le\infty\end{cases} \quad (2.11.6)$$

2.12 Computational procedure

Based on the theoretical formalism, the important parameters needed to ensure stability, accuracy, and convergence of our computational procedure are λ, θ, and N. The procedure is enumerated as follows:

1. For small enough fixed value of N and a chosen eigenvalue, we vary the value of θ and the scaling parameter λ. The study of the variation of λ and θ will show a plateau visible over the range of the parameters. The plateau is an indication of stability of the eigenvalue.
2. From the plot of the plateau of stability, we choose the value of λ and θ from the middle of the plateau, we then proceed to calculate the bound states for $\theta=0$, and $\theta>0$ for resonance energies by employing the complex scaling method.
3. Having achieved stability, we set to improve the accuracy of the result by increasing the dimension of the space N. This increase is carefully done up to the precision that maintain stability of the results.

CHAPTER 3

TWO DIMENSIONAL J-MATRIX

3.1 Introduction to two dimensional scattering

Two dimensional quantum scattering has been discussed by a number of authors [51-53]. The Spherical Bessel and Neumann functions in three dimensions become ordinary Bessel (regular at the origin) and Neumann (irregular) functions, owing to circular symmetry in two dimensions. The mathematical formalism involved in two dimensional scattering is similar to the one used in scattering of cylindrical waves in three dimensions [54]. As such, it has many of the complexities inherent in three dimensional scattering. In the past, Lapidus presented a mathematical description of two dimensional quantum scattering [55], while Adhikari [56] went further to study the analytical properties of the scattering amplitude.

In the following two sections we consider the two dimensional problem where the reference Hamiltonian is the radial part of the free Hamiltonian. We find two independent sets of expansion coefficients for the asymptotic reference wavefunction. We show that one of these two wavefunctions is the exact regular solution of the reference problem. The other one is uniquely regularized in that it is asymptotically identical to the exact irregular solution of the reference problem. We show that scattering information is contained in the phase difference between these two asymptotic solutions.

3.2 Regular J-matrix solution of the reference problem

A point particle in a certain short range potential $V(r,\phi)$ with cylindrically symmetric potential and of mass M can be described by a two-dimensional time-independent Schrödinger wave equation as follows

$$\left(H-E\right)\psi(r,\phi)=\left[-\frac{\hbar^2}{2M}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right)+V(r)-E\right]\psi(r,\phi)=0, \quad (3.2.1)$$

where $\psi(r,\phi)$ is the wave function and r and ϕ represent the particle's polar coordinates [57].

By employing the J-matrix formalism, we can expand the wave function ψ in a set of square integrable functions with discrete basis elements $\{\phi_n\}_{n=0}^{\infty}$ as $|\psi(\vec{r},E)\rangle=\sum_n f_n(E)|\phi_n(\vec{r})\rangle$, where $\vec{r}$ is the set of real space coordinates and E represents energy of the particle. An important condition that characterize the discrete basis set is the compatibility with the Hamiltonian domain and vanishing conditions at the boundary for both $r = 0$ and $r = \infty$. The expression in (3.1) can be separated based on cylindrical symmetry of the potential such that $\psi(r,\phi)=R(r)F(\phi)/\sqrt{r}$, which then yield the equation

$$F(\phi)\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{1/4}{2r^2}-E\right]\chi\left(r\right)+\frac{\chi\left(r\right)}{r^2}\left[-\frac{1}{2}\frac{d^2}{d\phi^2}+r^2V\left(r,\phi\right)\right]F(\phi)=0 \qquad (3.2.2)$$

Where $\hbar = M = 1$ .The equation (3.2.2) above can be expressed for non-central potentials of the form

$$V(r,\phi) = V_1(r) + \frac{1}{r^2} V_2(\phi) \qquad (3.2.3)$$

The angular and radial parts then become

$$\left[-\frac{1}{2}\frac{d^2}{d\phi^2} + V_2(\phi)\right] F(\phi) = k^2 F(\phi) \quad ; \quad \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{2r^2} + V_1(r)\right] \chi(r) = E\chi(r) (3.2.4$$

with E and k representing the eigenvalues of the radial and angular equations, respectively. Considering the exact solvability of the above angular equation, we choose a specific angular potential $V_2(\phi)$ that satisfies the periodicity condition

$V_2(\phi) = V_2(\phi + 2\pi)$. Some of these angular potentials have been studied [58], for the purpose of ensuring a clear quantization process for the inter-related physical constants E and k, we settled for a simple form of the well-known Poschl-Teller potential

$$V_2(\phi) = \frac{B}{(\sin p\phi)^2} \qquad (3.2.5)$$

B and p are physical constants. For the angular potential to satisfy the periodicity requirement, it is important that p must be an integral multiple of ½. Also, the potential is continuous with singularity at $\phi = 0, \frac{\pi}{p}$ thereby restricting the angular variable

$0<\phi<\pi/p$ and ensuring that $F(\phi)$ vanish at these boundaries $F(0)=F(\pi/p)=0$. For details on $F(\phi)$ see [58], the un-normalized angular wave function takes the form

$$F(\phi)=(\sin p\phi)^{\kappa}C_{n_1}^{\kappa}(\cos p\phi) \quad ; \quad \kappa=\frac{1}{2}+\frac{1}{2}\sqrt{1+4\frac{B}{p^2}} \quad ; \quad m=p(\kappa+n_1) \quad (3.2.6)$$

where $n_1 = 0,1,2\ldots$ is a positive integer and κ is a real parameter so that we require that $4B/p^2 + 1 > 0$. We now look at the radial equation (3.2.4). We have defined the reference Hamiltonian, termed H_0, as

$$H_0=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{m^2-1/4}{2r^2} \quad ; \quad m^2=p^2(\kappa+n_1)^2 \quad ; \quad n_1=0,1,2\cdots \qquad (3.2.7)$$

We begin by obtaining the solution to the reference problem analytically using the tools of the J-matrix method then after that we add the contribution of the scattering potential in the form of its matrix elements in a complete square integrable basis. Now, since the range of the potential is finite then its contribution is approximated by its matrix elements in a finite subset of the basis. The virtue of the J-matrix method is that it gives an exact solution of the problem for this truncated matrix model of the potential. Most other methods, on the other hand, give approximate solution of the problem for the exact potential. However, very often the truncated matrix elements of the potential give a faithful representation of the potential due to its short range. Nevertheless, the reference wave equation of the problem in 2D reads as follows

$$J(E)\chi(r,E)=\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{m^2-1/4}{2r^2}-E\right]\chi(r,E)=0, \qquad (3.2.8)$$

where $J(E)=H_0-E$ is the reference wave operator. The solution to this equation yields two independent solutions (for $E>0$), which represent the energy eigenfunctions of H_0, and has been obtained in most standard textbooks on quantum mechanics [59]. They are written in terms of the Bessel and Neumann functions as follows:

$$\chi_{reg}(r,E)=\sqrt{2kr}\,\mathcal{J}_{|m|}(kr)\,, \tag{3.2.9}$$

$$\chi_{irr}(r,E)=\sqrt{2kr}\,\mathcal{N}_{|m|}(kr)\,, \tag{3.2.10}$$

where $k=\sqrt{2E}$, $\mathcal{J}_{\mu}(x)$ and $\mathcal{N}_{\mu}(x)$ are the Bessel and Neumann functions, respectively. The regular solution is energy-normalized, $\left\langle \chi_{reg} \middle| \chi'_{reg} \right\rangle = \delta(k-k')$, whereas the irregular solution is not square integrable (with respect to the integration measure, *dr*). Near the origin they behave as $\chi_{reg}\to r^{|m|+1/2}$ and $\chi_{irr}\to r^{-|m|+1/2}$. On the other hand, asymptotically ($r\to\infty$) they are sinusoidal: $\chi_{reg}\to\frac{2}{\sqrt{\pi}}\cos\left(kr-|m|\frac{\pi}{2}-\frac{\pi}{4}\right)$ and $\chi_{irr}\to\frac{2}{\sqrt{\pi}}\sin\left(kr-|m|\frac{\pi}{2}-\frac{\pi}{4}\right)$ [60]. Now, in the J-matrix method, the emphasis is on the scattering information, which is contained in the phase difference between the two asymptotic sinusoidal solutions of (3.2.9) and (3.2.10). For that, the method replaces these two solutions with an equivalent series representation, in an L^2 basis, that is identical to it asymptotically. Such L^2 basis functions, $\{\phi_n\}_{n=0}^{\infty}$, must be complete and should support an infinite tridiagonal matrix representation for the reference wave operator $J = H_0 - E$. These requirements endow the method with its powerful analytic and computational tools. On the one hand, the analytic tools of orthogonal polynomials associated with tridiagonal matrices and three-term recursion relation. On the other hand, the stability and accuracy of the computational routines that favors tridiagonal matrices (e.g., in the calculation of their eigenvalues and eigenvectors) in addition to the use of Gauss quadrature approximation associated with tridiagonal representations. Now, one such basis, which is compatible with the domain of our problem (i.e., defined in the same range $r \in [0, \infty]$ and satisfies the boundary conditions), well behaved at the origin, and square integrable is [61]

$$\phi_n(y) = A_n (\lambda r)^{|m|+\frac{1}{2}} e^{-y/2} L_n^{\nu}(y)\,, \tag{3.2.11}$$

where λ is a positive basis parameter of inverse length dimension, and $L_n^{\nu}(y)$ is the associated Laguerre polynomial of order n with $\nu > -1$. We choose to work in, what is referred to as, the "Laguerre basis" for which $y = (\lambda r)$. The normalization constant A_n is chosen in this basis to be $A_n = \sqrt{\lambda \Gamma(n+1)/\Gamma(n+\nu+1)}$. In Appendix B, we repeat the same development in the "oscillator basis" for which $y = (\lambda r)^2$. Using the differential equation of the Laguerre polynomials [62], their differential formula, $x \frac{d}{dx} L_n^{\nu} = n\, L_n^{\nu} - (n+\nu) L_{n-1}^{\nu}$, and recursion relation we can show that the matrix representation of the wave operator J in the Laguerre basis will be tridiagonal only if $\nu = 2|m|$ giving

$$\begin{aligned} &\frac{2}{\lambda^2} J_{nm}(E) = \frac{2}{\lambda^2} \langle \phi_n | H_0 - E | \phi_m \rangle = \left(\tfrac{1}{4} + \mu^2\right) \times \\ &\left[-2\left(n + \ell + \tfrac{1}{2}\right) x\, \delta_{n,m} + \sqrt{n(n+2\ell)}\, \delta_{n,m+1} + \sqrt{(n+1)(n+2\ell+1)}\, \delta_{n,m-1} \right] \end{aligned} \tag{3.2.12}$$

where $\ell = |m|$, $x = \frac{\mu^2 - 1/4}{\mu^2 + 1/4} = \cos\theta$ with $0 < \theta \leq \pi$ and $\mu = k/\lambda$. The reference wave function, which is regular at the origin and which we refer to from now on by $\chi_{\sin}(r,E)$, can be expanded as follows

$$\chi_{\sin}(r,E) \equiv \chi_{reg}(r,E) = \sum_{n=0}^{\infty} s_n(E)\phi_n(r) \qquad (3.2.13)$$

