AN APPLICATION OF THE RAYLEIGH-RITZ METHOD TO THE INTEGRAL-EQUATION REPRESENTATION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
MIDDLE EAST TECHNICAL UNIVERSITY

BY

RUŞEN KAYA

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF MASTER OF SCIENCE
IN
MATHEMATICS

JULY 2019

Approval of the thesis:

AN APPLICATION OF THE RAYLEIGH-RITZ METHOD TO THE INTEGRAL-EQUATION REPRESENTATION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

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ABSTRACT

AN APPLICATION OF THE RAYLEIGH-RITZ METHOD TO THE INTEGRAL-EQUATION REPRESENTATION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

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July 2019, 52 pages

In this thesis, the theory of the relations between differential and integral equations is analyzed and is illustrated by the reformulation of the one-dimensional Schrödinger equation in terms of an integral equation employing the Green's function. The Rayleigh-Ritz method is applied to the integral-equation formulation of the one-dimensional Schrödinger equation in order to approximate the eigenvalues of the corresponding singular problem within the desired accuracy. The outcomes are compared with those resulting from the methods applied to the original formulation of the problem. Consecutive symmetries are observed throughout the symmetric structure of the problem, the symmetric Green's function, the symmetric potentials used in the method and the symmetric matrices obtained eventually.

Keywords: Integral Equations, Green's Function, Schrödinger equation, Rayleigh-Ritz Method

ÖZ

RAYLEIGH-RITZ YÖNTEMİNİN BİR BOYUTLU SCHRÖDINGER DENKLEMİNİN İNTEGRAL-DENKLEM GÖSTERİLİMİNE UYGULANMASI

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Tez Yöneticisi: Prof. Dr. Hasan Taşeli

Temmuz 2019, 52 sayfa

Bu tezde, diferansiyel ve integral denklemler arasındaki ilişkilerin teorisi incelenmiş ve bir boyutlu Schrödinger denkleminin Green fonksiyonu yardımıyla integral denklem olarak yeniden formülleştirilmesiyle örneklenmiştir. Karşılık gelen sonsuz problemin özdeğerlerini yaklaşık olarak istenilen doğrulukta hesaplamak için bir boyutlu Schrödinger denkleminin integral-denklem formülüne Rayleigh-Ritz yöntemi uygulanmıştır. Sonuçlar, problemin asıl formülüne uygulanan yöntemlerden elde edilenler ile karşılaştırılmıştır. Problemin simetrik yapısı, simetrik Green fonksiyonu, yöntemde kullanılan simetrik potansiyeller ve sonuç olarak elde edilen simetrik matrisler boyunca birbirini izleyen simetriler gözlenmiştir.

Anahtar Kelimeler: İntegral Denklemler, Green Fonksiyonu, Schrödinger Denklemi, Rayleigh-Ritz Yöntemi

To my wife

ACKNOWLEDGMENTS

I would like to express the greatest thankfulness to my supervisor, Prof. Dr. Hasan Taşeli, who has been not only an inspiration, but also a patient persuader to me in every part of this study.

I would also express my gratitude to each member of my family, to my wife, Elif, in particular, for their moral supports.

I would like to offer special thanks to Prof. Dr. Yıldıray Ozan, Prof. Dr. Songül Kaya Merdan, Dr. Muhiddin Uğuz, Prof. Dr. Melike Sayıl, Prof. Dr. Turgut Önder, Prof. Dr. Murat Yurdakul and Assoc. Prof. Dr. Mehmet Turan for their encouragements.

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LIST OF ABBREVIATIONS

2D	2 Dimensional
3D	3 Dimensional

CHAPTER 1

INTRODUCTION

"When you look at objects from different perspectives, the views fairly change. For instance, if you look at a cube through a bagel, you see an equator; if you look at it from one of its faces, you see a square; if you look at it from one of its edges, you see an angle. According to your point of view, you see objects and nature in different shapes as a result of your perception.", says Cahit Arf, the great mathematician, at the beginning of his speech within the scope of seminars of "Zeta Function Days" held in the Department of Mathematics of METU on May 26, 1991. One may define "mathematics" as a human endeavour to express the properties of infinite universe in terms of equations. In view of Cahit Arf's sentences, mathematicians develop varying techniques for the solutions of equations when they look at them from different perspectives. Differential equations, in particular, which form one of the vast field in engineering sciences and applied mathematics, require various methods to reach exact or numerical solutions. From one's perspective, a differential equation needs reducing to an algebraic equation by means of a numerical method. From our perspective, however, it is, equivalently, an integral equation in which the unknown function is presented under an integral sign.

Integral equations arise in many problems of mathematical physics and engineering sciences. Namely, they are used in potential theory, diffraction problems, water waves, conformal mapping and scattering in quantum mechanics. Other fields in which integral equations appear are functional analysis and stochastic process. Certain problems which are formulated by differential equations are solved more efficiently when they are formulated in terms of the corresponding integral equations. To be more precise, certain initial value or boundary value problems, together with the specified initial or boundary conditions, respectively, can be contracted into single integral-equation formulations. Conversely, certain integral equations can be converted into the corresponding initial value or boundary value problems. In other words, there exists an exact equivalence between initial value or boundary value problems and their corresponding integral-equation formulations. Furthermore, due to the fact that integration is a smooth process, more accurate outcomes are obtained through most of all numerical techniques applied to integral equations than those of the ones applied to differential equations when approximate solutions are searched for.

This thesis mainly involves the procedures composed of the construction of the equivalent integral-equation formulation of a famous quantum mechanical problem; namely, the one-dimensional Schrödinger equation, the employment of an advantageous numerical method; namely, the Rayleigh-Ritz method, to the formulation so obtained in order to compute the eigenvalues of the corresponding singular problem within the desired accuracy, and the comparison of the outcomes with those resulting from the methods applied to the original formulation of the one-dimensional Schrödinger equation. This thesis wherein an introductory theory of relations between differential and integral equations is elaborated and is supported by illustrative examples can also be regarded as a motivational guide for those who target further research in integral equations. The thesis also arouses interest in the sense that the one who reads it in a diligent manner will observe the advantages and firm consequences of **"symmetry"**. More precisely, throughout the thesis, there exists a succession of symmetries starting by the **symmetry** of the structure of our self-adjoint problem and persisting with the construction of the **symmetric** Green's function G, the process of the application of the numerical method in which reflective **symmetric** potentials are used and the achievement of **symmetric** matrices resulting from the eigenvalue problem brought about by the method. The effect of symmetry is observed not only on the reduction of orders of matrices but also on the elimination of complicated integrations and hence yields the simplicity of computations.

CHAPTER 2

INTEGRAL EQUATIONS

2.1 Definition and Classification of Integral Equations

A differential equation involves an unknown function y and its derivatives of several orders y', y'', ... , $y^{(n)}$. An integral equation, however, is an equation in which an unknown function y takes place under an integral sign. Integral equations are classified into two main categories: "linear integral equations" [2] and "nonlinear integral equations". Linear integral equations involve only linear forms of the unknown function y, whereas nonlinear integral equations involve some nonlinear functions of y. The following equations comprise two classifications of linear integral equations, which mainly hold our attention.

$$\alpha(x)y(x) = F(x) + \lambda \int_a^b K(x,\xi)y(\xi)d\xi \tag{2.1.1}$$

$$\alpha(x)y(x) = F(x) + \lambda \int_a^x K(x,\xi)y(\xi)d\xi, \tag{2.1.2}$$

where $x, \xi \in [a,b]$, $\lambda \neq 0$, a, b are constants, α, F, K are given functions and $y(x)$ is the unknown function. The given function $K(x,\xi)$ of the variables x and ξ is called the kernel of the integral equation.

Nonlinear integral equations, which are not considered here, can be illustrated with the following example

$$\alpha(x)y(x) = F(x) + \lambda \int_a^b K(x,\xi)[y(\xi)]^2 d\xi \tag{2.1.3}$$

due to the appearance of a nonlinear form $[y(\xi)]^2$ of the unknown function y in (2.1.3).

As we are back to our main concern, equations (2.1.1) and (2.1.2) are said to be the Fredholm equation and the Volterra equation, respectively. It is clear that the Volterra equation is obtained by interchanging the fixed upper limit of the integration in the Fredholm equation with the variable x.

Equations (2.1.1) and (2.1.2) are called the integral equations of the first kind if $\alpha(x) \equiv 0$, while they are called the equations of the second kind if $\alpha(x) \equiv 1$. The equations, in particular, are called homogeneous if $F(x) \equiv 0$. For example, a homogeneous Fredholm equation of the second kind is of the form

$$y(x) = \lambda \int_a^b K(x, \xi) y(\xi) d\xi. \qquad (21)$$

It is possible to rewrite an integral equation in the form of an equation of the second kind by means of a manipulation. For instance, when $\alpha(x) > 0$ for all $x \in [a, b]$, equation (2.1.1) can be converted into the form of

$$\sqrt{\alpha(x)}y(x) = \frac{F(x)}{\sqrt{\alpha(x)}} + \lambda \int_a^b \frac{K(x,\xi)}{\sqrt{\alpha(x)\alpha(\xi)}} \sqrt{\alpha(\xi)} y(\xi) d\xi, \qquad (2.1.4)$$

which is an integral equation of the second kind whose unknown function and altered kernel are $\sqrt{\alpha(x)}y(x)$ and $\dfrac{K(x,\xi)}{\sqrt{\alpha(x)\alpha(\xi)}}$, respectively. In addition, if the kernel $K(x,\xi)$ of (2.1.1) is symmetric; that is, if $K(x,\xi) = K(\xi, x)$, then the altered kernel $\dfrac{K(x,\xi)}{\sqrt{\alpha(x)\alpha(\xi)}}$ of (2.1.4) is also symmetric in the sense that $\dfrac{K(\xi,x)}{\sqrt{\alpha(\xi)\alpha(x)}} = \dfrac{K(x,\xi)}{\sqrt{\alpha(x)\alpha(\xi)}}$. Symmetric kernels are of great significance in linear integral equations as are symmetric matrices in linear algebra. The detailed consideration of linear integral equations with symmetric kernels is given by the Hilbert-Schmidt Theory [1].

Equation (2.1.1), by the way, possesses a continuous solution $y(x)$ provided that the given functions $F(x)$, $\alpha(x)$ and $K(x,\xi)$ are continuous in (a, b).

2.2 Relations between Differential and Integral Equations

Certain differential equations can be converted to integral equations and, conversely, certain integral equations can be transformed to differential equations. More specifically, certain initial value problems and boundary value problems are exactly equivalent to their corresponding integral-equation formulations. In Subsection 2.2.1, the procedure of showing the equivalence of an initial value problem and its corresponding integral-equation formulation is given for an illustrative example. Subsection 2.2.2, however, involves a complete construction of the integral-equation formulation of a boundary value problem by the determination of the Green's function.

2.2.1 Relations between Initial Value Problems and Integral Equations

The following lemma is required to indicate the strong relation between initial value problems and integral equations as an illustrative example.

Lemma 2.1.1. If f is an integrable function, then

$$\int_a^x \int_a^u f(t)dtdu = \int_a^x (x-\xi)f(\xi)d\xi$$

for some constant a.

