STUDIES ON THE PERTURBATION PROBLEMS IN QUANTUM MECHANICS

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I certify that this thesis satisfies all the requirements as a thesis for the degree of Master of Science.

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This is to certify that we have read this thesis and that in our opinion it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

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ABSTRACT

STUDIES ON THE PERTURBATION PROBLEMS IN QUANTUM MECHANICS

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In this thesis, the main perturbation problems encountered in quantum mechanics have been studied. Since the special functions and orthogonal polynomials appear very extensively in such problems, we emphasize on those topics as well. In this context, the classical quantum mechanical anharmonic oscillators described mathematically by the one-dimensional Schrödinger equation have been treated perturbatively in both finite and infinite intervals, corresponding to confined and non-confined systems, respectively.

Keywords: Schrödinger Equation, Anharmonic Oscillators, Perturbation Theory, Special Functions, Orthogonal Polynomials.

ÖZ

KUANTUM MEKANİKTEKİ PERTÜRBASYON PROBLEMLERİ

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Bu tezde, kuantum mekaniğinde karşılaşılan belli başlı pertürbasyon problemleri ele alınmıştır. Bu tür problemler geniş ölçüde özel fonksiyonlar ve ortogonal polinomları kullandığı için, ayrıca bu konular üzerinde de durulmuştur. Bu çerçevede, tek boyutlu Schrödinger denklemi ile tanımlanan kuantum mekaniksel anharmonik salınıcılar hem sonlu hem de sonsuz aralıklarda pertürbatif olarak incelenmiştir.

Anahtar Kelimeler: Schrödinger Denklemi, Anharmonik Salınıcılar, Pertürbasyon Teorisi, Özel Fonksiyonlar, Ortogonal Polinomlar.

To my family and husband

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CHAPTER 1

INTRODUCTION

1.1 The nature of Perturbation Theory

Perturbation theory first appeared in one of the oldest branches of applied mathematics; celestial mechanics, the study of the motions of the planets. From antiquity, various mathematical methods were used to describe these motions (as seen from earth), usually with no attempt to state their causes. After Newton's formulation of the law of gravity, it became possible to deduce the planetary motions from physical laws which were considered to be more fundamental. If only the sun and one planet are considered, the result is elliptical motion with the sun at a focus. However, this does not quite correspond to the actually observed motion. The explanation is that the planets exert gravitational forces on each other, and therefore "perturb", that is, modify, their motions. Perturbation theory in its original sence refers to various ways of taking these modifications into account. In essence, one begins with the "unperturbed solution", that is with purely elliptical motion, as a first approximation, then computes the forces which the planets would exert on each other if this unperturbed motion were correct, and then corrects the unperturbed solution accordingly. The first corrections are still not accurate, since their construction depended upon the unperturbed solution, and so a second set of corrections can be computed, and so on. The sum of the unperturbed solution and the sequence of corrections forms a series, and one hopes that a partial sum of a reasonable number of terms gives an adequate approximation to the motion for perhaps a few hundred years.

The scope of perturbation theory [2], [11], [21], [23] at the present time is much broader than its applications to celestial mechanics, but the main idea is the same. One begins with a solvable problem, called the unperturbed or reduced problem, and uses the solution of this problem as an approximation to the solution of a more complicated problem that differs from the reduced problem only by some small terms in the equations. Then one looks for a series of successive corrections to this initial approximation, most often in the form of a power series in a small quantity called "perturbation parameter". Finally one attempts to show that the use of only a few of these correction terms (usually one or two) provides a useful approximate solution to the actual problem at hand.

The simplest problem which can be addressed by perturbation theory is that of finding roots of polynomials. This problem illustrates many of the important ideas: proper formulation of perturbation families; degenerate and nondegenerate cases; uniform and nonuniform solutions; rescaling coordinates; rescaling parameters.

The problem is purely mathematical, so it is not necessary to address physical and mathematical issues simultaneously. There are no differential equations involved, so the only mathematical diffuculties are those coming from perturbation theory itself.

What does it mean to solve a polynomial equation by a perturbation method? Suppose the problem is

$$x^2 - 3.99x + 3.02 = 0. \tag{1.1.1}$$

Of course, this can be solved easily by the quadratic formula. But to approach it by perturbation theory, there are four steps:

1. The first is to notice that since $-3.99 = -4 + 0.01$ and $3.02 = 3 + 0.02$, equation (1.1.1) is almost the same as $x^2 - 4x + 3 = 0$, which can be solved easily by factoring: $(x-1)(x-3) = 0$, giving two roots $x_1 = 1,\ x_2 = 3$.

2. The second step is to create a family of problems intermediate between the easy, factorable problem and the original problem (1.1.1). This can be done by letting ϵ denote the small quantity 0.01, so that $-3.99 = -4+\epsilon$ and $3.02 = 3+2\epsilon$; then (1.1.1) can be written

$$x^2 + (\epsilon - 4)x + (3 + 2\epsilon) = 0. \tag{1.1.2}$$

Now allow ϵ to vary. Then (1.1.2) is no longer a single equation, but a family of equations, one equation for each value of ϵ. When $\epsilon = 0$, (1.1.2) reduces to the factorable problem, and when $\epsilon = 0.01$, it is the "target problem" (1.1.1). For $0 < \epsilon < 0.01$, it is midway between the two. Equation (1.1.2) is an example of a *perturbation family*, a family of problems depending on a small parameter ϵ which is easily solvable when $\epsilon = 0$.

3. The third step is to find approximate solutions of (1.1.2), in the form of polynomials (truncated power series) in the small parameter ϵ. In this example suitable solutions turn out to be

$$\begin{aligned} x_1 &\cong 1 + \frac{3}{2}\,\epsilon + \frac{15}{8}\,\epsilon^2, \\ x_2 &\cong 3 - \frac{5}{2}\,\epsilon - \frac{15}{8}\,\epsilon^2. \end{aligned} \tag{1.1.3}$$

Evaluating these solutions at $\epsilon = 0.01$ gives an approximate solution of the original problem (1.1.1) namely $x_1 \cong 1.0151875$, $x_2 \cong 2.9748125$.

4. The fourth step is, whenever possible, to say something about the amount of error in these approximations.

This brief example already reveals a good deal about perturbation theory. First of all, the method can only be applied when the "target" problem is close to a solvable problem (that is, close to a problem solvable exactly or approximately by some method other than perturbation theory). A polynomial equation chosen at random can probably not be solved by perturbation theory, since it is unlikely to be close to a factorable polynomial.

Next, the example shows that in solving a problem by perturbation theory, one solves not only a single target problem such as (1.1.1), but every problem belonging to the perturbation family (1.1.2), as long as ϵ is "sufficiently small". The meaning of "sufficiently small" is not clear until the error analysis has been completed.