This is a solution of the homogeneous differential equation, $\left(H_0 - E\right)\chi_{\sin}(r,E) = 0$. Using (3.2.13) and the fact that the basis set $\{\phi_n\}_{n=0}^{\infty}$ is complete and orthonormal we arrive at a three term recursion relation for the expansion coefficients, $\{s_n\}_{n=0}^{\infty}$, of the from $\sum_m J_{nm} s_m = 0$, which explicitly reads

$$2\left(n + \ell + \tfrac{1}{2}\right) x\, s_n = \sqrt{n(n+2\ell)}\, s_{n-1} + \sqrt{(n+1)(n+2\ell+1)}\, s_{n+1}, \qquad (3.2.14)$$

with the initial condition

$$\left(2\ell + 1\right) x\, s_0 - \sqrt{(2\ell+1)}\, s_1 = 0. \qquad (3.2.15)$$

This recursion relation could be solved (modulo an arbitrary non-zero function of the energy) by correspondence with those of known orthogonal polynomials. However, in this work, we pursue a direct integration approach to obtain the expansion coefficients $\{s_n\}_{n=0}^{\infty}$ by writing (3.2.13) as

$$\chi_{reg}(r,E) = \sqrt{2\mu y}\, \mathcal{J}_{\ell}(\mu y) = \sum_{n=0}^{\infty} s_n(E)\phi_n(y) \qquad (3.2.16)$$

After multiplication with the proper factor, this equation could be integrated using the orthogonality of the Laguerre polynomials giving

$$s_n(E)=\lambda^{-1}\sqrt{2\mu}A_n\int_0^\infty y^{\ell}e^{-y/2}L_n^{2\ell}(y)\mathcal{J}_\ell(\mu y)dy\ . \qquad (3.2.17)$$

This integral could be evaluated using the result in [63] giving

$$s_n(E)=\frac{1}{\sqrt{\lambda\pi}}\sqrt{\frac{\Gamma(n+1)}{\Gamma(n+2\ell+1)}}\,\Gamma\left(\ell+\tfrac{1}{2}\right)\left(2\sin\theta\right)^{\ell+\frac{1}{2}}C_n^{\ell+\frac{1}{2}}(\cos\theta)\,, \quad (3.2.18)$$

where $C_n^{\ell+1/2}(x)$ is the ultra-spherical Gegenbauer polynomial. Using the differential equation of these polynomials [64], one can show that the sine-like coefficients satisfy the following second order energy differential equation

$$\left[\left(1-x^2\right)\frac{d^2}{dx^2}-x\,\frac{d}{dx}-\frac{\ell^2-1/4}{1-x^2}+\left(n+\ell+\tfrac{1}{2}\right)^2\right]s_n(E)=0\,. \qquad (3.2.19)$$

In the following section, we calculate the other independent asymptotic solution of the reference problem (the cosine-like solution, $\chi_{\cos}$).

3.3 J-matrix regularization of the irregular reference solution

Now, we look for a second independent solution, $\left\{G_n\right\}_{n=0}^{\infty}$, of the above recursion relation that satisfies (3.2.14) but with the following inhomogeneous initial relation

$$\left(2\ell+1\right)xG_0-\sqrt{(2\ell+1)}\,G_1=\gamma\,, \qquad (3.3.1)$$

where γ is a real parameter that depends on E and ℓ, which is fixed by the asymptotic boundary conditions as follows. The cosine-like solution (also called regularized solution) is defined by

$$\chi_{\cos}(r,E)=\sum_{n=0}^{\infty}G_n(E)\phi_n(r)\,. \tag{3.3.2}$$

In Dirac notation, we can write $J\left|\chi_{\cos}\right\rangle = J\sum_n G_n\left|\phi_n\right\rangle$. Using completeness of the bi-orthogonal basis, $\sum_{n=0}^{\infty}\left|\bar{\phi}_n\right\rangle\left\langle\phi_n\right|=1$ where $\left\langle\bar{\phi}_m\middle|\phi_n\right\rangle=\delta_{mn}$, and the fact that the J operator is tridiagonal in this representation we get

$$J\left|\chi_{\cos}\right\rangle=\sum_{m=0}^{\infty}\left(J_{m,m}G_m+J_{m,m+1}G_{m+1}+J_{m,m-1}G_{m-1}\right)\left|\bar{\phi}_m\right\rangle. \tag{3.3.3}$$

Due to the fact that the set $\left\{c_n\right\}_{n=0}^{\infty}$ satisfy the recursion (3.2.14) with its initial relation (3.3.1), all terms in the above equation vanish except for m = 0, which then gives

$$J\left|\chi_{\cos}\right\rangle=\left(J_{00}G_0+J_{01}G_1\right)\left|\bar{\phi}_0\right\rangle. \tag{3.3.4}$$

Using the J-matrix element as can be identified easily from (3.3.1) we obtain $J\left|\chi_{\cos}\right\rangle=\gamma\left|\bar{\phi}_0\right\rangle$, which is written in r-space as

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell^2-1/4}{2r^2}-E\right]\chi_{\cos}(r,E)=\gamma\,\bar{\phi}_0(r)\,. \tag{3.3.5}$$

The Green's function $g(r,r')$ associated with the reference wave operator J, which satisfies $J(E)g(r,r')=-\delta(r-r')$, is given by

$$g(r,r') = \frac{2}{W(E)} \chi_{reg}(r_<)\chi_{irr}(r_>) , \tag{3.3.6}$$

where $r_>$ and $r_<$ stands for the largest and smallest among r and r'. $W(E)$ is the Wronskian of the two independent solutions shown in (3.2.9 & 3.2.10), which reads $W = 4k/\pi = \left(4\lambda/\pi\right)\mu$. Using the Green function, the solution of (3.3.5) becomes

$$\begin{aligned} \chi_{\cos}(r,E) &= -\gamma\int_0^\infty g(r,r')\overline{\phi}_0(r')dr' \\ &= -\frac{2\gamma}{W}\left[\chi_{irr}(r)\int_0^r \chi_{reg}(r')\overline{\phi}_0(r')dr' + \chi_{reg}(r)\int_r^\infty \chi_{irr}(r')\overline{\phi}_0(r')dr' \right] \end{aligned} \tag{3.3.7}$$

Imposing the asymptotic boundary condition $\lim\limits_{r\to\infty}\chi_{irr}(r,E) = \chi_{\cos}(r,E)$ gives $\gamma = -W/2s_0$. Using the Wronskian and the value of s_0 as given by Eq. (3.2.18) we obtain

$$\gamma = \frac{-2\lambda\sqrt{\lambda/\pi}}{\Gamma\left(\ell+1/2\right)}\sqrt{\Gamma(2\ell+1)}\,\mu\left(2\sin\theta\right)^{-\ell-1/2} \tag{3.3.8}$$

and $W = \dfrac{4k}{\pi} = \dfrac{2\lambda}{\pi}\sqrt{\dfrac{1+x}{1-x}}$ while $s_0 = \dfrac{2^\ell}{\sqrt{\pi}}\dfrac{\Gamma\left(\ell+\frac{1}{2}\right)}{\sqrt{\lambda\Gamma(2\ell+1)}}\left(1-x^2\right)^{\frac{\ell}{2}+\frac{1}{4}}$, (recall: $x = \cos\theta$)

Moreover, G_n obey the recursion relation (3.3.1) which can be brought into a simpler form through the transformation

$$G_n(x) = \sqrt{\tfrac{\Gamma(n+1)\Gamma(2\ell+1)}{\Gamma(n+2\ell+1)}}\,c_n(x) , \tag{3.3.9}$$

Leading to

$$\left(2n+2\ell+1\right)x\,c_n = (n+2\ell)c_{n-1} + (n+1)c_{n+1} \quad ; \quad n = 1,2,3,.... \tag{3.3.10}$$

The initial condition (3.3.4) can then be written explicitly as follows

$$-(2\ell+1)x\,c_0+c_1=\frac{2\gamma}{\lambda^2\left(\mu^2+\frac{1}{4}\right)}\,. \tag{3.3.11}$$

Iterating the above recursion relation (3.3.10) starting from the initial condition (3.3.4) for successive values of *n* leads us to the following general structure of the solution

$$c_n=c_0\,C_n^{\ell+1/2}(x)-\eta\,Q_{n-1}(x)\,, \tag{3.3.12}$$

where

$$\eta=\frac{-2\gamma}{\lambda^2\left(\mu^2+\frac{1}{4}\right)}=-\frac{2^{\frac{3}{2}+\ell}}{\sqrt{\pi}}\frac{\sqrt{\lambda\Gamma(2\ell+1)}}{\Gamma\left(\ell+\frac{1}{2}\right)}(1-x^2)^{\frac{1}{4}-\frac{\ell}{2}} \tag{3.3.13}$$

and the new polynomials Q_n satisfy the following recursion relation

$$\begin{aligned}&\left(2n+2\ell+3\right)x\,Q_n=(2\ell+n+1)\,Q_{n-1}+(n+2)Q_{n+1};\quad n\geq 1\\&\left(2\ell+3\right)xQ_0-2Q_1=0\quad;\quad Q_0=1\end{aligned} \tag{3.3.14}$$