Proof. Let

$$\int_a^x \int_a^u f(t)dtdu = y_1(x) \quad \text{and} \quad \int_a^x (x-\xi)f(\xi)d\xi = y_2(x).$$

Then, the fundamental theorem of calculus and the Leibnitz's Rule [7] yield

$$y_1'(x) = \int_a^x f(t)dt \quad \text{and} \quad y_2'(x) = \int_a^x f(\xi)d\xi, \quad \text{respectively.}$$

It is obvious that $y_1'(x) = y_2'(x)$. Therefore, $y_1(x)$ and $y_2(x)$ differ by some constant and that constant, however, is precisely zero since $y_1(x)$ and $y_2(x)$ both vanish at $x = a$, which simply follows that $y_1(x) = y_2(x)$.

Example 2.1.1. The initial value problem consisting of the linear second-order differential equation

$$y''(x) + p(x)y'(x) + q(x)y(x) = f(x) \tag{2.2.5}$$

and the initial conditions $y(a) = y_0$, $y'(a) = y_0'$ is equivalent to the Volterra equation of the second kind

$$y(x) = F(x) + \int_a^x K(x, \xi)y(\xi)d\xi, \tag{2.2.6}$$

where

$$F(x) = \int_a^x (x - \xi)f(\xi)d\xi + \big(p(a)y_0 + y_0'\big)(x - a) + y_0 \tag{2.2.7a}$$

and

$$K(x, \xi) = (\xi - x)\big(q(\xi) - p'(\xi)\big) - p(\xi). \tag{2.2.7b}$$

Solution. The exact equivalence of the initial value problem consisting of (2.2.5) with the specified initial conditions and the integral equation (2.2.6) is shown in two parts:

Part 1. Let us assume the initial value problem consisting of (2.2.5) and the specified initial conditions. Integration of each member of (2.2.5) over (a, x) leads to the equation

$$y'(x) - y_0' + \int_a^x p(t)y'(t)dt + \int_a^x q(t)y(t)dt = \int_a^x f(t)dt$$

and the evaluation of the first integral on the left by parts yields

$$y'(x) - y_0' + p(x)y(x) - p(a)y_0 - \int_a^x y(t)p'(t)dt = \int_a^x f(t)dt.$$

A second integration, together with the help of lemma (2.2.1), results in

$$\begin{aligned} y(x) &= \int_a^x (x - \xi)f(\xi)d\xi + \big(p(a)y_0 + y_0'\big)(x - a) + y_0 + \int_a^x [(\xi - x)\big(q(\xi) - p'(\xi)\big) - p(\xi)]y(\xi)d\xi \\ &= F(x) + \int_a^x K(x, \xi)y(\xi)d\xi, \end{aligned}$$

where $F(x)$ and $K(x, \xi)$ are the same as identified by (2.2.7a) and (2.2.7b).

Therefore, the integral equation (2.2.6) is deduced from the initial value problem consisting of (2.2.5) and the specified initial conditions.

Part 2. Conversely, given the Volterra equation of the second kind (2.2.6), differentiation of (2.2.6) leads to

$$y'(x) = F'(x) + K(x, x)y(x) + \int_a^x \frac{\partial K(x, \xi)}{\partial x} y(\xi)d\xi \tag{2.2.8}$$

with the help of the Leibnitz's Rule. Making use of the explicit forms (2.2.7a) and (2.2.7b) of $F(x)$ and $K(x,\xi)$, respectively, we rewrite

$$y'(x) = \int_a^x f(\xi)d\xi + p(a)y_0 + y_0' - p(x)y(x) + \int_a^x p'(\xi)y(\xi)d\xi - \int_a^x q(\xi)y(\xi)d\xi. \tag{2.2.9}$$

Integration of the fifth term on the right by parts gives

$$\begin{aligned} y'(x) = &\int_a^x f(\xi)d\xi + p(a)y_0 + y_0' - p(x)y(x) + p(x)y(x) \\ &- p(a)y(a) - \int_a^x p(\xi)y'(\xi)d\xi - \int_a^x q(\xi)y(\xi)d\xi \\ = &\int_a^x [f(\xi) - p(\xi)y'(\xi) - q(\xi)y(\xi)]d\xi + p(a)(y_0 - y(a)) + y_0'. \end{aligned} \tag{2.2.10}$$

A second differentiation of $y(x)$ results in

$$y''(x) = f(x) - p(x)y'(x) - q(x)y(x). \tag{2.2.11}$$

As a result of (2.2.11), we obtain

$$y''(x)+p(x)y'(x)+q(x)y(x) = f(x)-p(x)y'(x)-q(x)y(x)+p(x)y'(x)+q(x)y(x) = f(x).$$

That is, y satisfies the linear second-order differential equation (2.2.5). Further, setting $x = a$ in (2.2.6), (2.2.7a) and (2.2.10), we, respectively, acquire $F(a) = y(a)$, $F(a) = y_0$ and $y'(a) = y_0$.

It is consequently deduced that the Volterra equation of the second kind (2.2.6) is reduced to the initial value problem consisting of (2.2.5) and the specified initial conditions.

As a result of part 1 and part 2, the conclusion is drawn that the Volterra equation of the second kind (2.2.6) and the initial value problem consisting of the linear second-order differential equation (2.2.5) and the specified initial conditions are exactly equivalent.

2.2.2 Relations between Boundary Value Problems and Integral Equations (The Green's Function)

In this section, an equivalent integral-equation formulation of a boundary value problem is established by constructing the Green's function, whose definition is still in progress.

Let us start with the boundary value problem consisting of the differential equation

$$Ly(x) + \Phi(x) = 0 \tag{2.2.12}$$

and the boundary conditions

$$k_1 y(x) + k_2 y'(x) = 0 \tag{2.2.13}$$

at the end points of the interval $[a, b]$ for some constants k_1 and k_2, where L is the self-adjoint differential operator [1] defined by

$$L = \frac{d}{dx}\big(p(x)\frac{d}{dx}\big) + q(x) = p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} + q(x); \tag{2.2.14}$$

$\Phi(x)$ is of the form $\Phi(x) = \phi(x)$ or $\Phi(x) = \phi\big(x, y(x)\big)$; $p'(x)$, $q(x)$ are continuous and $p(x) \neq 0$ in (a, b).

To set up an equivalent integral-equation formulation of the problem, we first aim the construction of the Green's function $G(x)$ for a fixed value of ξ in the form of

$$G(x) = \begin{cases} G_1(x) & \text{if} \quad a < x \leq \xi \\ G_2(x) & \text{if} \quad \xi \leq x < b \end{cases}, \tag{2.2.15}$$

which supplies the following conditions:

C1. $LG_1(x) = 0$ and $LG_2(x) = 0$ whenever $x < \xi$ and $x > \xi$, respectively.

C2. $G_1(x)$ and $G_2(x)$ satisfy the specified boundary conditions (2.2.13) at $x = a$ and $x = b$, respectively.

C3. $G(x)$ is continuous at $x = \xi$, from its definition with $G_1(\xi) = G_2(\xi)$.

C4. The measure of the jump discontinuity of G' at $x = \xi$ is $\dfrac{-1}{p(\xi)}$; that is, $G_2'(\xi) - G_1'(\xi) = \dfrac{-1}{p(\xi)}$.

Then, we show the equivalence of the integral-equation formulation

$$y(x) = \int_a^b G(x,\xi)\Phi(\xi)d\xi \tag{2.2.16}$$

to the boundary value problem consisting of (2.2.12) and the specified boundary conditions such that (2.2.16) determines the solution $y(x)$ if $\Phi(x) = \phi(x)$, while (2.2.16) forms the corresponding formulation of the problem if $\Phi(x) = \phi\big(x, y(x)\big)$.
Before making a start on the construction of the Green's function, it is required to mention the following theorem known as Abel's formula [1].

Theorem 2.2.1 (Abel's Formula). If $u(x)$ and $v(x)$ satisfy the equation $Ly = 0$, where L is the differential operator $L = p(x)\dfrac{d^2}{dx^2} + p'(x)\dfrac{d}{dx} + q(x)$, then

$$u(x)v'(x) - u'(x)v(x) = \frac{c}{p(x)}$$

for some constant c whenever $p'(x)$, $q(x)$ are continuous and $p(x) \neq 0$ in an interval (a, b).

Proof. With the abbreviation of prime notation of derivative, we write

$$pu'' + p'u' + qu = 0 \tag{2.2.17}$$

$$pv'' + p'v' + qv = 0. \tag{2.2.18}$$

Multiplication of each member of equations (2.2.17) and (2.2.18) by v and u, respectively, and subtraction of the resulting equations lead to

$$p'(uv' - u'v) + p(uv'' - vu'') = 0,$$

which implies

$$p'(uv' - u'v) + p(uv' - vu')' = 0, \tag{2.2.19}$$

where $(uv' - vu')' = uv'' - vu''$.
An equivalent form of (2.2.19) is derived as $[p(uv' - vu')]' = 0$, which follows that

$$u(x)v'(x) - u'(x)v(x) = \frac{c}{p(x)} \tag{2.2.20}$$

for some constant c.

Construction of the Green's Function

To set up G, we propose two nontrivial solutions $u(x)$ and $v(x)$ of $Ly = 0$ with the associated boundary conditions (2.2.13) at $x = a$ for $u(x)$ and at $x = b$ for $v(x)$. Then, $G_1(x) = c_1 u(x)$ and $G_2(x) = c_2 v(x)$ automatically satisfy the conditions C1 and C2. It remains to set the values of c_1 and c_2 in terms of ξ. The conditions C3 and C4 imply $G_1(\xi) = G_2(\xi)$ and $G_2'(\xi) - G_1'(\xi) = \dfrac{-1}{p(\xi)}$, respectively. Then, one has

$$c_2 v(\xi) - c_1 u(\xi) = 0 \tag{2.2.21a}$$

$$c_2 v'(\xi) - c_1 u'(\xi) = \frac{-1}{p(\xi)}. \tag{2.2.21b}$$

The system of equations (2.2.21a) and (2.2.21b) possesses a unique solution for c_1 and c_2 if the Wronskian

$$W\big(u(\xi), v(\xi)\big) = \begin{vmatrix} u(\xi) & v(\xi) \\ u'(\xi) & v'(\xi) \end{vmatrix}$$

of the solutions u and v of $Ly = 0$ is nonzero. When u and v are linearly independent,

$$W\big(u(\xi), v(\xi)\big) = u(\xi)v'(\xi) - v(\xi)u'(\xi) \neq 0. \tag{2.2.22}$$

Employment Abel's formula for u and v gives rise to

$$u(\xi)v'(\xi) - v(\xi)u'(\xi) = \frac{c}{p(\xi)}, \tag{2.2.23}$$

where c is nonzero by (2.2.22). Multiplication of each member of (2.2.23) by $\frac{-1}{c}$ leads to $\frac{-u(\xi)}{c}v'(\xi) - \frac{-v(\xi)}{c}u'(\xi) = \frac{-1}{p(\xi)}$, where $\frac{-u(\xi)}{c}$ and $\frac{-v(\xi)}{c}$ stand for c_1 and c_2, respectively, in (2.2.21b).

The ultimate format of (2.2.15) becomes

$$G(x) = \begin{cases} \frac{-1}{c}u(x)v(\xi) & \text{if} \quad a < x \leq \xi \\ \frac{-1}{c}u(\xi)v(x) & \text{if} \quad \xi \leq x < b \end{cases}, \tag{2.2.24}$$

which completes the construction of G. It is clearly seen that the Green's function is symmetric; that is, $G(x,\xi) = G(\xi,x)$.