Often a physical problem is stated at first in terms suited to the application, and rescaled several times in the course of analysis; then the solutions must be interpreted carefully to see how they apply to the original problem. The easy example of finding roots is a good introduction to those ideas.

1.2 The methods to solve the Quantum Mechanical problems (Schrödinger Equation)

Let $y = y(x)$ be a solution of the equation

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0 \tag{1.2.4}$$

of hypergeometric type, and let $\rho(x)$, a solution of $(\sigma\rho)' = \tau\rho$, be bounded on (a, b) and satisfy the conditions that $\tau(x)$ has to vanish at some point of (a, b) and has a negative derivative, $\tau' < 0$. Then nontrivial solutions of the equation of hypergeometric type for which $y(x)\sqrt{\rho(x)}$ is bounded and square integrable on (a,b), exist only when

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma'', \quad (n = 0, 1, 2, \cdots) \tag{1.2.5}$$

and they have the form

$$y(x, \lambda_n) = y_n(x) = \frac{B_n}{\rho(x)} \frac{d^n}{dx^n} \left[\sigma^n(x)\rho(x)\right], \tag{1.2.6}$$

i.e. they are the classical polynomials that are orthogonal with weight $\rho(x)$ on (a, b).

This property is used in quantum mechanics [6], [9], [18], [20] for solving problems about the energy levels and wave functions of a particle in a potential field. To find the wave functions $\psi(r)$ and corresponding enegy levels E, one solves the time-independent Schrödinger equation

$$\frac{-h^2}{2\mu}\Delta\psi + U\psi = E\psi \tag{1.2.7}$$

where h is Planck's constant, μ is the mass of the particle, $U = U(r)$ is the potential and r is the radius-vector.

For many problems of quantum mechanics [25], the Schrödinger equation reduces to a generalized equation of hypergeometric type;

$$u'' + \frac{\tilde{\tau}(x)}{\sigma(x)} u' + \frac{\tilde{\sigma}(x)}{\sigma^2(x)} u = 0 \quad (a < x < b). \tag{1.2.8}$$

Equation (1.2.8) can be transformed by the substitution $u = \phi(x)y$ into an equation of hypergeometric type

$$\frac{d}{dx}\left[\sigma\rho\frac{dy}{dx}\right] + \lambda\rho y = 0, \tag{1.2.9}$$

where $(\sigma\rho)' = \tau\rho, \quad \tau = \tilde{\tau} + 2(\phi'/\phi)\sigma$ and $y(x)\sqrt{\rho(x)}$ is bounded and square integrable on (a,b).

The values of λ for which our problem has non-trivial solutions are the eigenvalues and the corresponding functions $y(x, \lambda)$ are the eigenfunctions.

Exactly solvable models have played a relevant role in the development of quantum mechanics [8]. Sometimes they provide simple explanations of the most relevant features of actual physical phenomena and also they become the starting point for more or less accurate aproximations based, for instance, on the variational method, perturbation theory or both [27].

Perturbation theory is a large collection of iterative methods for obtaining approximate solutions to problems involving a small parameter ϵ. When $\epsilon = 0$, the problem becomes solvable.

Perturbation methods attempt to solve a given problem by approximating it by simpler problems whose solutions are more or less explicitly known. For example, the differential equation,

$$y'' = [1 + \epsilon/(1 + x^2)]y \tag{1.2.10}$$

can only be solved in terms of elementary functions when $\epsilon = 0$. A perturbative solution is written as a series of powers of ϵ:

$$y(x) = y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2(x) + \cdots .$$

This series is called perturbation series. If ϵ is very small, $y(x)$ will be well approximated by only a few terms of perturbation series.

By using the methods of perturbation theory it is possible to approximate the eigenvalues and eigenfunctions of the Schrödinger equation [1], [12], [24] of the form,

$$(H_0 + \epsilon H_1)\psi = E\psi \tag{1.2.11}$$

where H_0 and H_1 are operators and ϵ is the perturbation parameter. We remark, at this point, that if the Hamiltonion can be written as a convergent power series in a certain parameter ϵ, with H_1 being a bounded operator, then the perturbed eigenvalues and eigenfunctions are analytic functions of ϵ, and their power series are convergent power series in a neighbourhood of $\epsilon = 0$. So, we formally expand the eigenfunctions and the energy eigenvalues in the form of power series in ϵ [41].

Then, our task is the determination of the serial expansions of $E(\epsilon)$ and $\psi(\xi, \epsilon)$ in nonnegative powers of ϵ, i.e.

$$\begin{cases} E_n(\epsilon) &= \displaystyle\sum_{k=0}^{\infty} w_k(n)\epsilon^k, \\ \psi_n(\xi,\epsilon) &= \displaystyle\sum_{k=0}^{\infty} F_n^{(k)}(\xi)\epsilon^k \end{cases} \tag{1.2.12}$$

By the substitution of (1.2.12) into (1.2.11), we have the sequence of equations and by comparing the powers of ϵ, we have an iterative procedure for calculating the coefficients in the perturbation series for E_n and $\psi_n(\xi)$. Once the coefficients $w_0(n), w_1(n), \cdots, w_{N-1}(n)$; $F_n^{(0)}, F_n^{(1)}, \cdots, F_n^{(N-1)}$ are known, $w_N(n)$ and $F_n^{(N)}$ can be calculated.

Although the evaluation of higher order terms seems to be, in principle, possible, the enormousness of the effort needed to handle the intermediate steps without mistakes, has to be prevented from continuing further in this direction. As a matter of fact, the scheme remains the same in higher order evaluations, however the appearance of many dimensional integrations which are elementary in concept, rapidly increases the number of manipulations.

The organization of this thesis is as follows: In Chapter 2, special functions of applied mathematics are reviewed. Chapter 3 deals with perturbation theory and its applications. Numerical applications are given in Chapter 4. Finally, we discuss the results in Chapter 5.

CHAPTER 2

A REVIEW OF SPECIAL FUNCTIONS

2.1 Theory of Special Functions

Consider

$$u'' + \frac{\tilde{\tau}(x)}{\sigma(x)}u' + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}u = 0 \tag{2.1.1}$$

where $\tilde{\tau}(x)$ is a polynomial of degree at most 1; $\sigma(x)$ and $\tilde{\sigma}(x)$ are the polynomials of degree at most 2. We may reduce (2.1.1) to a simpler form by introducing the transformation,

$$u = \phi(x)y$$

Substituting of u, u' and u'' into (2.1.1) we obtain,

$$y'' + \left(2\frac{\phi'}{\phi} + \frac{\tilde{\tau}}{\sigma}\right)y' + \left(\frac{\tilde{\sigma}}{\sigma^2} + \frac{\tilde{\tau}}{\sigma}\frac{\phi'}{\phi} + \frac{\phi''}{\phi}\right)y = 0. \tag{2.1.2}$$