Comparing this recursion relation for Q_n with that associated with the Gegenbauer polynomial, we deduce that their recursion coefficients are shifted by one unit (i.e. $n\to n+1$). These are just the associated Gegenbauer or Wimp polynomials as defined in Sec. 5.7.1 of [64] by $Q_n=\mathcal{C}_n^{\ell+1/2}(x,1)$. In the literature, $\mathcal{C}_n^{\ell+1/2}(x,c)$ obeys the following recursion relation

$$\begin{aligned}&2\left(n+c+\ell+1/2\right)x\,\mathcal{C}_n^{\ell+1/2}=\left(2\ell+n+c\right)\mathcal{C}_{n-1}^{\ell+1/2}+\left(n+c+1\right)\mathcal{C}_{n+1}^{\ell+1/2};\quad n\geq 1\\&\mathcal{C}_0^{\ell+1/2}(x,c)=1\,;\quad \mathcal{C}_{-1}^{\ell+1/2}(x,c)=0.\end{aligned} \tag{3.3.15}$$

Thus, the general solution for the recursion relation (3.3.10) can written as follows

$$c_n(x) = c_0\, C_n^{\ell+1/2}\left(x\right) - \eta\, \mathcal{C}_{n-1}^{\ell+1/2}\left(x,1\right). \tag{3.3.16}$$

And
$$G_n(x) = s_n\left(x\right) - \eta\sqrt{\tfrac{\Gamma(n+1)\Gamma(2\ell+1)}{\Gamma(n+2\ell+1)}}\, \mathcal{C}_{n-1}^{\ell+1/2}\left(x,1\right) \tag{3.3.17}$$

The regularized cosine-like solution can then be written as follows

$$\begin{aligned}\chi_{\cos}(r,x) &= \sum_{n=0}^{\infty} G_n(x)\phi_n(r)\\ &= \sum_{n=0}^{\infty}\sqrt{\tfrac{\Gamma(n+1)\Gamma(2\ell+1)}{\Gamma(n+2\ell+1)}}\left[c_0\, C_n^{\ell+1/2}\left(x\right) - \eta\, \mathcal{C}_{n-1}^{\ell+1/2}\left(x,1\right)\right]\phi_n(\lambda r)\end{aligned} \tag{3.3.18}$$

To fix the parameter c_0 we require that for $\eta = 0$ the solution reduces to the regular one, with $s_n(x)$ as expansion coefficients, giving

$$c_0 = \sqrt{2}s_0 = \frac{2^{\ell+\frac{1}{2}}}{\sqrt{\pi}}\frac{\Gamma\left(\ell+\frac{1}{2}\right)}{\sqrt{\lambda\Gamma(2\ell+1)}}(1-x^2)^{\frac{1}{4}+\frac{\ell}{2}}. \tag{3.3.19}$$

Then our regularized cosine-like solution (3.3.18) becomes

$$\begin{aligned}\chi_{\cos}(r,E) &= \chi_{\sin}(r,E) - \eta\sum_{n=0}^{\infty}\sqrt{\frac{\Gamma(2\ell+1)\Gamma(n+1)}{\Gamma(n+2\ell+1)}}\, Q_{n-1}(x)\phi_n(\lambda r)\\ &= \chi_{\sin}(r,E) - \eta\sum_{n=0}^{\infty}\sqrt{\frac{\Gamma(2\ell+1)\Gamma(n+1)}{\Gamma(n+2\ell+1)}}\, \mathcal{C}_{n-1}^{\ell+1/2}\left(x,1\right)\phi_n(\lambda r)\end{aligned} \tag{3.3.20}$$

To verify the validity of our approach we perform computations of the sine-like and cosine-like solutions defined by their respective expansions

$$\chi_{\sin}(r,E) = \sum_{n=0}^{\infty} s_n(E)\phi_n(r)\,,\ \ \chi_{\cos}(r,E) = \sum_{n=0}^{\infty} G_n(E)\phi_n(r)\,. \tag{3.3.21}$$

Both should be regular at the origin and $\chi_{\sin}(r,E)=\chi_{reg}^{\nu}(r,E)=\sqrt{2kr}\,J_{\nu}(kr)$ whereas $\lim_{r\to\infty}\chi_{\cos}(r,E)=\lim_{r\to\infty}\chi_{irr}^{\nu}(r,E)=\lim_{r\to\infty}\sqrt{2kr}\,Y_{\nu}(kr)$. For illustration, we show in Figures 3.1 and 3.2 the sine-like and cosine-like solutions obtained from the series expansions (3.3.20) for a given energy and angular momentum. As expected, the sine-like solution is identical to the regular solution (3.2.9) while the cosine-like solution coincides with the irregular solution only asymptotically but deforms itself near the origin, as imposed by the J-matrix regularization scheme, to comply with the vanishing of the wave function at this boundary. On the other hand, Figure 3.3 shows that the phase difference between these two solutions is exactly $\pi/2$ asymptotically as required by construction. These two solutions, $\chi_{\sin}(r,E)$ and $\chi_{\cos}(r,E)$, are the carriers of the scattering information at the detector side (far from the interaction center). This information is stored in the phase difference between the two solutions. In the absence of interaction, this phase difference is exactly $\pi/2$ for all energies.

Using the J-matrix approach, the reference Hamiltonian matrix $\left(H_0\right)_{nm}$ is obtained from (3.2.12) by setting $E = 0$ whereas the matrix elements of the potential in the basis (3.2.11) are obtained by evaluating the integral

$$\begin{aligned} V_{nm} &= \langle\phi_n|V|\phi_m\rangle = \int_0^\infty \phi_n(\lambda r)\,V(r)\phi_m(\lambda r)dr \\ &= \lambda^{-1}A_nA_m\int_0^\infty y^{2\ell}e^{-y}L_n^{2\ell}(y)L_m^{2\ell}(y)\left[yV(y/\lambda)\right]dy \end{aligned} \qquad (3.3.22)$$

The evaluation of such an integral for a general short-range potential function *V*(*r*) is usually done numerically. We use Gauss quadrature approximation (see Appendix A in [4]), which gives

$$V_{nm} \cong \sum_{k=0}^{N-1} \Lambda_{nk} \Lambda_{mk} \left[\mu_k V\left(\mu_k / \lambda \right) \right], \tag{3.3.23}$$

where μ_k and $\left\{ \Lambda_{nk} \right\}_{n=0}^{N-1}$ are the N eigenvalues and corresponding normalized eigenvectors of the $N \times N$ tridiagonal basis overlap matrix $\left\langle \phi_n \middle| \phi_m \right\rangle$, which is obtained from (3.2.12) as the tridiagonal matrix multiplying $-E$

$$\left\langle \phi_n \middle| \phi_m \right\rangle = \left(2n + 2\ell + 1 \right) \delta_{n,m} - \sqrt{n(n+2\ell)}\, \delta_{n,m+1} - \sqrt{(n+1)(n+2\ell+1)}\, \delta_{n,m-1} \tag{3.2.24}$$

Table 3.1: The explicit form of the J-matrix kinematics quantities, $\left\{ T_n(E), R_n^{\pm}(E) \right\}$, the finite Green's function, $g_{N-1,N-1}(z)$, and $J_{N-1,N}(E)$ in the Laguerre basis. The eigenvalues of the finite $N \times N$ total Hamiltonian H are denoted by $\left\{ \varepsilon_n \right\}_{n=0}^{N-1}$ and the eigenvalues of the truncated H obtained by removing the last row and last column are $\left\{ \tilde{\varepsilon}_n \right\}_{n=0}^{N-2}$.

$g_{N-1,N-1}(z)$	$\frac{1}{N+2\ell} \left[\prod_{m=0}^{N-2} \left(\tilde{\varepsilon}_m - z \right) \Big/ \prod_{n=0}^{N-1} \left(\varepsilon_n - z \right) \right]$
$T_n(E)$	$\frac{G_n(E) - i s_n(E)}{G_n(E) + i s_n(E)}$
$R_n^{\pm}(E)$	$\frac{G_n(E) \pm i s_n(E)}{G_{n-1}(E) \pm i s_{n-1}(E)}$
$s_n^{\ell}(E)$	$\Gamma\left(\ell + \frac{1}{2} \right) \frac{A_n}{\lambda \sqrt{\pi}} (2 \sin\theta)^{\ell+\frac{1}{2}} C_n^{\ell+\frac{1}{2}}(\cos\theta)$
$G_n(E)$	$\sqrt{\frac{\Gamma(n+1)\Gamma(2\ell+1)}{\Gamma(n+2\ell+1)}} \left[c_0\, C_n^{\ell+1/2}\left(\cos\theta \right) - \eta\, \mathcal{C}_{n-1}^{\ell+1/2}\left(\cos\theta, 1 \right) \right]$
$J_{N-1,N}(E)$	$\left(E + \lambda^2/8 \right) \sqrt{N(N+2\ell)}$

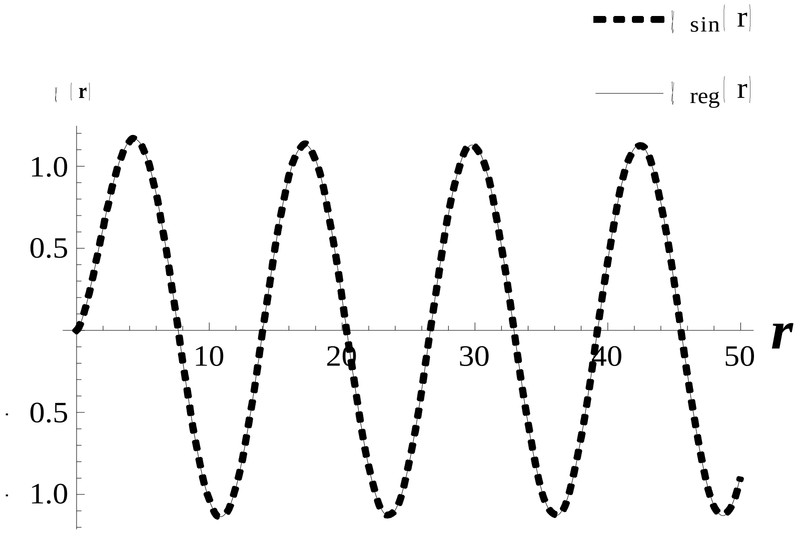

Fig. 3.1: Plot of the sine-like, and regular solutions for $\ell = 1$, $\lambda = 1$, $k = 0.5$. (Atomic units used)