Equivalence of the integral-equation formulation (2.2.16) to the boundary value problem consisting of (2.2.12) and the specified boundary conditions is established in two parts:

Part 1 (Reduction of the formulation (2.2.16) **to the boundary value problem consisting of** (2.2.12) **and the specified boundary conditions).**

Let us start by substituting the explicit form (2.2.24) of G into (2.2.16). Then, we obtain

$$y(x) = \frac{-1}{c}\Big[\int_a^x v(x)u(\xi)\Phi(\xi)d\xi + \int_x^b u(x)v(\xi)\Phi(\xi)d\xi\Big]. \tag{2.2.25}$$

Differentiation of each member of (2.2.25) yields

$$y'(x) = \frac{-1}{c}\left[v(x)u(x)\Phi(x) + \int_a^x v'(x)u(\xi)\Phi(\xi)d\xi - u(x)v(x)\Phi(x) + \int_x^b u'(x)v(\xi)\Phi(\xi)d\xi\right]$$
$$= \frac{-1}{c}\left[\int_a^x v'(x)u(\xi)\Phi(\xi)d\xi + \int_x^b u'(x)v(\xi)\Phi(\xi)d\xi\right]. \tag{2.2.26}$$

Second differentiation of $y(x)$ leads to

$$y''(x) = \frac{-1}{c}\left[\int_a^x v''(x)u(\xi)\Phi(\xi)d\xi + \int_x^b u''(x)v(\xi)\Phi(\xi)d\xi\right] - \frac{1}{c}\big[v'(x)u(x) - u'(x)v(x)\big]\Phi(x). \tag{2.2.27}$$

By recalling that $Ly = py'' + p'y' + qy$ and that u and v satisfy (2.2.20), equation (2.2.27) is transformed into

$$\begin{aligned}
Ly(x) = &\frac{-1}{c}\left[p(x)\int_a^x v''(x)u(\xi)\Phi(\xi)d\xi + p(x)\int_x^b u''(x)v(\xi)\Phi(\xi)d\xi\right] - \frac{p(x)}{c}\frac{c}{p(x)}\Phi(x) \\
&- \frac{1}{c}\left[p'(x)\int_a^x v'(x)u(\xi)\Phi(\xi)d\xi + p'(x)\int_x^b u'(x)v(\xi)\Phi(\xi)d\xi\right] \\
&- \frac{1}{c}\left[q(x)\int_a^x v(x)u(\xi)\Phi(\xi)d\xi + q(x)\int_x^b u(x)v(\xi)\Phi(\xi)d\xi\right] \\
= &-\frac{1}{c}\Bigg[\int_a^x \big[p(x)v''(x) + p'(x)v'(x) + q(x)v(x)\big]u(\xi)\Phi(\xi)d\xi \\
&\qquad + \int_x^b \big[p(x)u''(x) + p'(x)u'(x) + q(x)u(x)\big]v(\xi)\Phi(\xi)d\xi\Bigg] - \Phi(x) \\
= &-\frac{1}{c}\left[\int_a^x Lv(x)u(\xi)\Phi(\xi)d\xi + \int_x^b Lu(x)v(\xi)\Phi(\xi)d\xi\right] - \Phi(x) \\
= &-\Phi(x),
\end{aligned}$$

where $Lv(x) = 0 = Lu(x)$. Therefore, (2.2.16) implies (2.2.12).
Moreover, imposing $x = a$ on (2.2.25) and (2.2.26), we obtain

$$y(a) = \frac{-1}{c}u(a)\int_a^b v(\xi)\Phi(\xi)d\xi \tag{2.2.28a}$$

and

$$y'(a) = \frac{-1}{c} u'(a) \int_a^b v(\xi)\Phi(\xi) d\xi, \tag{2.2.28b}$$

respectively. Multiplying each member of (2.2.28a) and (2.2.28b) by $u'(a)$ and $u(a)$, respectively, we observe the equality $u'(a)y(a) = u(a)y'(a)$, which is equivalent to $u'(a)y(a) + \big(-u(a)\big)y'(a) = 0$, where $u'(a)$ and $-u(a)$ are the constants which stand for k_1 and k_2 in (2.2.13). A similar process guarantees the fulfillment of the condition for $x = b$. Therefore, y, determined by the formulation (2.2.16), satisfies the specified boundary conditions.

Part 2 (Deduction of the formulation (2.2.16) **from the boundary value problem consisting of** (2.2.12) **and the specified boundary conditions).**
Let us start by the simple equality

$$\int_a^b G(x,\xi)\Phi(x)dx = \int_a^b G(x,\xi)\big[-Ly(x)\big]dx = -\int_a^b G(x,\xi)\big[Ly(x)\big]dx. \tag{2.2.29}$$

Dividing the interval of the right member of (2.2.29) into two subintervals and applying the self-adjoint operator L in (2.2.14) to $y(x)$, we obtain

$$\begin{aligned}\int_a^b G(x,\xi)\Phi(x)dx &= -\int_a^\xi G_1(x,\xi)\big[\big(p(x)y'(x)\big)' + q(x)y(x)\big]dx \\ &\quad - \int_\xi^b G_2(x,\xi)\big[\big(p(x)y'(x)\big)' + q(x)y(x)\big]dx \\ &= -\int_a^\xi G_1(x,\xi)\big[\big(p(x)y'(x)\big)'\big]dx - \int_\xi^b G_2(x,\xi)\big[\big(p(x)y'(x)\big)'\big]dx \\ &\quad - \int_a^\xi G_1(x,\xi)q(x)y(x)dx - \int_\xi^b G_2(x,\xi)q(x)y(x)dx.\end{aligned} \tag{2.2.30}$$

Integration of the first two members by parts and condensation of the other members on the right of (2.2.30) yield

$$\int_a^b G(x,\xi)\Phi(x)dx = -p(\xi)G_1(\xi)y'(\xi) + G_1(a)p(a)y'(a) + \int_a^\xi G_1'(x)p(x)y'(x)dx \\ - G_2(b)p(b)y'(b) + G_2(\xi)p(\xi)y'(\xi) + \int_\xi^b G_2'(x)p(x)y'(x)dx \\ - \int_a^b G(x,\xi)q(x)y(x)dx. \tag{2.2.31}$$

By recalling that any linear combination (2.2.13) of the function $y(x)$ and its derivative $y'(x)$ vanishes at the endpoints of the interval $[a, b]$ due to the homogeneous specified boundary conditions, equation (2.2.31) is abbreviated as

$$\int_a^b G(x,\xi)\Phi(x)dx = -p(\xi)G_1(\xi)y'(\xi) + \int_a^\xi G_1'(x)p(x)y'(x)dx \\ + G_2(\xi)p(\xi)y'(\xi) + \int_\xi^b G_2'(x)p(x)y'(x)dx \\ - \int_a^b G(x,\xi)q(x)y(x)dx. \tag{2.2.32}$$

Due to the third condition C3 of G, (2.2.32) takes the simple form

$$\int_a^b G(x,\xi)\Phi(x)dx = \int_a^\xi G_1'(x)p(x)y'(x)dx + + \int_\xi^b G_2'(x)p(x)y'(x)dx \\ - \int_a^b G(x,\xi)q(x)y(x)dx. \tag{2.2.33}$$

Integration of the first two terms on the right of (2.2.33) by parts and employment of the specified boundary conditions lead to

$$\int_a^b G(x,\xi)\Phi(x)dx = G_1'(\xi)p(\xi)y(\xi) - \int_a^\xi \big(G_1'(x)p(x)\big)'y(x)dx \\ - G_2'(\xi)p(\xi)y(\xi) - \int_\xi^b \big(G_2'(x)p(x)\big)'y(x)dx \\ - \int_a^b G(x,\xi)q(x)y(x)dx. \tag{2.2.34}$$

Conditions C1 and C4 of G simplify (2.2.34) to

$$\begin{aligned}\int_a^b G(x,\xi)\Phi(x)dx &= \int_a^\xi G_1(x,\xi)q(x)y(x)dx + \int_\xi^b G_2(x,\xi)q(x)y(x)dx \\ &\quad - \int_a^b G(x,\xi)q(x)y(x)dx + p(\xi)\frac{1}{p(\xi)}y(\xi) \\ &= y(\xi).\end{aligned} \tag{2.2.35}$$

Changing the variables in (2.2.35) and using the symmetry of $G(x,\xi)$, we ultimately obtain

$$\int_a^b G(x,\xi)\Phi(\xi)d\xi = \int_a^b G(\xi,x)\Phi(\xi)d\xi = y(x).$$

Hence, the integral-equation formulation (2.2.16) is deduced from the boundary value problem consisting of (2.2.12) and the specified boundary conditions.

As a result, part 1 and part 2 together imply that the integral-equation formulation (2.2.16) and the boundary value problem consisting of (2.2.12) and the specified boundary conditions are exactly equivalent.

An excellent illustrative example of this equivalence is given by the installation of the integral-equation formulation of the one-dimensional Schrödinger equation in Section 2.3.

2.3 Integral Equation-Formulation of the One-Dimensional Schrödinger Equation

The Schrödinger equation is regarded as the fundamental equation of quantum theory in physics. In addition to the extensive affect of this equation in modern physics, it is of great interest to many researchers in applied mathematics. Despite the availability of various forms of the Schrödinger equation, we deal with its particular form called the one-dimensional Schrödinger equation [6], given by

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + v(x)\psi(x) = E\psi(x), \tag{2.3.36}$$

where the eigenfunction $\psi(x)$, the eigenvalue E, the constants $\hbar$ and m represent the wave function, the energy eigenvalue, the Planck constant and the mass of a particle, respectively, under a potential $v(x)$. Leaving aside the physical implications of (2.3.36) and turning our attention to its mathematical aspect, we obtain the eigenvalue problem [3]

$$-y''(x) + v(x)y(x) = \lambda y(x), \tag{2.3.37}$$

which is an equivalent modified form of (2.3.36). Together with the homogeneous boundary conditions $y(-l) = 0 = y(l)$, (2.3.37) becomes the boundary value problem on $[-l, l]$, explicitly given by

$$-y''(x) + v(x)y(x) = \lambda y(x), \quad y(-l) = 0 = y(l), \quad x \in (-l, l). \tag{2.3.38}$$

Boundary value problem (2.3.38) is called the Dirichlet boundary value problem, whose detailed consideration is given in Section 3.1.

For the reformulation of the problem useful for our numerical purpose introduced in chapter 3, (2.3.38) is simply converted to the equivalent form

$$-y''(t) + w(t)y(t) = \tilde{\lambda} y(t), \quad y(-\pi) = 0 = y(\pi), \quad t \in (-\pi, \pi). \tag{2.3.39}$$

by means of a scaling relation

$$x = \frac{l}{\pi}t, \tag{2.3.40a}$$

where

$$w(t) = \frac{l^2}{\pi^2} v\left(\frac{l}{\pi}t\right) \tag{2.3.40b}$$

and

$$\tilde{\lambda} = \frac{l^2}{\pi^2}\lambda. \tag{2.3.40c}$$

The exact self-adjoint form of (2.3.39) is expressed by

$$y''(t) + \big(\tilde{\lambda} - w(t)\big)y(t) = 0, \quad y(-\pi) = 0 = y(\pi), \quad t \in (-\pi, \pi), \tag{2.3.41}$$

which is equivalent to

$$Ly + \Phi(t) = 0, \quad y(-\pi) = 0 = y(\pi), \quad t \in (-\pi, \pi), \tag{2.3.42}$$

where $Ly(t) = y''(t)$ and $\Phi(t) = \big(\tilde{\lambda} - w(t)\big)y(t)$.