Require that the coefficient of y' is of the form,

$$\frac{\tau(x)}{\sigma(x)}$$

where $\tau(x)$ is a polynomial of degree at most 1. This requirement leads to,

$$2\frac{\phi'}{\phi} = \frac{\tau(x) - \tilde{\tau}(x)}{\sigma(x)},$$

$$\frac{\phi'(x)}{\phi(x)} = \frac{\pi(x)}{\sigma(x)} \tag{2.1.3}$$

where

$$\pi(x) = \frac{1}{2}[\tau(x) - \tilde{\tau}(x)] \tag{2.1.4}$$

is also a polynomial of degree at most 1. Equation (2.1.2) takes the form,

$$y'' + \frac{\tau(x)}{\sigma(x)}y' + \frac{\tilde{\tilde{\sigma}}(x)}{\sigma^2(x)}y = 0. \tag{2.1.5}$$

Here

$$\tau(x) = 2\pi(x) + \tilde{\tau}(x) \tag{2.1.6}$$

and

$$\tilde{\tilde{\sigma}}(x) = \pi^2(x) + [\tilde{\tau}(x) - \sigma'(x)]\pi(x) + [\tilde{\sigma}(x) + \pi'(x)\sigma(x)]. \tag{2.1.7}$$

We have derived a class of transformations induced by the substitution $u = \phi(x)y$ that do not change the type of the differential equation under consideration.

Now, for simplicity, we shall choose $\pi(x)$ so that $\tilde{\tilde{\sigma}}(x)$ in (2.1.7) is divisible by $\sigma(x)$, that is,

$$\tilde{\tilde{\sigma}}(x) = \lambda\sigma(x), \tag{2.1.8}$$

where λ is a constant. Then (2.1.5) can be written as,

$$y'' + \frac{\tau(x)}{\sigma(x)}y' + \lambda\frac{\sigma(x)}{\sigma^2(x)}y = 0$$

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0. \tag{2.1.9}$$

Equation (2.1.9) is referred to as a differential equation of the hypergeometric type and its solutions referred to as the functions of the hypergeometric type. Then equation (2.1.1) may be called a generalized differential equation of the hypergeometric type. Now, let us determine λ and $\pi(x)$. From (2.1.8) and (2.1.7), we write,

$$\pi^2 + (\tilde{\tau} - \sigma')\pi + (\tilde{\sigma} - k\sigma) = 0 \tag{2.1.10}$$

where k is a constant,

$$k = \lambda - \pi'(x). \tag{2.1.11}$$

Assume that k is given for a moment, we have;

$$\pi(x) = \frac{1}{2}[\sigma'(x) - \tilde{\tau}(x)] \mp \sqrt{\left[\frac{\tilde{\tau}(x) - \sigma'(x)}{2}\right]^2 - [\tilde{\sigma}(x) - k\sigma(x)]}.$$

Notice that the expression, say $P_2(x)$, under the square root sign, is a quadratic polynomial in x.

Notice also that it must be the square of a linear polynomial as $\pi(x)$ is a linear polynomial.

2.2 The Classical Orthogonal Polynomials

We know that the differential equation of hypergeometric type has the form;

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0$$

This equation has polynomial solutions given by Rodriguez formula,

$$y_n(x) = \frac{B_n}{\rho(x)}\frac{d^n}{dx^n}[\sigma^n(x)\rho(x)]$$

with B_n a normalization constant. The solutions are valid for the particular values of $\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma''$, $\;n = 0, 1, \cdots$. The function $\rho(x)$ satisfies the equation

$$[\sigma(x)\rho(x)]' = \tau(x)\rho(x)$$

and has the possible forms;

$$\rho(x) = \begin{cases} (1-x)^\alpha(1+x)^\beta & \text{for} \quad \sigma(x) = 1 - x^2 \\ x^\alpha e^{-x} & \text{for} \quad \sigma(x) = x \\ e^{-x^2} & \text{for} \quad \sigma(x) = 1 \end{cases}$$

depending on $\sigma(x)$, where α and β are constants.

Now, we shall be concerned with the main properties of the classical polynomials; Jacobi, Laguerre and Hermite respectively [26], [30], [31].

2.2.1 Jacobi Polynomials

Let $\sigma(x) = 1-x^2$ and $\rho(x) = (1-x)^\alpha(1+x)^\beta$. We find $\tau(x)$ and λ_n as follows;

$$\begin{aligned}
\tau(x) &= -(\alpha+\beta+2)x+\beta-\alpha \\
\lambda_n &= n(n+\alpha+\beta+1), \qquad n = 0,1,2,\cdots.
\end{aligned}$$

Then, the corresponding polynomials are defined by;

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}[(1-x)^{n+\alpha}(1+x)^{n+\beta}]. \qquad (2.2.12)$$

The Jacobi polynomials are orthogonal on $[-1,1]$ with the weight function $\rho(x) = (1-x)^\alpha(1+x)^\beta$. The orthogonal polynomials with the weight function on the finite interval $[a,b]$ can be expressed in the form

$$cP_n^{(\alpha,\beta)}\left\{2\frac{x-a}{b-a}-1\right\} \qquad (2.2.13)$$

where c is a constant. The Rodriguez formula implies that;

$$P_n^{(\alpha,\beta)}(x) = (-1)^n P_n^{(\beta,\alpha)}(-x) \qquad (2.2.14)$$

Theorem 2.2.1. *The Jacobi polynomials $y = P_n^{(\alpha,\beta)}(x)$ satisfy the following linear homogeneous differential equation of the second order:*

$$(1-x^2)y'' + [\beta-\alpha-(\alpha+\beta+2)x]y' + n(n+\alpha+\beta+1)y = 0. \qquad (2.2.15)$$

Proof. Proof is given in [31]. □

Theorem 2.2.2. *Let $\alpha > -1$, $\beta > -1$. The differential equation*

$$(1-x^2)y'' + [\beta-\alpha-(\alpha+\beta+2)x]y' + \lambda y = 0, \qquad (2.2.16)$$

where λ is a parameter, has a polynomial solution not identically zero if and only if λ has the form $n(n+\alpha+\beta+1)$, $n = 0,1,2,\cdots$. This solution is $cP_n^{(\alpha,\beta)}(x)$ where c is a constant and no solution which is linearly independent of $P_n^{(\alpha,\beta)}(x)$, *can be a polynomial.*

Proof. Proof is given in [31]. □

Substitution of $x = 1 - 2x'$ in (2.2.15) yields

$$x'(1-x')\frac{d^2y}{dx'^2} + [\alpha + 1 - (\alpha+\beta+2)x']\frac{dy}{dx'} + n(n+\alpha+\beta+1)y = 0, \quad (2.2.17)$$

which is the hypergeometric equation of Gauss. For $n \geq 1$, we obtain the important representation:

$$P_n^{(\alpha,\beta)}(x) = \binom{n+\alpha}{n} \, {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right) \quad (2.2.18)$$

where

$$P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}.$$

From the equation (2.2.14), we obtain an equivalent form of (2.2.18),

$$P_n^{(\alpha,\beta)}(x) = (-1)^n \binom{n+\beta}{n} \, {}_2F_1\left(-n, n+\alpha+\beta+1; \beta+1; \frac{1+x}{2}\right) \quad (2.2.19)$$

Another application of (2.2.18) is the useful formula;

$$\frac{d}{dx}\{P_n^{(\alpha,\beta)}(x)\} = \frac{1}{2}(n+\alpha+\beta+1)P_{n-1}^{(\alpha+1,\beta+1)}(x). \quad (2.2.20)$$

According to the theory of hypergeometric functions, a second solution of (2.2.15) is given by

$$(1-x)^{-\alpha} \, {}_2F_1(-n-\alpha, n+\beta+1; 1-\alpha; \frac{1-x}{2}), \quad (2.2.21)$$

unless α is an integer.