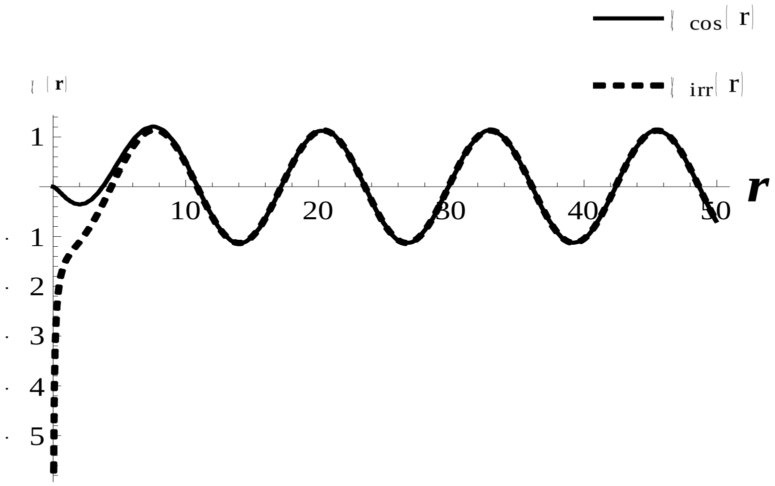

Fig. 3.2: Plot of the cosine-like, and irregular solutions for $\ell = 1$, $\lambda = 1$, $k = 0.5$ (Atomic units used)

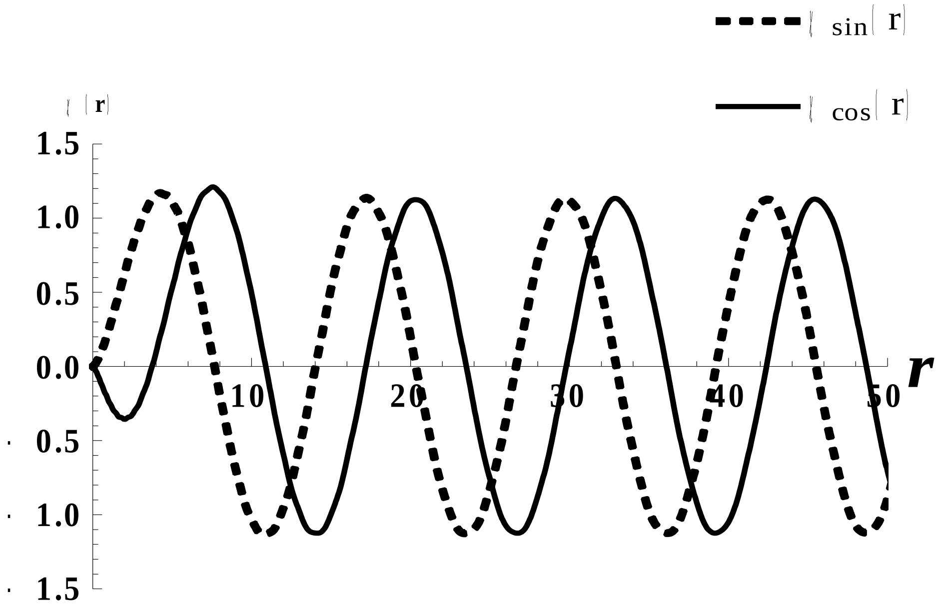

Fig. 3.3: Asymptotic plot of the sine-like and cosine-like solutions

CHAPTER 4

NUMERICAL RESULTS

4.1 Bound states for the Kratzer potential

To test the validity and show the utility of our 2D J-Matrix formalism we propose to consider the Kratzer potential as a model for the structure and dynamics of diatomic molecules and obtain the bound states and scattering phase shift for different diatomic molecules. Solutions of Schrodinger equation for motion of a particle under the influence of a central potential field is a very important problem in the field of theoretical Physics, as the solution thus obtained will help in understanding the structure and interaction of such system. One of such potential is the Kratzer potential, which was proposed a long time ago [65], and has been constantly revisited especially as its wave function can be used as basis set for diatomic molecules [66]. The role of Kratzer potential in the field of quantum and molecular chemistry cannot be overemphasized, owing to its extensive use in describing molecular structure and interactions [67-72]. Various numerical and analytical methods have been employed in solving Schrodinger equation with Kratzer potential in three dimensions, but not much has been done for two dimensional solutions. Some of the numerical approach for obtaining two and three dimensional solutions with Kratzer potential include Asymptotic iteration (AIM) [73], Supersymmetry (SUSY) [35], Exact quantization rule (EQR) [74], and the Nikifurov-Uvarov (NU) [75].

The Kratzer potential is defined by

$$V(r) = -D_e\left(\frac{2r_e}{r} - \frac{r_e^2}{r^2}\right)$$

(4.1.1)

where D_e is the dissociation energy and r_e is the equilibrium inter-nuclear separation. Figure 4.1 shows the shape of the Kratzer potential for different diatomic molecules, with minimum at r_e. The Kratzer potential is composed of both the coulombic repulsive part and the centripetal attractive part. The combinations of the two parts form an effective potential pocket, where a particle can be trapped in a Kratzer potential well. The r^{-1} term can be interpreted to be related to the coulombic potential energy for diatomic molecules, and the r^{-2} term is related to the electronic kinetic energy [76]. The figure also reveals that, as r goes to zero, V(r) goes to infinity owing to strong inter-nuclear orbital attraction, and as r goes to infinity, V(r) goes to zero.

The aim of this work is to present the two-dimensional J-matrix approach to calculate the non-zero angular momentum solution of the Schrodinger equation for the Kratzer potential and obtain the bound states for different diatomic molecules. It is important to study bound state processes so as to understand the molecular spectrum of diatomic molecules. The Kratzer potential was solved exactly in any arbitrary dimension D ≥ 2, and presented in the literature [74]. For D = 2 (two dimension), we obtain,

$$E_{n\ell} = -\left(\frac{2\mu {D_e}^2 {r_e}^2}{\hbar^2}\right)\left[n + \frac{1}{2} + \sqrt{\ell^2 + \frac{2\mu D_e {r_e}^2}{\hbar^2}}\right]^{-2} \qquad (4.1.2)$$

Here, μ is the reduced mass, which is equivalent to the mass M in our formalism.

The Kratzer potential is a singular potential with r^{-1} and r^{-2} singularities. Numerical solution is difficult to obtain as a result of the singularities. Hence, we need a numerical scheme like the J-matrix method where the singularities can be absorbed in the reference Hamiltonian and treated analytically.

In two dimension, the reference Hamiltonian can be absorbed as

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{2r^2} + \frac{\Omega}{r} \tag{4.1.3}$$

The Schrodinger equation can be described in the form (two dimensions)

$$\begin{aligned} H\psi(r) &= [H_0 + V(r)]\psi(r) = [-\frac{1}{2}\frac{d^2}{dr^2} + \frac{b^2 - 1/4}{2r^2} + \frac{Z}{r} + V(r)]\psi(r) \\ H\psi(r) &= -\frac{1}{2}\frac{d^2}{dr^2} + \frac{b^2 - 1/4}{2r^2} + \frac{Z}{r} + \frac{D_e r_e^2}{r^2} - \frac{2D_e r_e}{r} \end{aligned} \tag{4.1.4}$$

Comparing (4.1.3) and (4.1.4)

$$\begin{aligned} & m^2 - \tfrac{1}{4} = b^2 - \tfrac{1}{4} + 2D_e r_e^2 \\ & m = \pm\sqrt{b^2 + 2D_e r_e^2} \\ & \Omega = Z - 2D_e r_e \\ & \ell = |m| \end{aligned} \tag{4.1.5}$$

The above formalism set the stage for the code development.

To determine the existence of bound states and resonances, we consider an electron trapped in a Kratzer potential. Adding the two dimensional centrifugal barrier results in an effective potential:

$$V_{eff}(r) = \frac{D_e r_e^2}{r^2} - \frac{2D_e r_e}{r} + \frac{\ell^2 - 1/4}{2r^2} \tag{4.1.6}$$

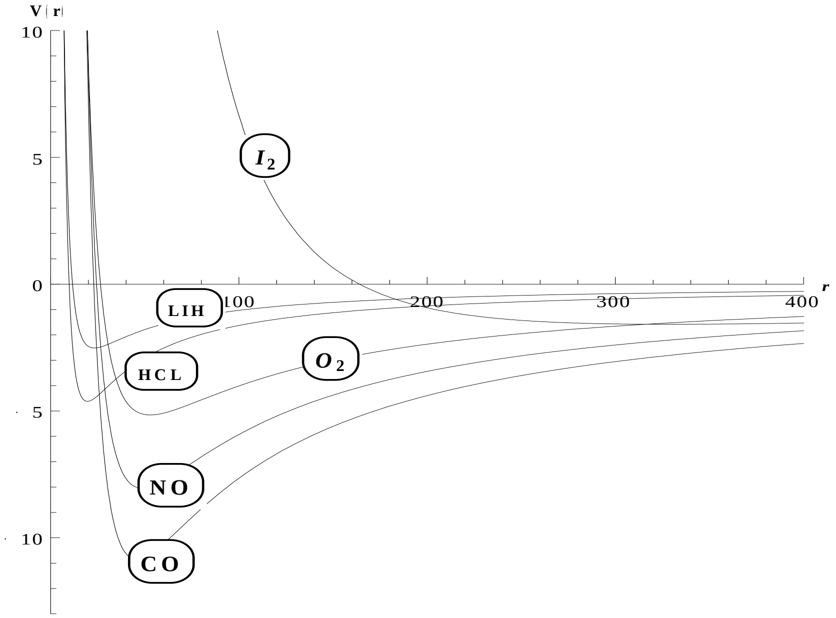

Figure 4.1: Shape of the Kratzer potential for relevant diatomic molecules

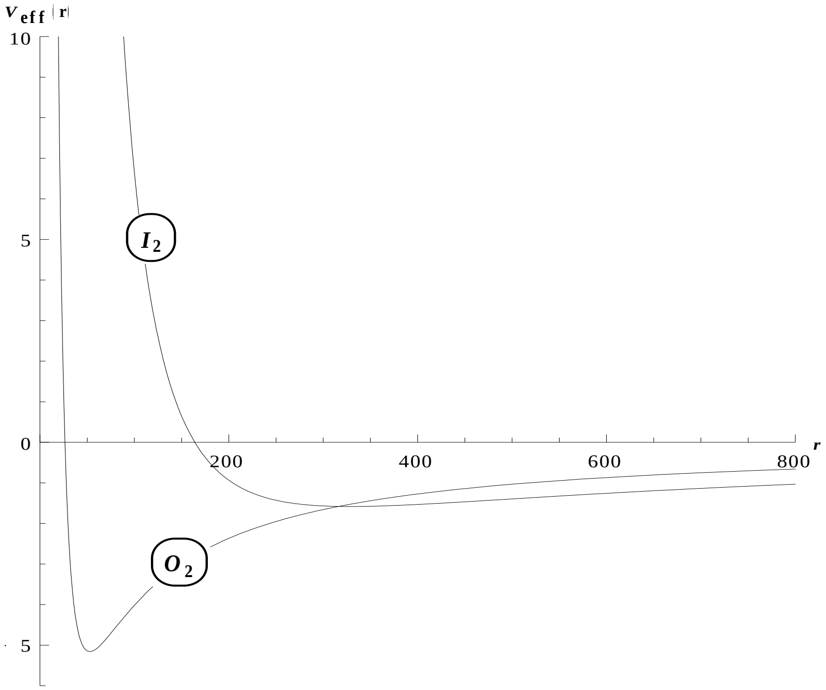

Figure 4.2: The effective Kratzer potential for relevant molecules at ℓ =1

Resonances occur if the Potential function contains a barrier behind which localization of positive energy electron exists. Mathematically, we first obtain the derivative of the effective potential with respect to r.