The equivalent integral-equation formulation of (2.3.41) is

$$\begin{aligned} y(t) &= \int_{-\pi}^{\pi} G(t,\xi)\big(\tilde{\lambda} - w(\xi)\big)y(\xi)d\xi \\ &= -\int_{-\pi}^{\pi} G(t,\xi)w(\xi)y(\xi)d\xi + \tilde{\lambda}\int_{-\pi}^{\pi} G(t,\xi)y(\xi)d\xi, \end{aligned} \tag{2.3.43}$$

which is a Fredholm equation of the second kind, where the Green's function $G(t)$ is to be determined.

For the construction of the Green's function G, let us propose the general solution $y = c_1 + c_2 t$ of $Ly(t) = 0$. If $u(t)$ and $v(t)$ are two nontrivial solutions satisfying the homogeneous boundary conditions $u(-\pi) = 0$ and $v(\pi) = 0$, then $u(t)$ and $v(t)$ are taken as $u(t) = \pi + t$ and $v(t) = t - \pi$. Therefore, G is expressed in the form of (2.2.24) as

$$G(t) = \begin{cases} \dfrac{-1}{c}(\pi + t)(\xi - \pi) & \text{if} \quad -\pi < t \le \xi \\ \dfrac{-1}{c}(\pi + \xi)(t - \pi) & \text{if} \quad \xi \le t < \pi \end{cases}. \tag{2.3.44}$$

Condition C4 of G implies $G_2'(\xi) - G_1'(\xi) = \dfrac{-1}{p(\xi)}$, where $G_1(t) = \dfrac{-1}{c}(\pi + t)(\xi - \pi)$, $G_2(t) = \dfrac{-1}{c}(\pi + \xi)(t - \pi)$ and $p(x) \equiv 1$. It immediately follows that $c = 2\pi$.

(2.3.44), then, becomes

$$G(t) = \begin{cases} \frac{1}{2\pi}(t+\pi)(\pi-\xi) & \text{if} \quad -\pi < t \leq \xi \\ \frac{1}{2\pi}(\pi+\xi)(\pi-t) & \text{if} \quad \xi \leq t < \pi \end{cases} . \tag{2.3.45}$$

Substitution of (2.3.45) into (2.3.43) permits us to deduce the corresponding integral-equation formulation

$$y(t) = -\int_{-\pi}^{\pi} G(t,\xi)w(\xi)y(\xi)d\xi + \tilde{\lambda}\int_{-\pi}^{\pi} G(t,\xi)y(\xi)d\xi, \tag{2.3.46}$$

of the scaled form (2.3.41) of (2.3.38), where

$$G(t,\xi) = \begin{cases} \frac{1}{2\pi}(\pi+\xi)(\pi-t) & \text{if} \quad -\pi < \xi \leq t \\ \frac{1}{2\pi}(\pi+t)(\pi-\xi) & \text{if} \quad t \leq \xi < \pi \end{cases} . \tag{2.3.47}$$

acts as a function of ξ.

As are clearly seen from (2.3.45) and (2.3.47), two formulations $G(t,\xi)$ and $G(\xi,t)$ are unchanged when t and ξ are interchanged; that is, $G(t,\xi) = G(\xi,t)$ and hence G is symmetric, as expected.

The symmetry of G has an enormous effect on simplifications of our further computations in chapter 4.

CHAPTER 3

A REVIEW OF NUMERICAL APPROACHES TO SINGULAR PROBLEMS THROUGH THE FINITE BOUNDARY VALUE PROBLEMS

In addition to the Dirichlet boundary value problem introduced by (2.3.38), if the equation (2.3.37) satisfies the homogeneous boundary conditions $y'(-l) = 0 = y'(l)$, then the new boundary value problem takes the form of

$$-y''(x) + v(x)y(x) = \lambda y(x), \quad y'(-l) = 0 = y'(l), \quad x \in (-l, l), \tag{3.0.1}$$

which is called the Neumann boundary value problem.

The Dirichlet and Neumann boundary value problems both become singular boundary value problems over $(-\infty, \infty)$ as l diverges to infinity.

3.1 Behaviours of the Eigenvalues of the One-Dimensional Schrödinger Equation

If the potential $v(x) = x^2$ is substituted into the one-dimensional Schrödinger equation (2.3.37), then the equation so obtained is expressed by

$$-y''(x) + x^2 y(x) = \lambda y(x), \tag{3.1.1}$$

known as the famous quantum mechanical harmonic oscillator problem. Moreover, (3.1.1) is analytically solvable in $(-\infty, \infty)$ with the exact associated eigenvalues $\lambda_n^\infty = 2n + 1$ for $n = 0, 1, 2, ...$, especially used for testing various numerical methods.

As a result of the consideration of that the singular boundary value problem is the limiting case of the finite boundary value problem on $[-l, l]$, we may observe the following remarkable corollary [3].

Corollary. The eigenvalues $\lambda^+(l)$ and $\lambda^-(l)$ of Dirichlet and Neumann boundary value problems, respectively, generate two-sided eigenvalue bounds for the eigenvalues λ^∞ of the singular boundary value problem in the sense that $\lambda^-(l) < \lambda^\infty < \lambda^-(l)$, where $l > l_0$ for some threshold value l_0 of l.

The core of this corollary can be reflected by Figure 3.1, see [3].

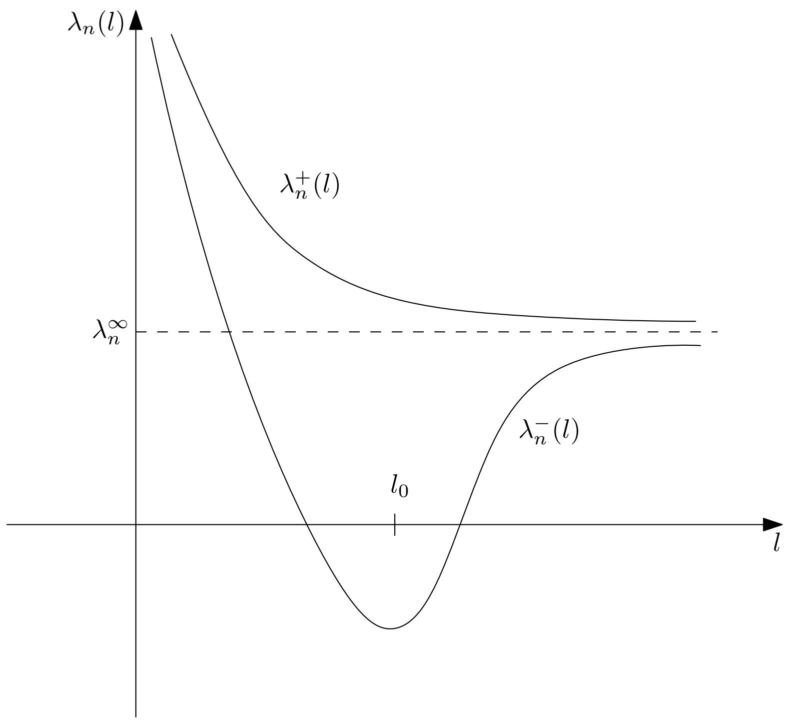

Figure 3.1: Asymptotic Behaviours of Dirichlet and Neumann Eigenvalues

It may be observed from 3.1 that the upper bound $\lambda^+(l)$ and the lower bound $\lambda^-(l)$ for λ^∞ both have asymptotic behaviours. Furthermore, $\lambda^+(l) - \lambda^-(l)$ can be regarded as the measure of the error in the computation of λ^∞, which is not directly calculated, but is approximately calculated by $\lambda^-(l)$ within negligible errors when l is sufficiently large.

It is also clear that $\lim_{l\to\infty}[\lambda^+(l) - \lambda^-(l)] = 0$; or, equivalently, for any given $\epsilon > 0$, there exists a threshold value l_0 of l such that $\lambda^+(l) - \lambda^-(l) < \epsilon$ whenever $l > l_0$, which implies that the error in the computation of λ^∞ can be made arbitrarily small by taking l sufficiently large. In other words, λ^∞ can be satisfactorily approximated within a desired accuracy.

An efficient methodology to demonstrate the successful approximation of λ^∞ is the Rayleigh-Ritz method, which is introduced in Section 3.2. The following remark, however, creates a motivational base that is essential for the construction of the procedure.

Remark.

- The sequences of trigonometric functions

$$\phi_{2k}(x) = \frac{1}{\sqrt{\pi}}\cos(k + \frac{1}{2})x, \quad k = 0, 1, 2, ... \tag{3.1.2a}$$

$$\phi_{2k+1}(x) = \frac{1}{\sqrt{\pi}}\sin(k + 1)x, \quad k = 0, 1, 2, ... \tag{3.1.2b}$$

  satisfies the Dirichlet boundary conditions and form orthonormal bases over $x \in [-\pi, \pi]$. The even functions in (3.1.2a) and the odd ones in (3.1.2b) decompose the spectrum of the finite boundary value problem in $[-\pi, \pi]$ into two disjoint subsets consisting of even and odd parity state eigenvalues, separately, if the potential $v(x)$ has a reflection symmetry; that is, if $v(x)$ is an even function [3]. Moreover, Taşeli and Eid [8] have shown that the bases formed by (3.1.2a) and (3.1.2b) give satisfactory results in two and three-dimensional Schrödinger equations as well.

- The choice of the basis of trigonometric functions, even or odd, separately, diminishes the dimensions of matrices arising from the matrix eigenvalue problem as an ultimate result of the Rayleigh-Ritz method. We will carry out the procedure with an even polynomial, and hence having the reflection symmetry, by utilizing the basis in (3.1.2a) to obtain even state eigenvalues. A similar procedure can be followed by (3.1.2b) to get odd state eigenvalues. The cases both, however, facilitate the computation of the eigenvalues avoiding the laboured evaluation of large matrices.