Recurrence Formula:

Here $P_{n+1}^{(\alpha,\beta)}(x)$ [or $P_{n-1}^{(\alpha,\beta)}(x)$] can be expressed in terms of $xP_n^{(\alpha,\beta)}(x)$, $P_n^{(\alpha,\beta)}(x)$, $P_{n-1}^{(\alpha,\beta)}(x)$ [or $P_{n+1}^{(\alpha,\beta)}(x)$]. This yields,

$$(2n+\alpha+\beta)(1-x^2)\frac{d}{dx}\{P_n^{(\alpha,\beta)}(x)\} = \quad (2.2.22)$$

$$= -n\{(2n+\alpha+\beta)x+\beta-\alpha\}P_n^{(\alpha,\beta)}(x)+2(n+\alpha)(n+\beta)P_{n-1}^{(\alpha,\beta)}(x),$$

$$(2n+\alpha+\beta+2)(1-x^2)\frac{d}{dx}\{P_n^{(\alpha,\beta)}(x)\} = \tag{2.2.23}$$

$$(n+\alpha+\beta+1)\{(2n+\alpha+\beta+2)x+\alpha-\beta\}P_n^{(\alpha,\beta)}(x)-$$

$$2(n+1)(n+\alpha+\beta+1)P_{n+1}^{(\alpha,\beta)}(x).$$

For particular values of α and β in the Jacobi polynomials, we introduce some very well known polynomials. For example, if $\alpha = \beta = 0$ the Jacobi polynomials $P_n^{(0,0)}(x) := P_n(x)$ are known as the "Legendre polynomials" satisfying

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0, \qquad n = 0, 1, 2, \cdots . \tag{2.2.24}$$

2.2.2 Laguerre Polynomials

Let $\sigma(x) = x$ and $\rho(x) = x^\alpha e^{-x}$. We find $\tau(x)$ and λ_n as follows;

$$\begin{aligned} \tau(x) &= \alpha + 1 - x \quad \text{and} \\ \lambda_n &= n, \qquad n = 0, 1, 2, \cdots . \end{aligned}$$

Then the corresponding polynomials are defined by ;

$$e^{-x}x^\alpha L_n^{(\alpha)}(x) = \frac{1}{n!}\frac{d^n}{dx^n}[e^{-x}x^{n+\alpha}]. \tag{2.2.25}$$

Also, we define the Laguerre polynomials $\{L_n^{(\alpha)}(x)\}$, for $\alpha > -1$, by the following conditions of orthogonality and normalization:

$$\int_0^\infty e^{-x}x^\alpha L_n^{(\alpha)}(x)L_m^{(\alpha)}(x)dx = \Gamma(\alpha+1)\binom{n+\alpha}{n}\delta_{nm}; n, m = 0, 1, 2, \cdots . \tag{2.2.26}$$

We also write $L_n^{(0)}(x) := L_n(x)$. We have the differential equation;

$$xy'' + (\alpha + 1 - x)y' + \lambda y = 0 \tag{2.2.27}$$

which has a polynomial solution when $\lambda = n$. Also, $L_n^{(\alpha)}(x)$ is the only polynomial solution. Further, we have the explicit representation

$$L_n^{(\alpha)}(x) = \sum_{\nu=0}^{n} \binom{n+\alpha}{n-\nu} \frac{(-x)^\nu}{\nu!}, \tag{2.2.28}$$

the formula

$$L_n^{(\alpha)}(0) = \binom{n+\alpha}{n} \tag{2.2.29}$$

and the expression

$$\ell_n^{(\alpha)} = \frac{(-1)^n}{n!} \tag{2.2.30}$$

for the coefficient $\ell_n^{(\alpha)}$ of x^n in $L_n^{(\alpha)}(x)$.

Recurrence Formula:

$$nL_n^{(\alpha)}(x) = (-x + 2n + \alpha - 1)L_{n-1}^{(\alpha)}(x) - (n + \alpha - 1)L_{n-2}^{(\alpha)}(x), \quad n = 2, 3, 4, \cdots, \tag{2.2.31}$$

$$L_0^{(\alpha)}(x) = 1, \quad L_1^{(\alpha)}(x) = -x + \alpha + 1.$$

We obtain from the explicit representation of $L_n^{(\alpha)}(x)$ that :

$$\sum_{\nu=0}^{n} L_\nu^{(\alpha)}(x) = L_n^{(\alpha+1)}(x), \tag{2.2.32}$$

$$L_n^{(\alpha)}(x) = L_n^{(\alpha+1)}(x) - L_{n-1}^{(\alpha+1)}(x), \tag{2.2.33}$$

$$\frac{d}{dx} L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x) = x^{-1}\{nL_n^{(\alpha)}(x) - (n+\alpha)L_{n-1}^{(\alpha)}(x)\}. \tag{2.2.34}$$

2.2.3 Confluent Hypergeometric Series; relation between Jacobi and Laguerre Polynomials; second solution

In the notation of Pochhammer - Barnes, the Confluent hypergeometric series is,

$$ {}_1F_1(\alpha;\gamma;x) = 1 + \sum_{\nu=1}^{\infty} \frac{\alpha(\alpha+1)\cdots(\alpha+\nu-1)}{\gamma(\gamma+1)\cdots(\gamma+\nu-1)} \frac{x^\nu}{\nu!}. \tag{2.2.35} $$

This is obtained from the ordinary hypergeometric series by the limiting process

$$ \lim_{\beta\to\infty} {}_2F_1(\alpha,\beta;\gamma;\beta^{-1}x) \tag{2.2.36} $$

we have,

$$ L_n^{(\alpha)}(x) = \binom{n+\alpha}{n} {}_1F_1(-n;\alpha+1;x) \tag{2.2.37} $$

and using (2.2.18) we obtain the following important relation between Laguerre and Jacobi polynomials:

$$ L_n^{(\alpha)}(x) = \lim_{\beta\to\infty} P_n^{(\alpha,\beta)}(1-2\beta^{-1}x). \tag{2.2.38} $$

This holds uniformly in every closed part of the complex x-plane.