$$\frac{dV(r)}{dr} = -\frac{2D_e r_e^2 + m^2 - 1/4}{r^3} + \frac{2D_e r_e}{r^2}$$

$$\frac{dV(r)}{dr} = 0$$

$$r = \frac{2D_e r_e^2 + m^2 - 1/4}{2D_e r_e} \qquad (4.1.7)$$

$$g(r) = C$$

$$g(r) = r; C = \frac{2D_e r_e^2 + m^2 - 1/4}{2D_e r_e}$$

$$\frac{dg(r)}{dr} = 1$$

Since $\frac{dg(r)}{dr}$ is independent of r. Therefore V(r) has no extremum, and does not support resonance.

However, bound states exist in certain regions where $V_{eff}(r) < 0$ as shown in figure 4.2, that is, the minimum of the potential must be below the asymptote. We can therefore conclude that the Kratzer potential can support a finite number of bound states but no resonance.

4.2 Resonance states for the Inverted Kratzer potential

In continuation of our test for the validity of the 2D J-Matrix formalism, we choose to consider the inverted Kratzer potential, having been treated as a model for electron scattering by negative ions [77], and obtain the resonances for different potential parameter. The inverted Kratzer potential is defined by

$$V(r) = \frac{1}{r} - \frac{f}{2r^2} \tag{4.2.1}$$

where $f > 0$. We calculated the resonances for the inverted Kratzer potential in two-dimensional for first few n, ℓ quantum numbers with model parameter f = 5, 10, 20, and 50 and compare the results obtained with the exact analytical solution given by Complex dimensional scaling [78], and 1/η expansion technique [79].

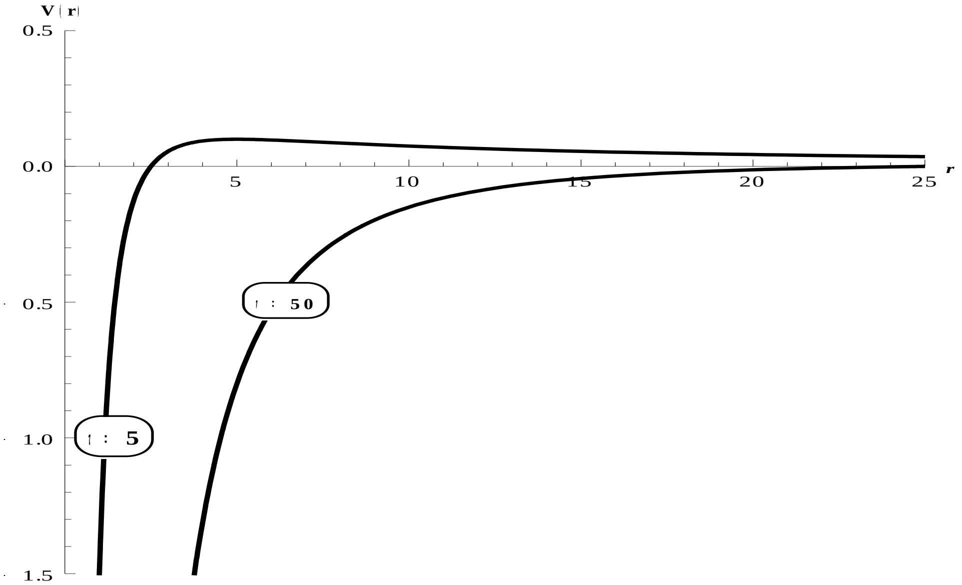

Fig. 4.3: inverted Kratzer potential for different values of *f*

Figure 4.3 shows the shape of the inverted Kratzer potential for different *f*. The inverted Kratzer potential is the sum of the columbic repulsive term, 1/r and the centripetal attractive term, - $f/2r^2$. $V(r)$ goes to a maximum at r = *f*, and as *r* goes to infinity, $V(r)$ goes to zero from above.

The inverted Kratzer potential was solved exactly in any arbitrary dimension D, and presented in the literature [78, 79]. For D = 2 (two dimension), we obtain the corresponding complex energy eigenvalue, $E = E_r - \frac{i}{2}\Gamma$ as,

$$E_r = \frac{(f - (n + \frac{1}{2})^2 - \ell^2)}{2(f + (n + \frac{1}{2})^2 - \ell^2)^2}$$
$$\Gamma = \frac{((2n+1)\sqrt{f - \ell^2})}{(f + (n + \frac{1}{2})^2 - \ell^2)^2} \qquad (4.2.2)$$

The Kratzer and inverted Kratzer potential are singular potentials with r^{-1} and r^{-2} singularities, hence, we need a numerical scheme like the J-matrix method where the singularities can be handled and treated analytically. Based on the theoretical formalism, the important parameters needed to ensure stability, accuracy, and convergence of our computational procedure are λ, θ, and N.

Numerical computations were carried out with the standard parameters in Table 4.1 [80-82] using the Laguerre basis set with N = 150 for the diatomic molecules. The energy eigenvalues obtained (Table 4.2-4.11) using the J-matrix approach is in excellent agreement with the exact results up to the precision that maintained numerical stability. At such significant digit, the numbers are rather truncated than rounded off.

4.3 Phase-shift for the Inverted Kratzer potential

Using the sine- and cosine-like solutions obtained above, we can write the asymptotic solution to the full scattering problem, $H = H_0 + V$, as

$$\lim_{r\to\infty} \psi(r,E) = \chi_-(r,E) + e^{2\mathrm{i}\delta(E)}\chi_+(r,E)\,, \tag{4.3.1}$$

where $\chi_\pm(r,E) = \chi_{\cos}(r,E) \pm \mathrm{i}\,\chi_{\sin}(r,E)$ and $\delta(E)$ is the energy-dependent phase shift that contains the contribution of the short range scattering potential $V(r)$. We calculate $\delta(E)$ using the conventional formulation of the S-matrix in the J-matrix formalism [1-2], which reads as follows

$$S(E) = e^{2\mathrm{i}\delta(E)} = T_{N-1}(E)\,\frac{1 + g_{N-1,N-1}(E)\,J_{N-1,N}(E) R_N^-(E)}{1 + g_{N-1,N-1}(E)\,J_{N-1,N}(E) R_N^+(E)}\,, \tag{4.3.2}$$

for some large enough integer N and where $T_n = \dfrac{c_n - \mathrm{i}s_n}{c_n + \mathrm{i}s_n}$, $R_n^{\pm} = \dfrac{c_n \pm \mathrm{i}s_n}{c_{n-1} \pm \mathrm{i}s_{n-1}}$ and $J_{n-1,n} = \frac{1}{2}\lambda^2\left(\frac{1}{4}+\mu^2\right)\sqrt{n(n+2\ell)}$. The finite Green's function $g_{N-1,N-1}(E)$ could be written in the Laguerre basis as follows

$$g_{N-1,N-1}(E) = \frac{1}{N+2\ell}\left[\prod\nolimits_{m=0}^{N-2}\left(\tilde{\varepsilon}_m - E\right)\Big/\prod\nolimits_{n=0}^{N-1}\left(\varepsilon_n - E\right)\right], \qquad (4.3.3)$$

Where $\{\varepsilon_n\}_{n=0}^{N-1}$ is the set of eigenvalues of the finite $N\times N$ matrix representation of the total Hamiltonian in the basis and $\{\tilde{\varepsilon}_n\}_{n=0}^{N-2}$ are the eigenvalues of the truncated H obtained by deleting the last row and last column. For the phase shift computation, we considered the scattering region E>0, and examine energy and angular momentum dependence on the phase shift.

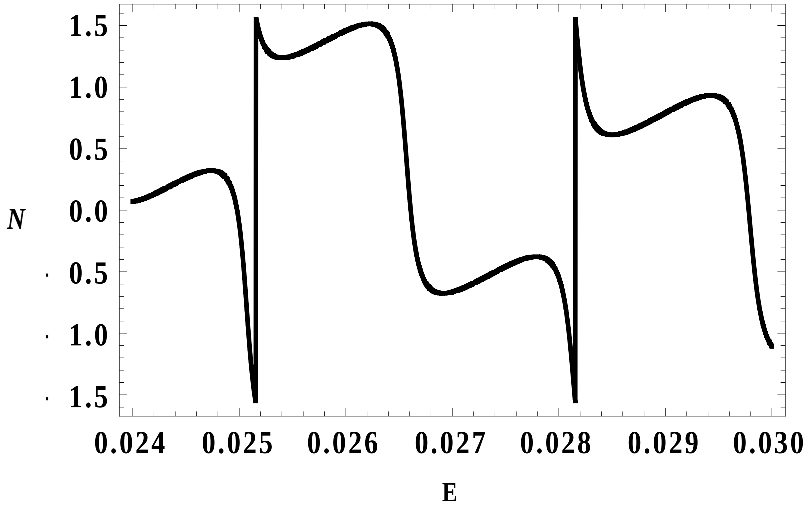

Fig. 4.4: Scattering phase shift $\delta(E)$ as a function of energy for Er = 0.0266-i0355, with f = 10 and ℓ =1.