3.2 The Rayleigh-Ritz Method

The Rayleigh-Ritz method, used together with a basis of trigonometric functions in (3.1.2a) or (3.1.2b) satisfying the Dirichlet boundary conditions, is quite effective to accurately compute eigenvalues of the one-dimensional Schrödinger equation with an even polynomial [4] . This method enables the even and odd state eigenvalues, separately, of an unbounded problem to be approximated by making use of the basis sets (3.1.2a) and (3.1.2b), respectively, with negligible errors whenever the boundary parameter l of the associated bounded problem remains greater than a critical value l_{cr}. Taking the above remark into account, we may expand an even state eigenfunction of the bounded problem in $[-\pi, \pi]$ in terms of the basis elements in (3.1.2a). In other words, any even state eigenfunction $\psi_T(x)$, called the trial function, is expressible as a linear combination of the basis elements in (3.1.2a) and hence it satisfies

$$-y''(x) + v(x)y(x) = \lambda y(x), \quad y(-\pi) = 0 = y(\pi) \tag{3.2.3}$$

when $v(x)$ is an even polynomial in the form of

$$v(x) = \sum_{i=1}^{M} v_{2i}x^{2i}. \tag{3.2.4}$$

Therefore, the substitution of $\psi_T(x) = \sum_{k=0}^{\infty} c_k\phi_{2k}(x)$ into (3.2.3), the application of the inner product of each member of the so obtained equation by $\phi_{2j}(x)$ and the truncation of the series expansion of ψ_T with the size N yield the eigenvalue problem

$$\sum_{k=0}^{N-1} H_{jk}c_k = \lambda \sum_{k=0}^{N-1} \delta_{jk}c_k, \tag{3.2.5}$$

where $H_{jk} = - < \phi''_{2k}(x), \phi_{2j}(x) > + < v(x)\phi_{2k}(x), \phi_{2j}(x) >$ and δ_{jk} represents the elements of the matrix $\mathbf{H}$ and Kronecker's delta, respectively. Further evaluation of the inner products gives rise to the results

$$H_{jk} = \big(j - \frac{1}{2}\big)^2 \delta_{jk} + \sum_{i=1}^{M} v_{2i}[R^{(i)}_{j+k-1} + R^{(i)}_{j-k}], \tag{3.2.6}$$

where

$$R^{(i)}_n = \frac{1}{\pi} \int_0^{\pi} x^{2i} cos(nx) dx. \tag{3.2.7}$$

More explicit equivalent forms are given by

$$R^{(i)}_n = \sum_{p=0}^{i-1} \frac{(-1)^{p+n}}{n^{2(p+1)}} \binom{2i}{2p+1} (2p+1)! \pi^{2(i-1-p)}, \quad n > 0 \tag{3.2.8a}$$

$$R^{(i)}_0 = \frac{\pi^{2i}}{2i+1}, \quad n = 0 \tag{3.2.8b}$$

or

$$n^2 R^{(i)}_n = 2i\pi^{2(i-1)}(-1)^k - 2i(i-1)R^{(i-1)}_n, \quad i \geq 1 \tag{3.2.9}$$

with the initial condition $R^{(0)}_k = 0$.

CHAPTER 4

APPLICATION OF THE RAYLEIGH-RITZ METHOD TO THE INTEGRAL-EQUATION FORMULATION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

4.1 Introduction

The equivalence of the Dirichlet boundary value problem (2.3.38) and its corresponding integral- equation formulation (2.3.46) enables us to apply the Rayleigh-Ritz method, together with the basis elements in (3.1.2a), to (2.3.46) in order to approximate the even state eigenvalues λ_n^∞, $n = 0, 2, 4, ...$, of the singular boundary value problem up to 15 digits accuracy employing the even polynomial potential $v(x) = x^2 + \beta x^4$, known as the anharmonic quartic oscillator, so long as the boundary parameter l remains greater than a critical value l_{cr} of l.

In particular, $\beta = 0$ case is used as a testing ground for our method since the singular problem becomes the famous harmonic oscillator problem whose even state eigenvalues are exactly known as $\lambda_n^\infty = 2n + 1$, $n = 0, 2, 4, ...$ over $x \in (-\infty, \infty)$.

4.2 The Process of the Application of the Method

Proposing an even state truncated solution of type

$$y(t) = \sum_{k=0}^{N-1} c_k \phi_{2k}(t) \tag{4.2.1}$$

for (2.3.46), where $\phi_{2k}(t) = \frac{1}{\sqrt{\pi}} cos(k + \frac{1}{2})t$, $k = 0, 1, ..., N-1$, given by (3.1.2a) and substituting (4.2.1) into (2.3.46), we obtain

$$\sum_{k=0}^{N-1} c_k \phi_{2k}(t) = -\int_{-\pi}^{\pi} \big[G(t,\xi)w(\xi) \sum_{k=0}^{N-1} c_k \phi_{2k}(\xi)\big] d\xi + \tilde{\lambda} \int_{-\pi}^{\pi} \big[G(t,\xi) \sum_{k=0}^{N-1} c_k \phi_{2k}(\xi)\big] d\xi. \tag{4.2.2}$$

Multiplication of each member of (4.2.2) by $\phi_{2j}(t)$ and integration with respect to t over $(-\pi, \pi)$ yield

$$\begin{aligned} \sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi} \phi_{2j}(t)\phi_{2k}(t)dt = &- \sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} G(t,\xi)w(\xi)\phi_{2k}(\xi)\phi_{2j}(t)d\xi dt \\ &+ \tilde{\lambda} \sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} G(t,\xi)\phi_{2k}(\xi)\phi_{2j}(t)d\xi dt. \end{aligned} \tag{4.2.3}$$

By making use of the symmetry of $G(t, \xi)$ and reversing the order of each integration on the right, (4.2.3) is converted to

$$\begin{aligned} \sum_{k=0}^{N-1} \delta_{jk} c_k = &- \sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi} w(\xi)\phi_{2k}(\xi) \int_{-\pi}^{\pi} G(\xi,t)\phi_{2j}(t)dtd\xi \\ &+ \tilde{\lambda} \sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi} \phi_{2k}(\xi) \int_{-\pi}^{\pi} G(\xi,t)\phi_{2j}(t)dtd\xi, \end{aligned} \tag{4.2.4}$$

where δ_{jk} is Kronecker's delta and G is the relevant Green's function acting as a function of t.

Abbreviations

$$I_j(\xi) = \int_{-\pi}^{\pi} G(\xi,t)\phi_{2j}(t)dt, \tag{4.2.5}$$

$$B_{jk} = \int_{-\pi}^{\pi} \phi_{2k}(\xi) I_j(\xi) d\xi \tag{4.2.6a}$$

and

$$A_{jk} = -\int_{-\pi}^{\pi} w(\xi)\phi_{2k}(\xi)I_j(\xi)d\xi \tag{4.2.6b}$$

transform (4.2.4) into

$$\sum_{k=0}^{N-1} \delta_{jk}c_k = \sum_{k=0}^{N-1} A_{jk}c_k + \tilde{\lambda}\sum_{k=0}^{N-1} B_{jk}c_k, \tag{4.2.7}$$

which is equivalent to the generalized matrix eigenvalue problem

$$(\mathbf{I} - \mathbf{A})\mathbf{c} = \tilde{\lambda}\mathbf{B}\mathbf{c} \tag{4.2.8}$$

where B_{jk}, A_{jk}, c_k stand for the elements of matrices $\mathbf{A}$, $\mathbf{B}$, the column matrix $\mathbf{c}$, respectively, and $\mathbf{I}$ is the identity matrix generated by Kronecker's delta δ_{jk}. Matrix $\mathbf{B}$, further, is shown to be invertible and diagonal in Section 4.3, so (4.2.8) is reduced to a simpler form

$$\hat{\mathbf{A}}\mathbf{c} = \tilde{\lambda}\mathbf{c}, \tag{4.2.9}$$

where

$$\hat{\mathbf{A}} = \mathbf{B}^{-1}(\mathbf{I} - \mathbf{A}). \tag{4.2.10}$$

4.3 Evaluation of Exact Formulations of Entries of the Matrices (The Effect of the Symmetry of the Green's Function)

Implicit formulations of entries of the matrices were obtained in their simple forms with the help of the assumed symmetry of G in Section 4.2. An alternative procedure of acquirement and computation of the same formulations is given in Appendix A to show how evaluations are much more complicated without making use of the symmetry of G. In this section, however, all the computations are simply carried out to obtain the exact formulation of entires of the matrices appeared in Section 4.2.

4.3.1 Evaluation of the Integral Formulation $I_j(\xi)$

Substitution of G, given in (2.3.45) by

$$G(t) = \begin{cases} \frac{1}{2\pi}(t+\pi)(\pi-\xi) & \text{if} \quad -\pi < t \le \xi \\ \frac{1}{2\pi}(\pi+\xi)(\pi-t) & \text{if} \quad \xi \le t < \pi, \end{cases}$$

and $\phi_{2j}(t)$, given in (3.1.2a) by $\phi_{2j}(t) = \dfrac{1}{\sqrt{\pi}} \cos(j + \frac{1}{2})t$, into (4.2.5) leads to the equation

$$I_j(\xi) = \frac{1}{2\pi\sqrt{\pi}} \left[(\pi-\xi) \int_{-\pi}^{\xi} (\pi+t) \cos(j+\frac{1}{2})t dt + (\xi+\pi) \int_{\xi}^{\pi} (\pi-t) \cos(j+\frac{1}{2})t dt \right]. \tag{4.3.11}$$

Integration of each term on the right by parts, together with the abbreviations, yields

$$I_j(\xi) = \frac{4}{\sqrt{\pi}} \frac{\cos(j+\frac{1}{2})\xi}{(2j+1)^2}. \tag{4.3.12}$$

4.3.2 Evaluation of the Entries of B

Substitution of ϕ_{2k} in (3.1.2a) and $I_j(\xi)$ in (4.3.12) into (4.2.6a) yields

$$\begin{aligned} B_{jk} &= \frac{2}{\pi(j+\frac{1}{2})^2} \int_0^{\pi} \cos\left((k+\frac{1}{2})\xi\right) \cos\left((j+\frac{1}{2})\xi\right) d\xi \\ &= \begin{cases} \frac{4}{(2k+1)^2}, & \text{if} \quad k = j \\ 0, & \text{if} \quad k \neq j. \end{cases} \end{aligned} \tag{4.3.13}$$

It immediately follows that $\mathbf{B}$ is a diagonal matrix, whose inverse $\mathbf{B}^{-1}$ is generated by the entries

$$B_{jk}^{-1} = \begin{cases} \dfrac{(2k+1)^2}{4}, & \text{if} \quad k = j. \\ 0, & \text{if} \quad k \neq j. \end{cases} \tag{4.3.14}$$

4.3.3 Evaluation of the Entries of A and $\hat{\text{A}}$ (The result of the Symmetry of $\hat{\text{A}}$)

As is clearly seen from the implicit formulation of the entries of $\mathbf{A}$ in (4.2.6b), evaluation of the general entry A_{jk} is determined by the potential w, where $w(t) = \frac{l^2}{\pi^2} v(\frac{l}{\pi} t)$ given by (2.3.40b), $v(x)$ is the potential of the original formulation of the problem in (2.3.38) and $x = \frac{l}{\pi} t$ is the scaling relation in (2.3.40a) that maps the domain from $x \in [-l, l]$ to $t \in [-\pi, \pi]$. Therefore, the entries of $\mathbf{A}$ are dependent upon the choice of the potentials $v(x)$ for which we try the harmonic and anharmonic quartic oscillators.

4.3.3.1 Harmonic Oscillator ($v(x) = x^2$)

Substitution of $w(t) = \frac{l^2}{\pi^2} v(\frac{l}{\pi} t) = \frac{l^4}{\pi^4} t^2$, given by (2.3.40b), ϕ_{2k} given by (3.1.2a), and $I_j(\xi)$, given by (4.3.12), into (4.2.6b) leads to

$$A_{jk} = \frac{-2l^4}{\pi^5 (2j+1)^2} \int_{-\pi}^{\pi} [\xi^2 \cos(k+j+1)\xi + \xi^2 \cos(k-j)\xi] d\xi. \tag{4.3.15}$$

Two integrations of the members on the right by parts result in

$$A_{jk} = \begin{cases} \dfrac{2l^4}{\pi^4 (2k+1)^2} \left[\dfrac{4}{(2k+1)^2} - \dfrac{2\pi^2}{3} \right], & \text{if} \quad k = j \\ \dfrac{8l^4 (-1)^{k+j}}{\pi^4 (2j+1)^2} \left[\dfrac{1}{(k+j+1)^2} - \dfrac{1}{(k-j)^2} \right], & \text{if} \quad k \neq j. \end{cases} \tag{4.3.16}$$

If use is made of (4.2.10), the general entry of $\hat{A}_{jk}$ of $\hat{\mathbf{A}}$ is obtained by

$$\hat{A}_{jk} = \begin{cases} B_{kk}^{-1} (1 - A_{kk}), & \text{if} \quad k = j \\ -B_{jj}^{-1} A_{jk}, & \text{if} \quad k \neq j. \end{cases} \tag{4.3.17}$$

Insertion of (4.3.14) and (4.3.16) in (4.3.17) yields

$$\hat{A}_{jk} = \begin{cases} \dfrac{(2k+1)^2}{4} - \dfrac{l^4}{\pi^4}\left(\dfrac{2}{(2k+1)^2} - \dfrac{\pi^2}{3}\right), & \text{if} \quad k = j \\ \dfrac{2l^4(2k+1)(2j+1)(-1)^{k+j}}{\pi^4(k-j)^2(k+j+1)^2}, & \text{if} \quad k \neq j. \end{cases} \tag{4.3.18}$$

It is not surprising that matrix $\hat{\mathbf{A}}$ is symmetric; that is $\hat{A}_{jk} = \hat{A}_{kj}$, since it reflects the symmetry of our self-adjoint problem whose eigenvalues are all real!