2.2.4 Hermite Polynomials

Let $\sigma(x) = 1$ and $\rho(x) = e^{-x^2}$. We find $\tau(x)$ and λ_n as follows;

$$ \begin{aligned} \tau(x) &= -2x \qquad \text{and} \\ \lambda_n &= 2n, \qquad n = 0,1,2,\cdots. \end{aligned} $$

Then, the corresponding polynomials are defined by;

$$ H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}[e^{-x^2}]. \tag{2.2.39} $$

Also, we define the Hermite polynomials by the conditions,

$$ \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \pi^{1/2} 2^n n! \delta_{nm}, n,m = 0,1,2,\cdots. \tag{2.2.40} $$

The coefficient of x^n in the $n-th$ polynomial is positive. On the other hand, the

Hermite polynomials are the solutions of the Hermite equation;

$$y'' - 2xy' + 2\nu y = 0 \qquad \text{where} \qquad \nu = n = 0, 1, 2, \cdots .$$

We know the following properties of Hermite polynomials:

$$\frac{H_n(x)}{n!} = \sum_{\nu=0}^{[n/2]} \frac{(-1)^\nu}{\nu!} \frac{(2x)^{n-2\nu}}{(n-2\nu)!}, \tag{2.2.41}$$

$$\lim_{x\to\infty} x^{-n} H_n(x) = 2^n. \tag{2.2.42}$$

Recurrence Formula:

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x), \qquad n = 2, 3, 4, \cdots ; \tag{2.2.43}$$

$$H_0(x) = 1, \qquad H_1(x) = 2x.$$

We notice the following “individual” properties:

$$H_n'(x) = 2nH_{n-1}(x), \quad H_n(x) = 2xH_{n-1}(x) - H_{n-1}'(x). \tag{2.2.44}$$

2.2.5 Relation of Hermite Polynomials to those of Laguerre

(1) Hermite polynomials can be entirely reduced to Laguerre polynomials with the parameters $\alpha = \mp\frac{1}{2}$, for we have

$$\begin{gathered} H_{2m}(x) = (-1)^m 2^{2m} m! L_m^{(-\frac{1}{2})}(x^2), \\ H_{2m+1}(x) = (-1)^m 2^{2m+1} m! x L_m^{(\frac{1}{2})}(x^2). \end{gathered} \tag{2.2.45}$$

Combining above equations with (2.2.38), we obtain a representation of Hermite polynomials as limits of Jacobi;

$$e^{(2xw-w^2)} = \lim_{\lambda\to\infty}(1-2\frac{x}{\lambda}w+\frac{w^2}{\lambda})^{-\lambda}, \tag{2.2.46}$$

so that

$$\frac{H_n(x)}{n!} = \lim_{\lambda\to\infty}\lambda^{-n/2}P_n^{(\lambda)}(\lambda^{-1/2}x). \tag{2.2.47}$$

(2) Conversely, Laguerre polynomials can, to a certain extent, be reduced to Hermite polynomials. We have,

$$L_n^{(\alpha)}(x) = \frac{(-1)^n\pi^{-1/2}}{\Gamma(\alpha+\frac{1}{2})}\frac{\Gamma(n+\alpha+1)}{(2n)!}$$

$$\int_{-1}^{+1}(1-t^2)^{\alpha-\frac{1}{2}}H_{2n}(x^{\frac{1}{2}}t)dt, \quad \alpha > -\frac{1}{2}. \tag{2.2.48}$$

2.3 Eigenvalue problems in Quantum Mechanics that can be solved by means of the Classical Orthogonal Polynomials

Consider the solution of the equation

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0 \tag{2.3.49}$$

of hypergeometric type for various values of λ, when $\rho(x)$ satisfies the equation;

$$(\sigma\rho)' = \tau\rho, \tag{2.3.50}$$

is bounded on an interval (a,b), and satisfies the conditions imposed on $\rho(x)$ for the classical orthogonal polynomials.

As we have seen, the simplest solutions of (2.3.49) are the classical orthogonal polynomials $y_n(x)$, which correspond to,

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma'', \quad n = 0, 1, \cdots . \tag{2.3.51}$$

It turns out that the classical orthogonal polynomials [29] are distinguished among the solutions of (2.3.49) corresponding to various values of λ not only by their simplicity, but also they are the only non-trivial solutions of (2.3.49) for which $y(x)\sqrt{\rho(x)}$ is both bounded and square integrable on (a,b).

This property is extensively used in quantum mechanics for solving problems about the energy levels and wave functions of a particle in a potential field. If external forces restrict the particle to a bounded part of space, so that it cannot move off to infinity, one says that the particle is in a bound state. To find the wave functions $\psi(r)$ that describe these states, and the corresponding energy levels λ, one solves the time - independent Schrödinger equation,

$$\frac{-h^2}{2\mu}\Delta\psi + U\psi = \lambda\psi, \tag{2.3.52}$$

where h is Planck's constant, μ is the mass of the particle, $U = U(r)$ is the potential and r is the radius - vector.

Here the wave function $\psi(r)$ must be bounded for all finite $|r|$ and be normalized by

$$\int_V |\psi(r)|^2 dV = 1. \tag{2.3.53}$$

For many problems of quantum mechanics that can be solved analytically by the method of seperation of variables, the Schrödinger equation reduces to a generalized equation of hypergeometric type:

$$u'' + \frac{\tilde{\tau}(x)}{\sigma(x)}u' + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}u = 0 \quad (a < x < b). \tag{2.3.54}$$

We assume that $\sigma(x) > 0$ for $x \in (a,b)$ and that $\sigma(x) = 0$ at the endpoints of (a,b) if the endpoints are not at infinity. Since (2.3.54) has no singular points at any $x \in (a,b)$, the function $u(x)$ is continuously differentiable on (a,b). Therefore it can have singular points only as $x \to a$ or $x \to b$. In order to state the additional restrictions that should be imposed on $u(x)$ at the endpoints of (a, b), we rewrite (2.3.54) in self adjoint form:

$$(\sigma\tilde{\rho}u')' + (\tilde{\sigma}/\sigma)\tilde{\rho}u = 0 \tag{2.3.55}$$

here $\tilde{\rho}(x) > 0$ and $\tilde{\rho}(x)$ satisfies

$$(\sigma\tilde{\rho})' = \tilde{\tau}\tilde{\rho}. \tag{2.3.56}$$

The function $\psi(r)$ will be bounded and satisfy the normalization condition (2.3.53) if the problem is formulated in terms of (2.3.55) in the following way:

Find all values of λ for which (2.3.55) has a non-trivial solution on (a, b) s.t $u(x)\{\tilde{\rho}(x)\}^{1/2}$ is bounded and square integrable on (a, b), i.e. $|u(x)|\{\tilde{\rho}(x)\}^{1/2} < c$ where c is a constant

and

$$\int_a^b |u(x)|^2\tilde{\rho}(x)dx < \infty$$

(if a and b are finite, the last condition can be omitted.)