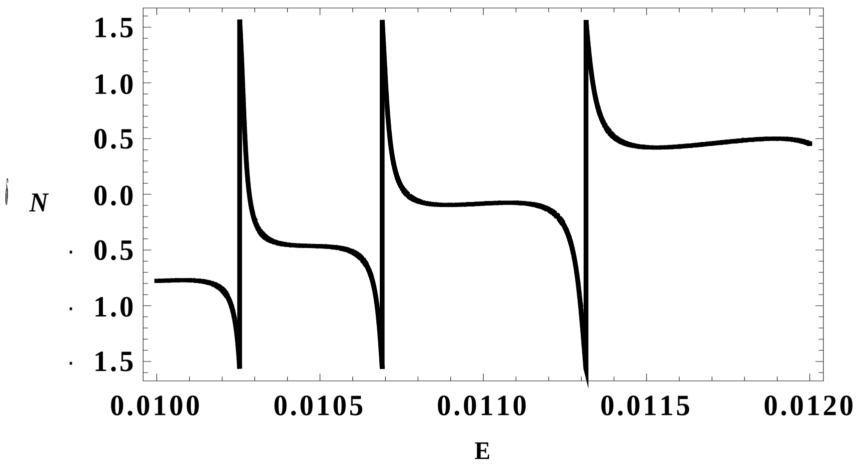

Fig. 4.5: Scattering phase shift $\delta(E)$ as a function of energy for Er = 0.0107-i0.00158, with f =50 and ℓ =2.

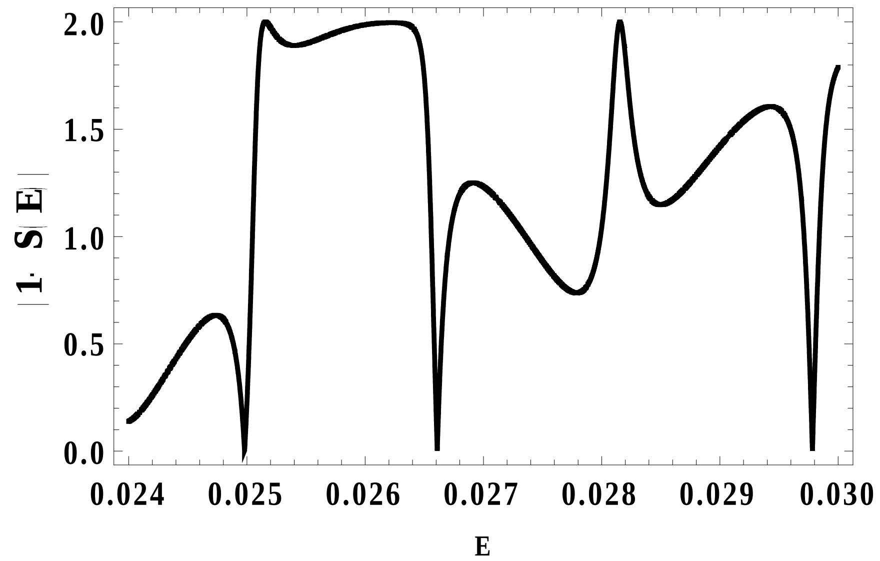

Fig. 4.6: Plot of Abs[1-S(E)] as a function of energy for Er = 0.0266-i0355, with

f =10 and ℓ =1.

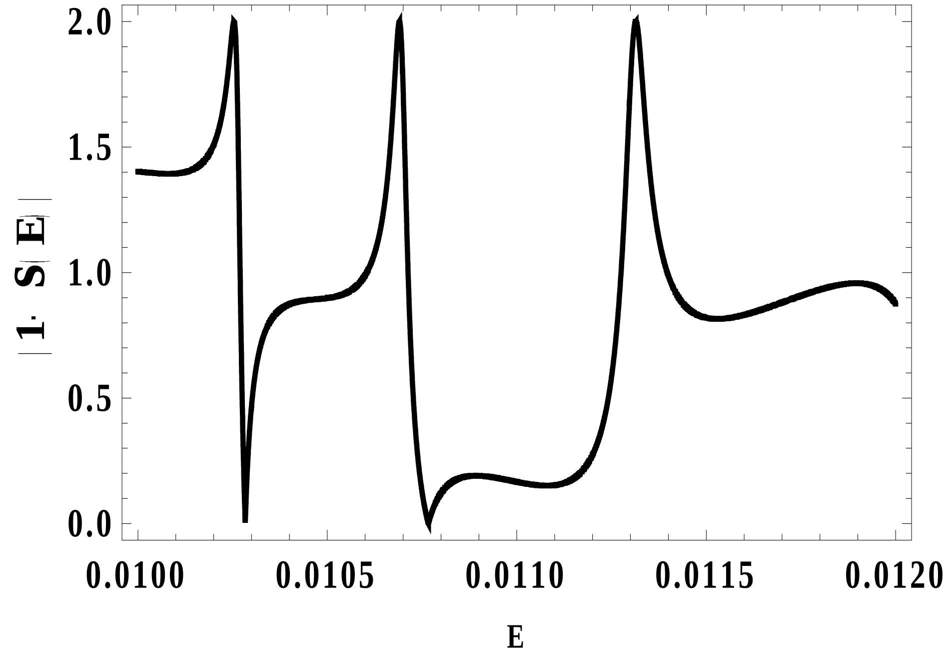

Fig. 4.7: Plot of Abs[1-S(E)] as a function of energy for Er = 0.01069- i0.00158, with *f* =50 and ℓ =2.

The above plots in Figures 4.4 to 4.7 shows that the Phase-shift and S-matrix are function of continuous energy. It also shows the resonance position (Er) of the resonance energy. That is 0.0266 in 4.4 and 4.6, and 0.01069 at 4.5 and 4.7. There is usually a pi-jump at the resonance energy as evident in these Plots.

Table 4.1: Reduced masses and spectroscopically determined properties of various diatomic molecules in the ground electronic state.

Parameters	LiH	I_2	O_2	HCl	NO	CO
D_e(eV)	2.515	1.582	5.157	4.619	8.044	10.845
r_e (A)	1.5956	2.662	1.208	1.2746	1.1508	1.1282
M (amu)	0.8801	63.4522	7.9975	0.9801	7.4684	6.8606

Table 4.2: Bound state energy eigenvalues of the Kratzer potential for LIH molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 3 to 8, N = 50)

ℓ	n	J-matrix	Exact
0	0	-2.4675368690593	-2.46753686905937
	1	-2.3760332946313	-2.37603329463134
	2	-2.2895267624327	-2.28952676243272
1	0	-2.4666308607095	-2.46663086070953
	1	-2.3751772079391	-2.37517720793913
	2	-2.2887169961193	-2.28871699611938
2	0	-2.4639168327684	-2.46391683276841
	1	-2.3726126718978	-2.37261267189782
	2	-2.2862911715811	-2.28629117158112

Table 4.3: Bound state energy eigenvalues of the Kratzer potential for HCL molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 4 to 10, N = 50)

ℓ	n	J-matrix	Exact
0	0	-4.542168208642	-4.5421682086427
	1	-4.3940324280697	-4.39403242806973
	2	-4.2530270471624	-4.25302704716240
1	0	-4.5408885637942	-4.54088856379422
	1	-4.3928148662300	-4.39281486623009
	2	-4.2518676164012	-4.25186761640124
2	0	-4.5370539607935	-4.53705396079355
	1	-4.3891662514363	-4.38916625143635
	2	-4.2483931537989	-4.24839315379893

Table 4.4: Bound state energy eigenvalues of the Kratzer potential for O_2 molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 5 to 9, N = 50)

ℓ	n	J-matrix	Exact
0	0	-5.1264030057928	-5.12640300579288
	1	-5.066684759179	-5.0666847591794
	2	-5.0080039672929	-5.00800396729292
1	0	-5.1262254913468	-5.12622549134686
	1	-5.0665103374949	-5.06651033749491
	2	-5.0078325669400	-5.00783256694002
2	0	-5.1256930218180	-5.12569302181801
	1	-5.0659871446473	-5.06598714464731
	2	-5.0073184365280	-5.00731843652801

Table 4.5: Bound state energy eigenvalues of the Kratzer potential for NO molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers(λ varies from 5 to 10, N = 50)

ℓ	n	J-matrix	Exact
0	0	-8.0027118464015	-8.00271184640152
	1	-7.9215084717111	-7.92150847171110
	2	-7.8415348092590	-7.84153480925909
1	0	-8.0025021493716	-8.00250214937160
	1	-7.9213019582383	-7.92130195823834
	2	-7.8413314152258	-7.84133141522582
2	0	-8.0018731242557	-8.00187312425579
	1	-7.9206824825447	-7.92068248254473
	2	-7.8407212966315	-7.84072129663154

Table 4.6: Bound state energy eigenvalues of the Kratzer potential for CO molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 7 to 10, N = 50)

ℓ	n	J-matrix	Exact
0	0	-10.7943747372950	-10.79437473729500
	1	-10.6938985116027	-10.69389851160270
	2	-10.5948186640957	-10.59481866409570
1	0	-10.7941370706252	-10.79413707062520
	1	-10.6936641555550	-10.69366415555500
	2	-10.59458755746670	-10.59458755746670
2	0	-10.79342413344230	-10.79342413344300
	1	-10.69296114914730	-10.69296114914730
	2	-10.5938942982473	-10.59389429824730

Table 4.7: Bound state energy eigenvalues of the Kratzer potential for I_2 molecule (in eV) with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 3 to 4, N = 50)

ℓ	n	J-matrix	Exact
0	0	-1.5790838270852	-1.57908382708525
	1	-1.5736883946428	-1.57368839464281
	2	-1.5683205677989	-1.56832056779893
1	0	-1.5790791906147	-1.57907919061474
	1	-1.5736837819149	-1.57368378191490
	2	-1.5683159786517	-1.56831597865178
2	0	-1.5790652813666	-1.57906528136663
	1	-1.5736699438935	-1.57366994389352
	2	-1.5683022113716	-1.56830221137165

Table 4.8: Resonances of the inverted Kratzer potential for *f* = 50 with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 0.2 to 1.2, N = 30)