4.3.3.2 Anharmonic Quartic Oscillator ($v(x) = x^2 + \beta x^4$)

Following the same procedure as in section (4.3.3.1), substitution of

$$w(t) = \frac{l^2}{\pi^2} v(\frac{l}{\pi}t) = \frac{l^4}{\pi^4}t^2 + \beta\frac{l^6}{\pi^6}t^4,$$

ϕ_{2k} and $I_j(\xi)$ given in (2.3.40b), (3.1.2a) and (4.3.12), respectively, into (4.2.6b) yields

$$A_{jk} = \frac{-4l^4}{\pi^5(2j+1)^2}\left[\int_0^\pi \xi^2\big(\cos(k+j+1)\xi + \cos(k-j)\xi\big)d\xi + \frac{\beta l^2}{\pi^2}\int_0^\pi \xi^4\big(\cos(k+j+1)\xi + \cos(k-j)\xi\big)d\xi\right]. \tag{4.3.19}$$

Two integrations of the first term and four integrations of the second term on the right by parts yield

$$A_{jk} = \begin{cases} \frac{4l^4}{\pi^4(2k+1)^2}\left[\frac{2}{(2k+1)^2} - \frac{\pi^2}{3} + \frac{\beta l^2}{\pi^2}\left(\frac{4\pi^2}{(2k+1)^4} - \frac{\pi^4}{5} - \frac{24}{(2k+1)^2}\right)\right], & \text{if} \quad k = j \\ \frac{-8l^4(2k+1)(-1)^{k+j}}{\pi^4(2j+1)(k-j)^2(k+j+1)^2}\left[1 + \frac{2\beta l^2}{\pi^2}\left(\pi^2 - \frac{6[(k+j+1)^2+(k-j)^2]}{(k-j)^2(k+j+1)^2}\right)\right], & \text{if} \quad k \neq j. \end{cases} \tag{4.3.20}$$

Insertion of (4.3.14) and (4.3.20) in (4.3.17) leads to

$$\hat{A}_{jk} = \begin{cases} \frac{(2k+1)^2}{4} - \frac{l^4}{\pi^4}\left(\frac{2}{(2k+1)^2} - \frac{\pi^2}{3}\right) + \beta\frac{l^6}{\pi^6}\left(\frac{\pi^4}{5} + \frac{24}{(2k+1)^4} - \frac{4\pi^2}{(2k+1)^2}\right), & \text{if} \quad k = j \\ \frac{2l^4(2k+1)(2j+1)(-1)^{k+j}}{\pi^4(k-j)^2(k+j+1)^2}\left[1 + \beta\frac{2l^2}{\pi^2}\left(\pi^2 - \frac{6[(k+j+1)^2+(k-j)^2]}{(k-j)^2(k+j+1)^2}\right)\right], & \text{if} \quad k \neq j \end{cases} \tag{4.3.21}$$

It is, again, clear that $\hat{A}_{jk} = \hat{A}_{kj}$ and hence matrix $\hat{\mathbf{A}}$ is symmetric as expected. Furthermore, it may be inductively shown that matrix $\hat{\mathbf{A}}$ is symmetric whenever the potential $v(x)$ is taken as the generalized anharmonic oscillator $x^2 + \beta x^{2m}$, $m = 2, 3, ...$ due to the symmetric structure of our self-adjoint problem. Note that formulations (4.3.18) and (4.3.21) agree when $\beta = 0$.

CHAPTER 5

NUMERICAL RESULTS AND DISCUSSION

By recalling from the eigenvalue problem (4.2.9) that $\hat{\mathbf{A}}$ is the matrix yielding the spectrum of the integral-equation formulation (2.3.46) of the corresponding scaled Dirichlet boundary value problem (2.3.41) of (2.3.38), the eigenvalues of (2.3.46) and hence the eigenvalues of (2.3.38) are simply computed since the exact formulations of all entries of the symmetric matrix $\hat{\mathbf{A}}$ were obtained for the harmonic and anharmonic quartic oscillators in Chapter 4. All numerical computations are performed by means of the MATLAB language. Numerical results of the even parity state eigenvalues for the harmonic and anharmonic quartic oscillators tabulated are up to 15 digits.

5.1 Even Parity State Eigenvalues for the Harmonic Oscillator

Tables 5.1, 5.2 and 5.3 include ground-state λ_0, second excited-state λ_2 and fourth excited-state λ_4 eigenvalues, respectively, corresponding to the number N of basis functions and the boundary parameter l. Tabulated eigenvalues λ_0, λ_2 and λ_4 are the upper bounds to the even state eigenvalues λ_0^∞, λ_2^∞ and λ_4^∞, respectively, of the unbounded harmonic oscillator problem whose eigenvalues are exact by $\lambda_0^\infty = 1$, $\lambda_2^\infty = 5$ and $\lambda_4^\infty = 9$.

As is clearly seen from Tables 5.1, 5.2 and 5.3, among the boundary parameters l, indicated, there is a critical value (distance) l_{cr} of l at which the eigenvalue of the unbounded problem is calculated up to 15 digits accuracy with an optimal truncation size N.

Table 5.1: Convergence of ground-state eigenvalues $\lambda_0(l, N)$ of the harmonic oscillator $v(x) = x^2$ up to 15 digits as a function of the boundary parameter l and the truncation order N.

l	N	$\lambda_0(l, N)$
5.5	8	1.000 000 001 147 89
	11	1.000 000 000 000 88
	14	1.000 000 000 000 89
	20	1.000 000 000 000 89
6.3	10	1.000 000 000 025 80
	11	1.000 000 000 000 12
	12	1.000 000 000 000 00
	13	1.000 000 000 000 00
6.5	11	1.000 000 000 000 86
	12	1.000 000 000 000 00
	13	1.000 000 000 000 00
6.7	12	1.000 000 000 000 03
	13	1.000 000 000 000 00
	14	1.000 000 000 000 00
8	14	1.000 000 000 000 17
	15	1.000 000 000 000 00
	16	1.000 000 000 000 00

Namely, according to Table 5.1, the critical value l_{cr} is observed to lie around 6.3, where the desired accuracy is obtained using 12 basis functions, whereas $l_{cr} = 6.6$ with $N = 14$ and $l_{cr} = 7.1$ with $N = 16$ in Tables 5.2 and 5.3, respectively. It is also clear from the tables that the boundary parameters l, less than the critical values l_{cr} indicated, do not yield the convergence of the eigenvalues of the bounded problem to those of the unbounded harmonic oscillator problem even though the truncation size is relatively large. Furthermore, the convergence with the same truncation size N as obtained at the critical distance to reach the desired accuracy is possibly acquired as the boundary parameter l is sufficiently close to l_{cr}. To illustrate, boundary parameters $l = 6.5$ around $l_{cr} = 6.3$ with $N = 12$ in Table 5.1, $l = 6.7$ around $l_{cr} = 6.6$ with

Table 5.2: Convergence of $n = 2$ excited-state eigenvalues $\lambda_2(l, N)$ of the harmonic oscillator $v(x) = x^2$ up to 15 digits as a function of the boundary parameter l and the truncation order N.

l	N	$\lambda_2(l, N)$
6	12	5.000 000 000 007 37
	13	5.000 000 000 007 34
	14	5.000 000 000 007 34
	15	5.000 000 000 007 34
6.6	12	5.000 000 000 023 24
	13	5.000 000 000 000 10
	14	5.000 000 000 000 00
	15	5.000 000 000 000 00
6.7	13	5.000 000 000 000 32
	14	5.000 000 000 000 00
	15	5.000 000 000 000 00
7	14	5.000 000 000 000 03
	15	5.000 000 000 000 00
	16	5.000 000 000 000 00
7.5	15	5.000 000 000 000 03
	16	5.000 000 000 000 00
	17	5.000 000 000 000 00

$N = 14$ in Table 5.2 and $l = 7.2$ around $l_{cr} = 7.1$ with $N = 16$ in Table 5.3 also lead to the convergence of the eigenvalues within the desired accuracy.

Larger boundary parameters l than the critical values l_{cr}, however, give rise to the convergence of the eigenvalues with larger truncation sizes N due to asymptotic behaviors of the eigenvalues in accordance with 3.1 given in Section 3.1. To illustrate, $l = 8 > l_{cr} = 6.3$ with $N = 15$ in Table 5.1, $l = 7.5 > l_{cr} = 6.6$ with $N = 16$ in Table 5.2 and $l = 8.5 > l_{cr} = 7.1$ with $N = 19$ in Table 5.3 yield the convergence, where the numbers of basis functions are relatively large.

Table 5.3: Convergence of $n = 4$ excited-state eigenvalues $\lambda_4(l, N)$ of the harmonic oscillator $v(x) = x^2$ up to 15 digits as a function of the boundary parameter l and the truncation order N.

l	N	$\lambda_4(l, N)$
	12	9.000 000 002 970 40
6.5	15	9.000 000 000 010 69
	20	9.000 000 000 010 69
	15	9.000 000 000 000 28
7.1	16	9.000 000 000 000 00
	17	9.000 000 000 000 00
	15	9.000 000 000 000 87
7.2	16	9.000 000 000 000 00
	17	9.000 000 000 000 00
	15	9.000 000 000 002 59
7.3	16	9.000 000 000 000 01
	17	9.000 000 000 000 00
	18	9.000 000 000 000 00
	18	9.000 000 000 000 33
8.5	19	9.000 000 000 000 00
	20	9.000 000 000 000 00

5.2 Even Parity State Eigenvalues for the Anharmonic Quartic Oscillator

In Tables 5.4, 5.5 and 5.6, β represents the anharmonicity constant of the quartic oscillator $v(x) = x^2 + \beta x^4$. λ_0, λ_2 and λ_4 are the first three even state eigenvalues of the integral equation formulation (2.3.46) of the scaled form (2.3.41) of the bounded Dirichlet boundary value problem (2.3.38) computed at indicated critical values l_{cr}. The first three even state eigenvalues of the bounded problem, indeed, are obtained at critical values l_{cr} using the required number N of basis functions in order to approximate the first three even state eigenvalues λ_0^∞, λ_2^∞ and λ_4^∞ of the corresponding unbounded problem correct to 15 digits. Critical values are dependent on the variational parameter β, so $l_{cr}(\beta)$ is regarded as a function of β.