Equation (2.3.54) can be transformed by the substitution $u = \phi(x)y$ into an equation of hypergeometric type

$$\frac{d}{dx}[\sigma\rho\frac{dy}{dx}] + \lambda\rho y = 0, \tag{2.3.57}$$

where $\rho(x)$ satisfies $(\sigma\rho)' = \tau\rho$ and $\tau(x)$ is connected with $\tilde{\tau}(x)$ and $\phi(x)$ by

$$\tau = \tilde{\tau} + 2(\phi'/\phi)\sigma.$$

It follows from this and (2.3.56) that

$$\rho(x) = \tilde{\rho}(x)\phi^2(x).$$

Hence the requirements on $u(x)\{\tilde{\rho}(x)\}^{1/2}$ become the requirements listed above on $y(x)\sqrt{\rho(x)}$.

The values of λ for which our problem has non-trivial solutions are the “eigenvalues" and the corresponding functions $y(x, \lambda)$ are the "eigenfunctions".

For the majority of the problems of quantum mechanics that admit explicit solutions, the transformation of the equation (2.3.54) to (2.3.57) can be done by using a $\rho(x)$ that is bounded on (a, b) and satisfies the conditions imposed on $\rho(x)$ for the classical orthogonal polynomials.

Remark 2.3.1 In order to satisfy the conditions imposed on $\rho(x)$ for the classical orthogonal polynomials, $\tau(x)$ has to vanish at some point of (a, b) and has a negative derivative, $\tau' < 0$.

Remark (2.3.1) lets us simplify the selection of a transformation of (2.3.54) to (2.3.57).

Theorem 2.3.1. *Let $y = y(x)$ be a solution of the equation*

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0$$

of hypergeometric type, and let $\rho(x)$ a solution of $(\sigma\rho)' = \tau\rho$, be bounded on (a, b) and satisfy the conditions imposed on $\rho(x)$ for the classical orthogonal polynomials. Then non-trivial solutions of the equation of hypergeometric type for which $y(x)\sqrt{\rho(x)}$ is bounded and square integrable on (a, b) exist only when

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma'', \quad n = 0, 1, \cdots \tag{2.3.58}$$

and they have the form

$$y(x, \lambda_n) = y_n(x) = \frac{B_n}{\rho(x)} \frac{d^n}{dx^n}[\sigma^n(x)\rho(x)], \tag{2.3.59}$$

i.e., they are the classical polynomials that are orthogonal with weight $\rho(x)$ on (a, b), (if a and b are finite, the condition of quadratic integrability can be omitted).

We illustrate the applicability of the previous theorem by means of some quantum mechanics problems in which the Schrödinger equation reduces to a generalized equation of hypergeometric type.

2.3.1 Harmonic Oscillator

We consider the problem of finding the eigenvalues and eigenfunctions for the linear harmonic oscillator [38], i.e. for a particle in a field with potential $U = mw^2x^2/2$ (m is the mass, x the displacement from equilibrium, w the angular frequency). The problem of the harmonic oscillator plays an important role in the foundations of quantum electrodynamics, and has applications to various types of oscillations in crystals and molecules.

The Schrödinger equation for the wave function $\psi(x)$ of the harmonic oscillator has the form:

$$\frac{-h^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}mw^2x^2\psi = E\psi, \qquad -\infty < x < \infty.$$

Here $\psi(x)$ must be bounded and satisfy the normalization condition

$$\int_{-\infty}^{\infty} \psi^2(x)dx = 1.$$

In solving the problem it is convenient to replace x and E by dimensionless variables ξ and ϵ:

$$x = \xi\sqrt{\frac{h}{mw}} = \alpha\xi, \quad E = hw\epsilon.$$

Then we obtain the equation

$$\psi'' + (2\epsilon - \xi^2)\psi = 0 \tag{2.3.60}$$

(Here primes denote differentiation w.r.t. ξ). This is a generalized equation of hypergeometric type for which

$$\sigma(\xi) = 1, \quad \tilde{\tau}(\xi) = 0, \quad \tilde{\sigma}(\xi) = 2\epsilon - \xi^2.$$

We now have a problem that can be solved by means of classical orthogonal polynomials. The requirement that $\sqrt{\tilde{\rho}(\xi)}\psi(\xi)$ is square integrable follows from the normalization condition. We transform the equation for ψ to an equation of hypergeometric type,

$$\sigma(\xi)y'' + \tau(\xi)y' + \lambda y = 0, \tag{2.3.61}$$

by putting $\psi(\xi) = \phi(\xi)y(\xi)$, where $\phi(\xi)$ satisfies the equation

$$\frac{\phi'}{\phi} = \frac{\pi(\xi)}{\sigma(\xi)}.$$

Then the equation (2.3.60) takes the form

$$y'' + \frac{2\phi'}{\phi}y' + \left(\frac{\phi''}{\phi} + 2\epsilon - \xi^2\right) y = 0. \tag{2.3.62}$$

Following the same procedure in the section 2.1, we may transform the equation (2.3.62) to hypergeometric type in (2.3.61) such that,

$$y'' + \frac{\tau}{\sigma}y' + \frac{\tilde{\tilde{\sigma}}}{\sigma^2}y = 0 \quad \text{where} \quad \tilde{\tilde{\sigma}} = \lambda\sigma. \tag{2.3.63}$$

The polynomial $\pi(\xi)$ is of the form,

$$\pi(\xi) = \pm\sqrt{k - 2\epsilon + \xi^2}.$$

The constant k can be determined from the condition that the function under the square root sign has a double zero, i.e. $k = 2\epsilon$. There are two possible polynomials $\pi(\xi) = \pm\xi$; we select the one for which

$$\tau(\xi) = \tilde{\tau}(\xi) + 2\pi(\xi)$$

has a negative derivative. The conditions on $\tau(\xi)$ are satisfied if we take
$\tau(\xi) = -2\xi$, in which case

$$\begin{aligned} \pi(\xi) &= -\xi,\ \phi(\xi) = e^{-\frac{\xi^2}{2}}, \\ \rho(\xi) &= e^{-\xi^2},\ \lambda = 2\epsilon - 1. \end{aligned}$$

The equation (2.3.63) takes the form,

$$y'' - 2\xi y' + \lambda y = 0, \quad \text{where} \quad \lambda = 2\nu. \tag{2.3.64}$$