ℓ	n	J-matrix	Exact
0	0	0.00985-0.001400 i	0.009851-0.0014001 i
	1	0.00874-0.003885 i	0.008745-0.0038851 i
	2	0.00691-0.005587 i	0.006913-0.0055870 i
1	0	0.01004-0.00144 i	0.010049-0.001442 i
	1	0.00889-0.00399 i	0.008899-0.003997 i
	2	0.00700-0.00573 i	0.007002-0.005732 i
2	0	0.01069-0.00158 i	0.010693-0.001585 i
	1	0.00939-0.00436 i	0.009396-0.004369 i
	2	0.00728-0.00621 i	0.007280-0.006210 i

Table 4.9: Resonances of the inverted Kratzer potential for *f* = 20 with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 0.2 to 3.0, N = 30)

ℓ	n	J-matrix	Exact
0	0	0.0240-0.0054 i	0.02408-0.00545 i
	1	0.0179-0.0135 i	0.01792-0.01355 i
	2	0.0099-0.0162 i	0.00997-0.01622i
1	0	0.025-0.005 i	0.0252-0.0058 i
	1	0.018-0.014 i	0.0185-0.0144 i
	2	0.009-0.017 i	0.0099-0.0170 i
2	0	0.029-0.007 i	0.0298-0.0075 i
	1	0.020-0.018i	0.0206-0.0180 i
	2	0.009-0.020 i	0.0098-0.0201 i

Table 4.10: Resonances of the inverted Kratzer potential for *f* = 10 with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 0.2 to 3.0, N = 30)

ℓ	n	J-matrix	Exact
0	0	0.046400-0.015049 i	0.0464009-0.0150495 i
	1	0.025822-0.031609 i	0.0258225-0.0316096 i
	2	0.007100-0.029938 i	0.0071005-0.0299387 i
1	0	0.0511-0.0175 i	0.05113-0.01753 i
	1	0.0266-0.0355 i	0.02666-0.03555 i
	2	0.0059-0.0322 i	0.00591-0.03224 i
2	0	0.07360-0.03135 i	0.073600-0.031353 i
	1	0.02754-0.05398 i	0.027548-0.053983 i
	2	-0.00083-0.04080 i	-0.000832-0.040807 i

Table 4.11: Resonances of the inverted Kratzer potential for *f* = 5 with different values of the rotational ℓ and vibrational n quantum numbers (λ varies from 0.8 to 4.0, N = 30)

ℓ	n	J-matrix	Exact
0	0	0.08616-0.040563 i	0.086167-0.0405635 i
	1	0.02615-0.063811 i	0.026159-0.0638116 i
	2	-0.00493-0.044169 i	-0.004938-0.0441692 i
1	0	0.103806-0.055363 i	0.1038062-0.0553633 i
	1	0.022400-0.076800 i	0.0224000-0.0768000 i
	2	-0.010707-0.047590 i	-0.0107079-0.0475907 i
2	0	0.240000-0.320000 i	0.2400000-0.3200000 i
	1	-0.059171-0.142011 i	-0.0591715-0.1420118 i
	2	-0.049940-0.047562 i	-0.0499405-0.0475624 i

CHAPTER 5

CONCLUSION

To sum up, we have succeeded in formulating the 2D J-matrix. This step completes the J-matrix formalism in all physical dimensions [1, 11]. Through our journey in the J-matrix formalism we have realized that reduction in space dimension makes the problem more demanding and mathematically trickier, contrary to our expectation. The 2D J-matrix can be used to handle all scattering phenomena that take place in real 2D space such as those scattering problems related to surfaces or effective 2D scattering problem that result from the application of high magnetic field or other confining potentials. We have tested the validity of the formalism by checking the expected behavior of the two independent solutions whose expansion coefficient characterizes the kinetic part of the J-matrix formalism. We also used the formalism to find the bound states and resonances for exactly solvable potentials, we selected the Kratzer potential, and inverted Kratzer potential, respectively. Our results are in excellent agreement with the exact ones and the accuracy of our results can be controlled by fine-tuning the basis parameters and the size of the basis set. However, we should mention that the most general formulating of the 2D J-matrix in Cartesian coordinates, that is in absence of cylindrical symmetry, still awaits its formulation.

APPENDIX A

J-MATRIX SOLUTION OF THE REFERENCE PROBLEM IN THE OSCILLATOR BASIS

In this appendix, we evaluate the solutions of the reference Hamiltonian using the oscillator basis defined by

$$\phi_n(y) = A_n y^{\left(\frac{\ell}{2}+\frac{1}{4}\right)} e^{-y/2} L_n^{\nu}(y) \quad ; \quad y = (\lambda r)^2 \tag{A1}$$

where $\nu > -1$, and λ is a positive scale parameter. The normalization constant A_n is chosen in this basis to be $A_n = \sqrt{2\lambda\Gamma(n+1)/\Gamma(n+1+\nu)}$. The reference Hamiltonian H_0 is just the free kinetic energy operator. Therefore, the reference wave equation for the J-matrix is given by Eq. (3.2.8). Using the differential equation of the Laguerre polynomials [61], their differential formula and recursion relation we can show that the matrix representation of the wave operator J will be tridiagonal only if $\nu = \ell$ giving

$$\begin{gathered}\frac{2}{\lambda^2} J_{mn}(E) = \frac{2}{\lambda^2} \langle \phi_m | H_0 - E | \phi_n \rangle = \\ \left[\left(2n+\ell+1-x\right)\delta_{n,m} + \sqrt{n(n+\ell)}\,\delta_{n,m+1} + \sqrt{(n+1)(n+\ell+1)}\,\delta_{n,m-1} \right]\end{gathered} \tag{A2}$$

where $x = \mu^2 = (k/\lambda)^2 = 2E/\lambda^2$. Thus, the expansion coefficients of the regular solution obey the following symmetric three-term recursion relation

$$\left(2n+\ell+1-x\right)s_n + \sqrt{n(n+\ell)}\,s_{n-1} + \sqrt{(n+1)(n+\ell+1)}\,s_{n+1} = 0\,. \tag{A3}$$

Using the following transformation to get rid of the square roots

$$s_n(x) = B_\ell (-1)^n \sqrt{\tfrac{\Gamma(n+1)}{\Gamma(n+\ell+1)}}\, Q_n(x)\,, \tag{A4}$$

with B_ℓ being a normalization constant that dependents on ℓ and will be fixed later. Equation (B3) reduces to

$$\begin{aligned}&\left(2n+\ell+1-x\right)Q_n-(n+1)Q_{n+1}-(n+\ell)Q_{n-1}=0\\&\left(\ell+1-x\right)Q_0-Q_1=0\end{aligned} \tag{A5}$$

Comparing the above equation with the one associated with generalized Laguerre polynomials

$$\left(2n+\sigma+1-x\right)L_n^\sigma-(n+1)L_{n+1}^\sigma-(n+\sigma)L_{n-1}^\sigma=0 \tag{A6}$$

We can deduce that $Q_n(x)=L_n^\ell(x)$ up to an overall factor that is independent of *n*. Similar to what we did for the Laguerre basis in the main text; we use direct integration and identify the regular solution of the reference wave equation with the sine-like solution

$$\begin{aligned}\chi_{reg}(E,y)&=\sqrt{2\mu}\,y^{1/4}J_\ell(\mu\sqrt{y})\\&=\sum_{n=0}^{\infty}s_n(\mu)\phi_n(y)=\sum_{n=0}^{\infty}s_n(\mu)A_n y^{\frac{\ell}{2}+\frac{1}{4}}e^{-y/2}L_n^\ell(y)\end{aligned} \tag{A7}$$

Using the orthogonality of the Laguerre polynomials, we obtain

$$s_n(E)=\sqrt{\frac{\mu\Gamma(n+1)}{\lambda\Gamma(n+\ell+1)}}\int_0^\infty y^{\ell/2}e^{-y/2}J_\ell(\mu\sqrt{y})L_n^\ell(y)dy\ . \tag{A8}$$

The result of this integral can be obtained from [62b] to give

$$s_n(E)=2(-1)^n\sqrt{\frac{\Gamma(n+1)}{\lambda\Gamma(n+\ell+1)}}\ \mu^{\ell+\frac{1}{2}}e^{-\mu^2/2}L_n^\ell(\mu^2)\,. \tag{A9}$$

Using the differential equation of the Laguerre polynomials, one can show that the sine-like coefficients (A9) satisfy the following second order energy differential equation

$$\hat{D}\, s_n(E) = \left[x\,\frac{d^2}{dx^2} + \frac{1}{2}\frac{d}{dx} - \frac{\ell^2 - 1/4}{4x} - \frac{1}{4}x + \frac{1}{2}\left(2n + \ell + 1\right) \right] s_n(E) = 0\,. \qquad \text{(A10)}$$

From this exact result, we can deduce the pre-factor in the transformation (A4) as $B_\nu = \frac{2}{\sqrt{\lambda}}\mu^{l+\frac{1}{2}} e^{-\mu^2/2}$. The expansion coefficients in the second regularized cosine-like solution,

$$\chi_{\cos}^{\nu}(r,E) \equiv \sum_{n=0}^{\infty} c_n(E)\phi_n(y)\,, \qquad \text{(A11)}$$

Which obey the same recursion relation (A3) but with the inhomogeneous initial condition

$$J_{00}\, c_0 + J_{01}\, c_1 = \gamma \quad ; \quad \gamma = -\frac{W}{2 s_0}\,, \qquad \text{(A12)}$$

Where W is the Wronskian of the two independent solutions. Using the transformation

(A4) in the form

$$c_n(x) = (-1)^n \sqrt{\frac{\Gamma(n+1)}{\Gamma(n+l+1)}}\, P_n(x)\,, \qquad \text{(A13)}$$

with P_n obeying the three term recursion relation

$$\begin{aligned} &\left(2n+\ell+1-\mu^2\right)P_n - (n+\ell)P_{n-1} - (n+1)P_{n+1} = 0 \\ &(\ell+1-\mu^2)P_0 - P_1 = \gamma \quad ; \quad \gamma = -\frac{k\sqrt{\lambda}}{\pi\,\lambda^2}\Gamma(\ell+1)\mu^{-\ell-\frac{1}{2}}\, e^{\mu^2/2} \end{aligned} \qquad \text{(A14)}$$

Following the same procedure for the Laguerre basis in the main text, the general solution of the recursion relation in A14 can be written in the form

$$P_n(\mu^2) = P_0(\mu^2)L_n^{\ell}(\mu^2) - \gamma L_n^{\ell}(\mu^2,1)\,, \qquad \text{(A15)}$$

where $L_n^\ell(x)$ are the normal Laguerre polynomials while $L_n^\ell(x,1)$ are the Laguerre polynomials of the second kind termed Wimp polynomials. They obey the same recursion relation as the Laguerre polynomials but with a recursion coefficient shifted by one unit (i.e., $n \to n+1$) [12]. Thus the cosine-like expansion coefficient are given by

$$c_n(\mu^2) = (-1)^n \sqrt{\frac{\Gamma(n+1)}{\Gamma(n+l+1)}} \left[P_0(\mu^2) L_n^\ell(\mu^2) - \gamma L_{n-1}^\ell(\mu^2,1) \right]. \qquad \text{(A16)}$$

To reduce the solution to a regularized one, we fixed the energy-dependent parameter P_0 , by taking γ = 0, our cosine-like solution in regularized form can be written as follows

$$\chi_{\cos}(r,E) = \chi_{\sin}(r,E) - \gamma \sum_{n=0}^{\infty} (-1)^n \sqrt{\frac{\Gamma(n+1)}{\Gamma(n+l+1)}} L_{n-1}^\ell(\mu^2,1) \phi_n(\lambda r) . \qquad \text{(A17)}$$

Having deduced all sine- and cosine-like coefficients, the two-dimensional J-matrix method in the Oscillator basis is completely defined.