Table 5.4: Ground-state eigenvalues λ_0 of the anharmonic quartic oscillator $v(x) = x^2 + \beta x^4$ up to 15 digits around the critical value $l_{cr}(\beta)$, as a function of β, estimated by the scaling relation $\beta^{-1/6} l_{cr}(1)$ for $\beta \geq 1$.

β	N	$l_{cr}(\beta)$	$\beta^{-1/6} l_{cr}(1)$	λ_0
0.0001	12	6.30	-	1.000 074 986 880 20
0.001	13	6.20	-	1.000 748 692 673 18
0.01	11	6.00	-	1.007 373 672 081 38
0.1	13	5.00	-	1.065 285 509 543 71
1	14	3.75	3.75	1.392 351 641 530 29
10	14	2.55	2.55	2.449 174 072 118 38
100	15	1.78	1.74	4.999 417 545 137 58
1000	16	1.18	1.18	10.639 788 711 328 0
40000	16	0.65	0.64	36.274 458 133 736 0

Table 5.5: $n = 2$ Excited-state eigenvalues λ_2 of the anharmonic quartic oscillator $v(x) = x^2 + \beta x^4$ up to 15 digits around the critical value $l_{cr}(\beta)$, as a function of β, estimated by the scaling relation $\beta^{-1/6} l_{cr}(1)$ for $\beta \geq 1$.

β	N	$l_{cr}(\beta)$	$\beta^{-1/6} l_{cr}(1)$	λ_2
0.0001	18	6.60	-	5.000 974 615 938 38
0.001	17	6.60	-	5.009 711 872 788 10
0.01	13	6.30	-	5.093 939 132 742 30
0.1	14	5.30	-	5.747 959 268 833 56
1	16	4.07	4.07	8.655 049 957 759 30
10	16	2.79	2.77	16.635 921 492 413 7
100	16	1.89	1.89	34.873 984 261 994 7
1000	17	1.29	1.29	74.681 404 200 164 8
40000	17	0.69	0.69	255.017 677 289 573

As β values range from the regime of small values to the regime of large values, critical values of boundary parameters l vary from the ones near the harmonic regime to the ones in the anharmonic regime. Determination of critical values of l is not a difficult task for the regime of small values of β due to the similarity between the behaviours of the anharmonic quartic oscillator and those of the harmonic oscillator.

Table 5.6: $n = 4$ Excited-state eigenvalues λ_4 of the anharmonic quartic oscillator $v(x) = x^2 + \beta x^4$ up to 15 digits around the critical value $l_{cr}(\beta)$, as a function of β, estimated by the scaling relation $\beta^{-1/6} l_{cr}(1)$ for $\beta \geq 1$.

β	N	$l_{cr}(\beta)$	$\beta^{-1/6} l_{cr}(1)$	λ_4
0.0001	17	7.2	-	9.003 072 972 044 61
0.001	17	7.2	-	9.030 549 566 074 71
0.01	15	6.9	-	9.289 479 816 311 88
0.1	16	6.0	-	11.098 595 622 633 0
1	19	4.85	4.85	18.057 557 436 303 2
10	20	3.29	3.30	35.885 171 222 253 8
100	20	2.25	2.25	75.877 004 028 669 7
1000	20	1.54	1.53	162.802 374 196 975
40000	20	0.84	0.82	556.200 474 630 523

As for determination of critical values of l for the regime of large values of β, a very useful scaling relation $\beta^{-1/6} l_{cr}(1)$, revealed by Taşeli [4], guides us to estimate. Critical values for the regime of large values of β are indicated together with the corresponding outputs of the scaling relation in Tables 5.4, 5.5 and 5.6 to be compared. Therefore, neither critical values of l for the regime of small values, nor those for the regime of large ones are difficult to estimate for acquirement of the eigenvalues within the desired accuracy using N basis functions. The Rayleigh-Ritz method enables us to accurately obtain the eigenvalues of the unbounded problem with optimal truncation sizes N. Tables 5.4, 5.5 and 5.6 show that no matter how large the values of β are, the desired accuracy is obtained by using required numbers N of basis functions ranging from $N = 12$ to $N = 20$. All numerical results reflected in Tables 5.4, 5.5 and 5.6 are compatible with the outcomes of an integration-free method published by Taşeli and Demiralp [5].

To summarize, Tables 5.4, 5.5 and 5.6, constructed as a result of the Rayleigh-Ritz method, reflect the first three even parity state eigenvalues of the integral-equation formulation of the corresponding finite Dirichlet boundary value problem. Moreover, these eigenvalues are not only upper bounds for those of the corresponding singular problem but also exact up to 15 digits around critical values $l_{cr}(\beta)$, roughly estimated by the scaling relation $\beta^{-1/6} l_{cr}(1)$, with optimal truncation sizes N as the anharmonicity constant β varies from the regime of small values to that of large ones.

CHAPTER 6

CONCLUSIONS

In this thesis, the exact equivalence of certain integral equations and differential equations is reflected by means of the application of the Rayleigh-Ritz method to the integral-equation formulation of the finite Dirichlet boundary value problem consisting of the one dimensional Schrödinger equation and its homogeneous boundary conditions. The outcome of the application of the numerical method reveals the even parity state eigenvalues of the corresponding singular problem within 15 digits accuracy which are compatible with those published by Taşeli [4] and Demiralp [5].

In accordance with the process of the method, reformulation of the problem is established for the scaled form of the Dirichlet boundary value problem utilizing a scaling relation mapping the domain from $x \in [-l, l]$ to $t \in [-\pi, \pi]$. The procedure is, then, sustained by making use of an orthonormal basis of even parity state trigonometric functions together with even polynomial potentials; namely, harmonic oscillator and anharmonic quartic oscillator.
Initially, the first three even parity state eigenvalues of the integral-equation formulation of the corresponding finite Dirichlet problem are compared with those of the famous singular harmonic problem whose spectrum is exactly known by

$$\{\lambda_n\}_{n=0}^{\infty} = \{2n+1\}_{n=0}^{\infty}.$$

After the successful completion of this test level, convergence of the even state eigenvalues of the integral-equation formulation of the bounded anharmonic quartic oscillator problem to those of the corresponding singular problem is observed. The admirable advantages of the method are taken in the aspects of computation of the eigenvalues with low-dimensional matrices and the convergence of the eigenvalues around critical distances l_{cr} whose rough estimations are not difficult thanks to a scaling relation [4]. As the variation of the anharmonicity constant β ranges from small values to large values, critical values l_{cr} change from those approximated around the harmonic regime to those, in the anharmonic regime, roughly calculated by the scaling relation.

As a result of this thesis, we form a chain of the following consequences which are connected with magic word "symmetry" of mathematics:

- Since the problem concerned is the Dirichlet boundary value problem consisting of the one-dimensional Schrödinger equation, of the **self-adjoint** form, and the specified homogeneous boundary conditions, its corresponding integral-equation formulation is achieved by the construction of the **symmetric** Green's function G.
- Employment of the Rayleigh-Ritz method with reflective **symmetric** polynomial potentials permits of the evaluation of eigenvalues with matrices of small orders, which prevents laborious computations.
- Exact formulation of the entries of matrix $\hat{\mathbf{A}}$, through which the eigenvalues are sought, is simply obtained with the help of the **symmetry** of G. (Difficulty of computations without using the symmetry of G is shown in Appendix A.)
- The formulation indicates that $\hat{\mathbf{A}}$ is **symmetric**, leading to all real eigenvalues, which is, indeed, the reflection of the **symmetric** structure of our **self-adjoint** problem.

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APPENDIX A

AN ALTERNATIVE PROCEDURE OF EVALUATION OF EXACT FORMULATIONS OF ENTRIES OF THE MATRICES

A.1 Introduction

The main target of this chapter is to show the great effect of the symmetry of the Green's function G on simplification of complicated integrations. The one who would prefer to cover this chapter rather than read Sections 4.2 and 4.3 misses the point of strong impact of the symmetry of G on difficult calculations. Conversely, Sections A.2 and A.3 are worth looking through to distinguish this impact from computational aspects despite their equivalence to Sections 4.2 and 4.3, respectively.

A.2 The Process of the Application of the Method

Proposing an even state truncated solution of type

$$y(t) = \sum_{k=0}^{N-1} c_k \phi_{2k}(t) \tag{A.2.1}$$

for (2.3.46), where $\phi_{2k}(t) = \frac{1}{\sqrt{\pi}} \cos(k + \frac{1}{2})t$, $k = 0, 1, ..., N-1$, given by (3.1.2a) and substituting (A.2.1) into (2.3.46), we obtain

$$\sum_{k=0}^{N-1} c_k \phi_{2k}(t) = -\int_{-\pi}^{\pi} \big[G(t,\xi) w(\xi) \sum_{k=0}^{N-1} c_k \phi_{2k}(\xi)\big] d\xi + \tilde{\lambda} \int_{-\pi}^{\pi} \big[G(t,\xi) \sum_{k=0}^{N-1} c_k \phi_{2k}(\xi)\big] d\xi. \tag{A.2.2}$$

Multiplication of each member of (A.2.2) by $\phi_{2j}(t)$ and integration with respect to t

over $(-\pi, \pi)$ yield

$$\sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi} \phi_{2j}(t)\phi_{2k}(t)dt = -\sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} G(t,\xi)w(\xi)\phi_{2k}(\xi)\phi_{2j}(t)d\xi dt$$
$$+ \tilde{\lambda}\sum_{k=0}^{N-1} c_k \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} G(t,\xi)\phi_{2k}(\xi)\phi_{2j}(t)d\xi dt. \tag{A.2.3}$$

Direction of the process differs from that of the one followed in Section 4.2 at this point omitting the usage of the symmetry of G made in Section 4.2.

Abbreviations

$$I_k(t) = \int_{-\pi}^{\pi} G(t,\xi)w(\xi)\phi_{2k}(\xi)d\xi \tag{A.2.4}$$

$$J_k(t) = \int_{-\pi}^{\pi} G(t,\xi)\phi_{2k}(\xi)d\xi \tag{A.2.5}$$

$$A_{jk} = -\int_{-\pi}^{\pi} I_k(t)\phi_{2j}(t)dt \tag{A.2.6}$$

and

$$B_{jk} = \int_{-\pi}^{\pi} J_k(t)\phi_{2j}(t)dt \tag{A.2.7}$$

transform (A.2.3) into

$$\sum_{k=0}^{N-1} \delta_{jk}c_k = \sum_{k=0}^{N-1} A_{jk}c_k + \tilde{\lambda}\sum_{k=0}^{N-1} B_{jk}c_k, \tag{A.2.8}$$

which is equivalent to the generalized matrix eigenvalue problem

$$(\mathbf{I} - \mathbf{A})\mathbf{c} = \tilde{\lambda}\mathbf{B}\mathbf{c}, \tag{A.2.9}$$

where B_{jk}, A_{jk}, c_j stand for the elements of the matrices $\mathbf{A}$, $\mathbf{B}$, the column matrix $\mathbf{c}$, respectively, and $\mathbf{I}$ is the identity matrix generated by Kronecker's delta δ_{jk}. Matrix