The differential equation (2.3.64) is the Hermite differential equation and it has polynomial solutions only when $\nu = n, \ n = 0, 1, 2, \cdots$. Furthermore, the energy eigenvalues are determined only when

$$\lambda + n\tau' + \frac{n(n-1)}{\tau}\sigma'' = 0.$$

Hence, the square integrability condition is satisfied, since $y(\xi)$ are polynomial solutions, so,

$$\int_{-\infty}^{\infty} e^{-\xi^2} y^2(\xi) d\xi < \infty.$$

Then,

$$\epsilon = \epsilon_n = n + \frac{1}{2}, \ i.e.$$

$$E = E_n = hw(n + \frac{1}{2}), \quad n = 0, 1, \cdots .$$

We obtain the eigenfunctions in the form

$$y_n(\xi) = B_n e^{\xi^2} \frac{d^n}{d\xi^n}(e^{-\xi^2}).$$

These are, up to numerical factors, the Hermite polynomials $H_n(\xi)$. The wave functions $\psi(x)$ are

$$\psi_n(x) = c_n e^{-\xi^2/2} H_n(\xi), \qquad x = \alpha\xi, \ \alpha = (h/(mw))^{1/2}.$$

Here c_n is a normalizing constant determined by

$$\int_{-\infty}^{\infty} \psi_n^2(x) dx = 1,$$

so

$$c_n = \frac{1}{2^{n/2}\sqrt{n!}\pi^{1/4}}.$$

2.3.2 Pöschl-Teller Potential

Consider the problem of finding the eigenvalues and eigenfunctions for the one-dimensional Schrödinger equation [37]

$$\frac{-h^2}{2m}\psi'' + U(x)\psi = E\psi, \qquad -\infty < x < \infty$$

for a particle in the field

$$U(x) = -\frac{U_0}{\cos h^2 \alpha x}, \text{ where } U_0 > 0.$$

Here $\psi(x)$ is to be bounded, and normalized by

$$\int_{-\infty}^{\infty} \psi^2(x)dx = 1.$$

Since $U(x) < 0$, only values of $E < 0$ are admissible. To simplify the form of the equation we make the change of independent variable $s = \tan h\alpha x$. (In many quantum mechanics problems that can be solved explicitly, the Schrödinger equation can be reduced to an equation with rational coefficients by a natural change of variable suggested by the form of $U(x)$, where the transformation must be one - to-one. In the present case the potential has a simple expression in terms of hyperbolic functions, so it is natural to try $\sin h\alpha x, \tan h\alpha x$, or $\exp(\pm\alpha x)$ as a new variable. We chose the substitution $s = \tan h\alpha x$.)

We then obtain the generalized equation of hypergeometric type

$$\Phi'' + \frac{\tilde{\tau}(s)}{\sigma(s)}\Phi' + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Phi = 0, \quad \Phi(s) = \psi(x),$$

for which $a = -1, \ b = 1$,

$$\sigma(s) = 1 - s^2, \ \ \tilde{\tau}(s) = -2s, \ \ \tilde{\sigma}(s) = -\beta^2 + \gamma^2(1 - s^2),$$

$$\beta^2 = -\frac{2mE}{h^2\alpha^2}, \ \ \gamma^2 = \frac{2mU_0}{h^2\alpha^2}, \ \ (\beta > 0, \ \gamma > 0).$$

This is again a problem of the kind we discussed. Here $\tilde{\sigma}(s) = 1$. Hence the square integrability of $\sqrt{\tilde{\rho}(s)}\Phi(s)$ follows from the normalization condition

$$\int_{-\infty}^{\infty} \psi^2(x)dx = 1. \qquad \text{In fact,}$$

$$\int_{-1}^{1} \Phi^2(s)ds = \alpha \int_{-\infty}^{\infty} \frac{\psi^2(x)}{\cos h^2 \alpha x} dx < \alpha \int_{-\infty}^{\infty} \psi^2(x)dx = \alpha.$$

The solution is obtained by the previous method. We transform the equation for $\Phi(s)$ to the equation of hypergeometric type

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0$$

by putting $\Phi(s) = \phi(s)y(s)$, where $\phi(s)$ satisfies

$$\phi'/\phi = \pi(s)/\sigma(s).$$

The polynomial $\pi(s)$ is now given by

$$\pi(s) = \pm\sqrt{\beta^2 - \gamma^2(1-s^2) + k(1-s^2)}.$$

The constant k determined by the condition that the expression under the square root sign has a double zero, that is $k = \gamma^2$ or $k = \gamma^2 - \beta^2$. In the first case $\pi(s) = \pm\beta$; in the second, $\pi(s) = \pm\beta s$. We choose the one for which $\tau(s) = \tilde{\tau}(s) + 2\pi(s)$ has a negative derivative and a zero on $(-1, +1)$. These conditions are satisfied by

$$\tau(s) = -2(1+\beta)s,$$

which correspond to

$$\pi(s) = -\beta s, \;\; \phi(s) = (1-s^2)^{\beta/2},$$

$$\lambda = \gamma^2 - \beta^2 - \beta, \;\; \rho(s) = (1-s^2)^{\beta}.$$

The energy eigenvalues are determined by

$$\lambda + n\tau' + \frac{1}{2}n(n-1)\sigma'' = 0, \quad n = 0, 1, \cdots,$$

which reduces to

$$\gamma^2 - \beta^2 - \beta = 2n(1+\beta) + n(n-1).$$

Hence the eigenvalues are

$$E_n = -\frac{h^2\alpha^2}{2m}\beta_n^2 \text{ where } \beta_n = -n - \frac{1}{2} + \sqrt{\gamma^2 + \frac{1}{4}},\ \beta_n > 0.$$

The condition $\beta_n > 0$ can be satisfied only for

$$n < \sqrt{\gamma^2 + \frac{1}{4}} - \frac{1}{2},$$

i.e., there are only finitely many eigenvalues. In this case the eigenfunctions $y_n(s)$ have the form

$$y_n(s) = P_n^{(\beta,\beta)}(s)$$

with

$$\beta = \beta_n.$$

The wave functions $\psi_n(x)$ are

$$\psi_n(x) = c_n(1-s^2)^{\beta/2} P_n^{(\beta,\beta)}(s),$$

with $\beta = \beta_n, \quad s = \tan h\alpha x$. Here c_n is a normalizing constant determined by

$$\int_{-\infty}^{\infty} \psi_n^2(x)dx = 1.$$

So,

$$c_n = \left\{ \frac{2^{2\beta+1}\Gamma^2(n+\beta+1)}{n!(2n+2\beta+1)\Gamma(n+2\beta+1)} \right\}^{1/2}.$$

2.3.3 Particle-in-a-box

Consider the problem of finding the eigenvalues and eigenfunctions of the equation,

$$-y'' + V(x)y = \lambda y, \quad x \in [-L, L], \; y(-L) = y(L) = 0$$

where the potential is in the form

$$V(x) = \begin{cases} \infty & , \; |x| \geq L \\ \\ 0 & , \; -L < x < L \end{cases}$$