APPENDIX B

The following are useful formulas and relations satisfied by the orthogonal polynomials that are relevant to the development carried out in this work. They are found in most books on orthogonal polynomials [62]. We list them here for ease of reference.

(1) The Laguerre polynomials $L_n^\nu(x)$, where $\nu > -1$:

$$xL_n^\nu = (2n+\nu+1)L_n^\nu - (n+\nu)L_{n-1}^\nu - (n+1)L_{n+1}^\nu \qquad \text{(B.1)}$$

$$L_n^\nu(x) = \tfrac{\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(\nu+1)}\, {}_1F_1(-n;\nu+1;x) \qquad \text{(B.2)}$$

$$\left[x\frac{d^2}{dx^2} + \left(\nu+1-x\right)\frac{d}{dx} + n\right]L_n^\nu(x) = 0 \qquad \text{(B.3)}$$

$$x\frac{d}{dx}L_n^\nu = nL_n^\nu - (n+\nu)L_{n-1}^\nu \qquad \text{(B.4)}$$

$$\int_0^\infty x^\nu e^{-x} L_n^\nu(x) L_m^\nu(x)\,dx = \tfrac{\Gamma(n+\nu+1)}{\Gamma(n+1)}\,\delta_{nm} \qquad \text{(B.5)}$$

(2) The Jacobi polynomials $P_n^{(\mu,\nu)}(x)$, where $\mu > -1, \nu > -1$:

$$\begin{aligned}\left(\tfrac{1\pm x}{2}\right)P_n^{(\mu,\nu)} &= \tfrac{2n(n+\mu+\nu+1)+(\mu+\nu)\left(\frac{\mu+\nu}{2}\pm\frac{\nu-\mu}{2}+1\right)}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\,P_n^{(\mu,\nu)} \\ &\pm \tfrac{(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}\,P_{n-1}^{(\mu,\nu)} \pm \tfrac{(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}\,P_{n+1}^{(\mu,\nu)}\end{aligned} \qquad \text{(B.6)}$$

$$P_n^{(\mu,\nu)}(x) = \tfrac{\Gamma(n+\mu+1)}{\Gamma(n+1)\Gamma(\mu+1)}\, {}_2F_1(-n, n+\mu+\nu+1;\mu+1;\tfrac{1-x}{2}) = (-)^n P_n^{(\nu,\mu)}(-x) \qquad \text{(B.7)}$$

$$\left\{\left(1-x^2\right)\frac{d^2}{dx^2} - \left[\left(\mu+\nu+2\right)x + \mu - \nu\right]\frac{d}{dx} + n\left(n+\mu+\nu+1\right)\right\}P_n^{(\mu,\nu)}(x) = 0 \qquad \text{(B.8)}$$

$$\left(1-x^2\right)\frac{d}{dx}P_n^{(\mu,\nu)} = -n\left(x+\frac{\nu-\mu}{2n+\mu+\nu}\right)P_n^{(\mu,\nu)} + 2\,\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\,P_{n-1}^{(\mu,\nu)} \tag{B.9}$$

$$\int_{-1}^{+1}(1-x)^{\mu}(1+x)^{\nu}P_n^{(\mu,\nu)}(x)P_m^{(\mu,\nu)}(x)dx = \frac{2^{\mu+\nu+1}}{2n+\mu+\nu+1}\,\frac{\Gamma(n+\mu+1)\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}\,\delta_{nm} \tag{B.10}$$

(3) The Pollaczek polynomials $P_n^{\mu}(x,\theta)$, where $\mu>0$ and $0<\theta<\pi$:

$$2\left[(n+\mu)\cos\theta + x\sin\theta\right]P_n^{\mu} - (n+2\mu-1)P_{n-1}^{\mu} - (n+1)P_{n+1}^{\mu} = 0 \tag{B.11}$$

$$P_n^{\mu}(x,\theta) = \frac{\Gamma(n+2\mu)}{\Gamma(n+1)\Gamma(2\mu)}\,e^{in\theta}\,{}_2F_1(-n,\mu+ix;2\mu;1-e^{-2i\theta}) \tag{B.12}$$

$$\int_{-\infty}^{+\infty}\rho^{\mu}(x,\theta)P_n^{\mu}(x,\theta)P_m^{\mu}(x,\theta)dx = \frac{\Gamma(n+2\mu)}{\Gamma(n+1)}\,\delta_{nm} \tag{B.13}$$

where $\rho^{\mu}(x,\theta) = \frac{1}{2\pi}(2\sin\theta)^{2\mu}e^{(2\theta-\pi)x}\left|\Gamma(\mu+ix)\right|^2$.

(4) The hyperbolic Pollaczek polynomials $P_n^{\mu}(x,\theta)$, where $\mu>0$ and θ > 0, are defined in terms of their recursion relation

$$2\left[(n+\mu)\cosh\theta + x\,\sinh\theta\right]P_n^{\mu} - (n+2\mu-1)P_{n-1}^{\mu} - (n+1)P_{n+1}^{\mu} = 0 \tag{B.14}$$

$$P_n^{\mu}(x,\theta) = P_n^{\mu}(-ix,i\,\theta) = \frac{\Gamma(n+2\mu)}{\Gamma(n+1)\Gamma(2\mu)}\,e^{-n\theta}\,{}_2F_1(-n,\mu+x;2\mu;1-e^{2\theta}) \tag{B.15}$$

$$\int_{-\infty}^{+\infty}\rho^{\mu}(x,\theta)P_n^{\mu}(x,\theta)P_m^{\mu}(x,\theta)dx = \frac{\Gamma(n+2\mu)}{\Gamma(n+1)}\,\delta_{nm} \tag{B.16}$$

Where $\rho^{\mu}(x,\theta) = \frac{1}{2\pi}(2\sinh\theta)^{2\mu}\left|\Gamma(\mu+x)\right|^2$

(5) The continuous dual Hahn polynomials $S_n^{\mu}(x;a,b)$, where $x^2>0$ and μ, a, b are positive except for a pair of complex conjugates with positive real parts:

$$\begin{aligned} x^2S_n^{\mu} &= \left[(n+\mu+a)(n+\mu+b)+n(n+a+b-1)-\mu^2\right]S_n^{\mu} \\ &\quad -n(n+a+b-1)S_{n-1}^{\mu}-(n+\mu+a)(n+\mu+b)S_{n+1}^{\mu} \end{aligned} \tag{B.17}$$

$$S_n^{\mu}(x;a,b) = {}_3F_2\left(\left.\begin{matrix}-n,\mu+ix,\mu-ix\\ \mu+a,\mu+b\end{matrix}\right|1\right) \tag{B.18}$$

$$\int_0^{\infty} \rho^{\mu}(x) S_n^{\mu}(x;a,b) S_m^{\mu}(x;a,b)\,dx = \frac{\Gamma(n+1)\Gamma(n+a+b)}{\Gamma(n+\mu+a)\Gamma(n+\mu+b)}\delta_{nm} \tag{B.19}$$

where $\rho^{\mu}(x) = \frac{1}{2\pi}\left|\frac{\Gamma(\mu+ix)\Gamma(a+ix)\Gamma(b+ix)}{\Gamma(\mu+a)\Gamma(\mu+b)\Gamma(2ix)}\right|^2$.

APPENDIX C

COMPUTATION OF INPUT PARAMETERS

The analytical result for bound states of Kratzer potential as evident in literature has been given in chapter 4, which is written below.

$$E_{n\ell} = -\left(\frac{2\mu D_e{}^2 r_e{}^2}{\hbar^2}\right)\left[n + \frac{1}{2} + \sqrt{\ell^2 + \frac{2\mu D_e r_e{}^2}{\hbar^2}}\right]^{-2} \tag{1}$$

The computed bound states in literatures were given in electron-volts (eV), as opposed to the J-matrix formalism used in this work, where we have used atomic mass units (a.m.u) with the assumption that $\hbar = M = \mu = 1$. To check with analytical results obtained in the literature, we have computed our results in eV.

For the purpose of computation, (1) can be re-written as

$$E_{n\ell} = -\left(\frac{B^2}{2}\right)\left[n + \frac{1}{2} + \sqrt{\ell^2 + 2A}\right]^{-2} \tag{2}$$

Where $A = \dfrac{\mu D_e r_e{}^2}{\hbar^2}$ and $B = \dfrac{2\sqrt{\mu} D_e r_e}{\hbar}$

Using the constants ($\hbar c = 1973.29 eV.A^0$, and $1 a.m.u = 931.5E06 eV / c^2$) and Table

4.1, the computed value of the input parameters in the calculation is summarized in the table below

Molecules	*A* (eV)	*B*
I_2	170143.0935	1037.5567
LIH	1348.27946	116.4698303
HCL	1759.445775	180.299614
O_2	14396.4751	544.9319609
NO	19032.3294	782.5392501
CO	22655.3469	991.3637385

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