TWO DIMENSIONAL J-MATRIX APPROACH TO QUANTUM SCATTERING

BY

ISMAIL ADEWALE OLUMEGBON

A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

PHYSICS

DECEMBER, 2013

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN- 31261, SAUDI ARABIA

DEANSHIP OF GRADUATE STUDIES

This thesis, written by **ISMAIL ADEWALE OLUMEGBON** under the direction his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN PHYSICS**.

Dr. Hocine Bahlouli
(Advisor)

Dr. Abdul Aziz Al-Jalal
Department Chairman

Dr. M.S. Abdelmonem
(Member)

Dr. Salam A. Zummo
Dean of Graduate Studies

Dr. Saeed Al-Marzoug
(Member)

6/2/14
Date

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

ACKNOWLEDGMENTS

It is important to state firstly that the writing of this thesis and my M.Sc Physics programme would not have been successful if not for the commitment, support and kindness of good people around me.

I would like to thank my thesis supervisor, Dr. Hocine Bahlouli, who was also instrumental to my joining the general Physics program upon leaving medical Physics. He saw my enthusiasm for theoretical Physics and gave the necessary academic support and research exposure. He facilitated my integration to the Saudi centre for theoretical Physics which made it possible for me to meet Professional Theoretical Physicist from different parts of the world. I say a big thank you.

In the same vein, I can only express my profound appreciation to other members of the thesis committee. I have learnt a lot from the superb computational skills of Dr. Saeed Al-Marzoug. He is solely responsible for the much I can do with Mathematica. In addition, he was always at hand to attend to my problems and correct my codes. Dr Abdelmonem treated me like a son and student. He was also my best critique of this thesis. He was not only concerned about my thesis, but also about how I become a better Theoretician.

To the chairman and faculty of the Physics department, I cannot thank you enough for providing a conducive academic atmosphere for me as a student. Most especially my teachers like Dr. Ibrahim Nasser whose support was crucial to the survival of my thesis.

Dr. Nabil Maalej and Dr. Khiari have also been helpful through their moral and academic support.

I would also like to acknowledge the support of Mr. Lateef Kareem on the successful implementation of this work. To other members of the Nigerian community, I indeed appreciate the moral and financial support of everyone especially Dr. S.O. Olatunji, Colleagues like Taoheed Owolabi and Ibrahim Alade, and my room- mate, Lookman Abdullah.

Above all, I would like to express my deepest love and appreciation to my loving wife, Lateefat, for her love, prayer, patience, support, and understanding throughout the period of this work. She experienced at first hand, my pains and frustrations at the critical stage of this work. She is indeed my backbone and life saver. Also, much thanks to my adorable daughter, Zainab, for her patience when daddy goes cranky.

Finally, I am very grateful to my mother for her consistent and persistent support and prayers. Of worthy mention is also my father and siblings for their unequivocal support and prayer at all times.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

Full Name : [Ismail Adewale Olumegbon]

Thesis Title : [Two dimensional J-matrix approach to quantum scattering]

Major Field : [Physics]

Date of Degree : [December, 2013]

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

عنوان الرسالة: تفسير التشتت الكمي بواسطة مصفوفة J ثناشية الأبعاد

التخصص: الفيزياء

تاريخ الدرجة العلمية: أكتوبر 2013م

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.

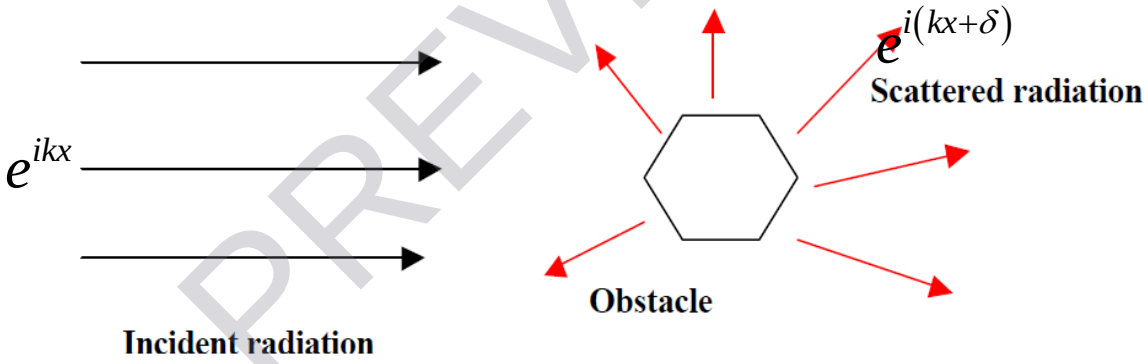

Figure 2.1: Schematic diagram of a typical scattering experiment

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