$\mathbf{B}$, further, is shown to be invertible and diagonal in section A.3, so (A.2.9) is reduced to a simpler form

$$\hat{\mathbf{A}}\mathbf{c} = \tilde{\lambda}\mathbf{c}, \tag{A.2.10}$$

where

$$\hat{\mathbf{A}} = \mathbf{B}^{-1}(\mathbf{I} - \mathbf{A}). \tag{A.2.11}$$

A.3 Evaluation of Exact Formulations of Entries of the Matrices

A.3.1 Evaluation of the Integral Formulations $I_k(t)$ and $J_k(t)$

Substitution of G given in (2.3.47) by

$$G(t,\xi) = \begin{cases} \frac{1}{2\pi}(\pi+\xi)(\pi-t), & \text{if} \quad -\pi < \xi \le t \\ \frac{1}{2\pi}(\pi+t)(\pi-\xi), & \text{if} \quad t \le \xi < \pi, \end{cases}$$

ϕ_{2k}, given in (3.1.2a), and $w(t) = \dfrac{l^2}{\pi^2}v\big(\dfrac{l}{\pi}t\big) = \dfrac{l^4}{\pi^4}t^2 + \beta\dfrac{l^6}{\pi^6}t^4$ into (A.2.4) leads to the equation

$$\begin{aligned} I_k(t) &= \frac{1}{2\pi\sqrt{\pi}}(\pi-t)\int_{-\pi}^{t}(\pi+\xi)\frac{l^4}{\pi^4}\big(\xi^2+\beta\frac{l^2}{\pi^2}\xi^4\big)\cos\Big((k+\frac{1}{2})\xi\Big)d\xi \\ &\quad + \frac{1}{2\pi\sqrt{\pi}}(\pi+t)\int_{t}^{\pi}(\pi-\xi)\frac{l^4}{\pi^4}\big(\xi^2+\beta\frac{l^2}{\pi^2}\xi^4\big)\cos\Big((k+\frac{1}{2})\xi\Big)d\xi \\ &= \frac{l^4}{2\pi^5\sqrt{\pi}}\Big[(\pi-t)\big[\pi R_2(t)+R_3(t)+\frac{\beta l^2}{\pi}R_4(t)+\frac{\beta l^2}{\pi^2}R_5(t)\big] \\ &\quad + (\pi+t)\big[\pi S_2(t)-S_3(t)+\frac{\beta l^2}{\pi}S_4(t)-\frac{\beta l^2}{\pi^2}S_6(t)\big]\Big], \end{aligned} \tag{A.3.12}$$

where

$$R_m(t) = \int_{-\pi}^{t}\xi^m\cos\Big((k+\frac{1}{2})\xi\Big)d\xi, \quad m = 2,3,4,5 \tag{A.3.13a}$$

and

$$S_m(t) = \int_t^\pi \xi^m \cos\left((k+\frac{1}{2})\xi\right) d\xi, \quad m = 2,3,4,5. \tag{A.3.13b}$$

The complexity of too many terms resulting from integrations of (A.3.13a) and (A.3.13b) by parts is reduced by the abbreviations

$$I_k(t) = H(t) + \beta H_a(t), \tag{A.3.14}$$

where

$$\begin{aligned} H(t) =& \frac{8\pi}{(2k+1)^2}\Bigg[t^2\cos(k+\frac{1}{2})t - \frac{8t}{2k+1}\sin(k+\frac{1}{2})t - \frac{24}{(2k+1)^2}\cos(k+\frac{1}{2})t \\ &+ \frac{8\pi}{(2k+1)}(-1)^k\Bigg], \end{aligned} \tag{A.3.15a}$$

$$\begin{aligned} H_a(t) =& \frac{8l^2}{\pi(2k+1)^2}\Bigg[t^4\cos(k+\frac{1}{2})t - \frac{16}{2k+1}t^3\sin(k+\frac{1}{2})t + \frac{16}{(2k+1)}\pi^3(-1)^k \\ &- \frac{144}{(2k+1)^2}t^2\cos(k+\frac{1}{2})t + \frac{768}{(2k+1)^3}t\sin(k+\frac{1}{2})t \\ &- \frac{768}{(2k+1)^3}\pi(-1)^k + \frac{1920}{(2k+1)^4}\cos(k+\frac{1}{2})t\Bigg], \end{aligned} \tag{A.3.15b}$$

H and H_a are determiners of the formulations of the elements of matrices for the harmonic and anharmonic quartic oscillators, respectively.

Substitution of G and ϕ_{2k} into (A.2.5) and evaluation of the so obtained integral yield

$$J_k(t) = \frac{4}{\sqrt{\pi}(2k+1)^2}\cos(t+\frac{1}{2})t. \tag{A.3.16}$$

A.3.2 Evaluation of the Entries of B

Substitution of ϕ_{2j} in (3.1.2a) and $I_k(t)$ in (A.3.16) into (A.2.7) results in

$$
\begin{aligned}
B_{jk} &= \int_{-\pi}^{\pi} \frac{4}{\sqrt{\pi}(2k+1)^2} \cos\left((k+\frac{1}{2})t\right) \frac{1}{\sqrt{\pi}} \cos\left((j+\frac{1}{2})t\right) dt \\
&= \frac{4}{\pi(2k+1)^2} \int_{0}^{\pi} \left(\cos(j+k+1)t + \cos(k-j)t\right) dt \\
&= \begin{cases} \dfrac{4}{(2k+1)^2}, & \text{if} \quad k = j \\ 0, \quad \text{if} \quad k \neq j, \end{cases}
\end{aligned}
\tag{A.3.17}
$$

where $\mathbf{B}$ is a diagonal matrix, whose inverse $\mathbf{B^{-1}}$ is generated by the entries

$$
B^{-1}_{jk} = \begin{cases} \dfrac{(2k+1)^2}{4}, & \text{if} \quad k = j \\ 0, \quad \text{if} \quad k \neq j, \end{cases}
\tag{A.3.18}
$$

Note that formulations (A.3.17) and (A.3.18) coincide with (4.3.13) and (4.3.14), respectively.

A.3.3 Evaluation of the Entries of A and Â

A.3.3.1 Harmonic Oscillator ($\beta = 0$)

Substitution of $I_k(t) = H(t)$ in (A.3.15a) into (A.2.6) and evaluation of the so obtained integral lead to

$$
A_{jk} = \begin{cases} \frac{-4l^4}{\pi^4(2k+1)^2}\left[\frac{\pi^2}{3} - \frac{2}{(2k+1)^2}\right], \quad \text{if} \quad k = j \\ \frac{-8l^4(-1)^{k+j}}{\pi^4(2k+1)^2}\left[\frac{(2k+1)(2j+1)}{(k+j+1)^2(k-j)^2} + \frac{4(2j+1)}{(2k+1)(k+j+1)(k-j)} + \frac{16}{(2k+1)(2j+1)}\right], \quad \text{if} \quad k \neq j \end{cases}
\tag{A.3.19}
$$

If use is made of (A.2.11), the general entry $\hat{A}_{jk}$ of $\hat{\mathbf{A}}$ is obtained by

$$\hat{A}_{jk} = \begin{cases} B_{kk}^{-1}(1 - A_{kk}), & \text{if} \quad k = j \\ -B_{jj}^{-1} A_{jk}, & \text{if} \quad k \neq j. \end{cases} \tag{A.3.20}$$

Insertion of (A.3.18) and (A.3.19) in (A.3.20) yields

$$\hat{A}_{jk} = \begin{cases} \frac{(2k+1)^2}{4} - \frac{l^4}{\pi^4}\left(\frac{2}{(2k+1)^2} - \frac{\pi^2}{3}\right), & \text{if} \quad k = j \\ \frac{2l^4}{\pi^4}\frac{(2j+1)^2(-1)^{k+j}}{(2k+1)^2}\left[\frac{(2j+1)(2k+1)}{(k+j+1)^2(k-j)^2} + \frac{4(2j+1)}{(2k+1)(k+j+1)(k-j)} + \frac{16}{(2k+1)(2j+1)}\right], & \text{if} \quad k \neq j. \end{cases} \tag{A.3.21}$$

One may concern that matrix $\hat{\mathbf{A}}$ is not symmetric. Two formulations (A.3.21) and (4.3.18), however, are exactly the same !

The equality is obvious when $k = j$. The case of $k \neq j$ is simply shown by a useful identity

$$(2k+1)^2 - (2j+1)^2 = 4(k+j+1)(k-j) \quad : \tag{A.3.22}$$

$$
\begin{aligned}
\hat{A}_{jk} &= \frac{2l^4}{\pi^4}\frac{(2j+1)^2(-1)^{k+j}}{(2k+1)^2}\left[\frac{(2j+1)(2k+1)}{(k+j+1)^2(k-j)^2} + \frac{4(2j+1)}{(2k+1)(k+j+1)(k-j)}\right. \\
&\qquad\qquad \left. + \frac{16}{(2k+1)(2j+1)}\right] \\
&= \frac{2l^4}{\pi^4}\frac{(2j+1)^3(-1)^{k+j}}{(2k+1)}\left[\frac{16}{\left[(2k+1)^2-(2j+1)^2\right]^2}\right. \\
&\qquad \left. + \frac{16}{(2k+1)^2\left[(2k+1)^2-(2j+1)^2\right]}\right] + \frac{16(2j+1)}{(2k+1)^3} \\
&= \frac{2l^4}{\pi^4}\frac{16(2j+1)(-1)^{k+j}}{(2k+1)^3}\left[\frac{(2j+1)^2[2(2k+1)^2-(2j+1)^2]}{\left[(2k+1)^2-(2j+1)^2\right]^2}\right. \\
&\qquad \left. + \frac{[(2k+1)^2-(2j+1)^2]^2}{\left[(2k+1)^2-(2j+1)^2\right]^2}\right] \\
&= \frac{2l^4}{\pi^4}\frac{16(2j+1)(-1)^{k+j}}{(2k+1)^3}\left[\frac{(2k+1)^4}{\left[(2k+1)^2-(2j+1)^2\right]^2}\right] \\
&= \frac{2l^4}{\pi^4}\frac{16(2j+1)(2k+1)(-1)^{k+j}}{16(k+j+1)^2(k-j)^2} \\
&= \frac{2l^4(2k+1)(2j+1)(-1)^{k+j}}{\pi^4(k-j)^2(k+j+1)^2},
\end{aligned}
$$

which is the same as $\hat{A}_{kj}$ when $k \neq j$ in (4.3.18).

A.3.3.2 Anharmonic Quartic Oscillator ($\beta > 0$)

Following the same procedure as in Section A.3.3.1, substitution of (A.3.15a), (A.3.15b) and ϕ_{2j} into (A.2.6) gives rise to the evaluation of the entries of $\mathbf{A}$ resulting from more complicated integrations. The entries of $\hat{\mathbf{A}}$, fortunately, are also obtained in the sense that the formulations

$$
\hat{A}_{jk} = \begin{cases} \frac{(2k+1)^2}{4} - \frac{l^4}{\pi^4}\left(\frac{2}{(2k+1)^2} - \frac{\pi^2}{3}\right) + \beta\frac{l^6}{\pi^6}\left(\frac{\pi^4}{5} + \frac{24}{(2k+1)^4} - \frac{4\pi^2}{(2k+1)^2}\right), & \text{if} \quad k = j \\ \frac{2l^4(2k+1)(2j+1)(-1)^{k+j}}{\pi^4(k-j)^2(k+j+1)^2}\left[1 + \beta\frac{2l^2}{\pi^2}\left(\pi^2 - \frac{6[(k+j+1)^2+(k-j)^2)]}{(k-j)^2(k+j+1)^2}\right)\right] & \text{if} \quad k \neq j \end{cases} \tag{A.3.23}
$$

and (4.3.21) agree with the help of abbreviations.