So, the equation takes the form;

$$y'' + \lambda y = 0$$

whose solutions are given in terms of circular functions,

$$y(x) = A\cos\sqrt{\lambda}x + B\sin\sqrt{\lambda}x. \tag{2.3.65}$$

If we substitute the boundary conditions in (2.3.65), we find

$$A\cos\sqrt{\lambda}L + B\sin\sqrt{\lambda}L = 0 \tag{2.3.66}$$

$$A\cos\sqrt{\lambda}L - B\sin\sqrt{\lambda}L = 0 \tag{2.3.67}$$

(2.3.66) + (2.3.67) gives the equation

$$\sqrt{\lambda}L = (n + \frac{1}{2})\pi, \quad n = 0, 1, 2, \cdots .$$

We define the even eigenvalues (that is, the eigenvalues which correspond to the even eigenfunctions) such that,

$$\lambda_{2n} = \frac{\pi^2}{L^2}(n + \frac{1}{2})^2, \quad n = 0, 1, 2, \cdots$$

and find the even eigenfunctions using the equation (2.3.66),

$$y_{2n} = A\cos\frac{\pi}{L}(n+\frac{1}{2})x, \quad A : \text{Arbitrary.} \tag{2.3.68}$$

In the same way (2.3.66) - (2.3.67) gives the equation

$$\sqrt{\lambda}L = (n+1)\pi, \quad n = 0, 1, 2, \cdots.$$

So, we may define the odd eigenvalues (that is, the eigenvalues which correspond to the odd eigenfunctions) as follows;

$$\lambda_{2n+1} = \frac{\pi^2}{L^2}(n+1)^2, \quad n = 0, 1, 2, \cdots$$

and find the odd eigenfunctions such that;

$$y_{2n+1} = B\sin\frac{\pi}{L}(n+1)x, \quad B : \text{Arbitrary.} \tag{2.3.69}$$

We may write the solutions in terms of the Chebyshev polynomials $V_n(x)$ and $W_n(x)$ of the third and fourth kinds of degree n as follows: We have already shown that the even eigenfunctions are in the form that,

$$y_{2n} = A\cos\frac{\pi}{L}(n+\frac{1}{2})x, \quad A : \text{Arbitrary.}$$

Let us define $\theta = \frac{\pi}{L}x$ and take $A = 1$.

$$y_{2n} = \cos(n+\frac{1}{2})\theta$$

$$y_{2n} = \cos\frac{\theta}{2}V_n(t) \quad \text{where}$$

$$V_n(t) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}, \text{ when } t = \cos\theta. \tag{2.3.70}$$

To justify the definition of $V_n(t)$, we first observe that $\cos(n+\frac{1}{2})\theta$ is an odd polynomial of degree $2n+1$ in $\cos\frac{1}{2}\theta$. Therefore the r.h.s. of (2.3.70) is an even polynomial of degree $2n$ in $\cos\frac{1}{2}\theta$, which is equivalent to a polynomial of degree

n in $\cos^2 \frac{1}{2}\theta = \frac{1}{2}(1+\cos\theta)$ and hence to a polynomial of degree n in $\cos\theta$. Thus $V_n(t)$ is indeed a polynomial of degree n in t. For example,

$$V_1(t) = \frac{\cos(1+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta} = \frac{4\cos^3\frac{1}{2}\theta - 3\cos\frac{1}{2}\theta}{\cos\frac{1}{2}\theta} =$$

$$= 4\cos^2\frac{1}{2}\theta - 3 = 2\cos\theta - 1 = 2t-1.$$

We may readily show that,

$$V_0(t) = 1,\ \ V_1(t) = 2t-1,\ \ V_2(t) = 4t^2-2t-1, \cdots .$$

In the same way, we may write the odd eigenfunctions by defining $\theta = \frac{\pi}{L}x$ and taking $B=1$ in (2.3.69) such that;

$$y_{2n+1} = \sin\frac{\theta}{2}W_n(t) \ \text{ where}$$

$$W_n(t) = \frac{\sin(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta} \quad \text{when } \ t=\cos\theta. \tag{2.3.71}$$

Similarly, $\sin(n+\frac{1}{2})\theta$ is an odd polynomial of degree $2n+1$ in $\sin\frac{1}{2}\theta$. Therefore the r.h.s. of (2.3.71) is an even polynomial of degree $2n$ in $\sin\frac{1}{2}\theta$, which is equivalent to a polynomial of degree n in $\sin^2\frac{1}{2}\theta = \frac{1}{2}(1-\cos\theta)$ and hence again to a polynomial of degree n in $\cos\theta$. For example,

$$W_1(t) = \frac{\sin(1+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta} = \frac{3\sin\frac{1}{2}\theta - 4\sin^3\frac{1}{2}\theta}{\sin\frac{1}{2}\theta} =$$

$$= 3 - 4\sin^2\frac{1}{2}\theta = 2\cos\theta + 1 = 2t+1.$$

We may readily show that,

$$W_0(t) = 1, W_1(t) = 2t+1, W_2(t) = 4t^2+2t-1, \cdots .$$

The polynomials $V_n(t)$ and $W_n(t)$ are, in fact, rescalings of two particular Jacobi polynomials $P_n^{(\alpha,\beta)}(t)$ with $\alpha = -\frac{1}{2}, \beta = \frac{1}{2}$ and vice versa. Explicitly,

$$\binom{2n}{n} V_n(t) = 2^{2n} P_n^{(-\frac{1}{2},\frac{1}{2})}(t),$$

$$\binom{2n}{n} W_n(t) = 2^{2n} P_n^{(\frac{1}{2},-\frac{1}{2})}(t).$$

These polynomials may be efficiently generated by the use of a recurrence relation. Since,

$$\cos(n+\frac{1}{2})\theta + \cos(n-2+\frac{1}{2})\theta = 2\cos\theta\cos(n-1+\frac{1}{2})\theta$$

and

$$\sin(n+\frac{1}{2})\theta + \sin(n-2+\frac{1}{2})\theta = 2\cos\theta\sin(n-1+\frac{1}{2})\theta,$$

it immediately follows that

$$V_n(t) = 2tV_{n-1}(t) - V_{n-2}(t), \quad n = 2, 3, \cdots,$$

and

$$W_n(t) = 2tW_{n-1}(t) - W_{n-2}(t), \quad n = 2, 3, \cdots,$$

with

$$V_0(t) = 1, \quad V_1(t) = 2t - 1$$

and

$$W_0(t) = 1, \quad W_1(t) = 2t + 1.$$

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CHAPTER 3

PERTURBATION THEORY

3.1 Introduction

Perturbation theory is a large collection of iterative methods for obtaining approximate solutions to problems involving a small parameter ϵ. These methods are so powerful that sometimes it is actually advisable to introduce a parameter ϵ temporarily into a difficult problem having no small parameter and then finally to set $\epsilon = 1$ to recover the original problem. This apparently artificial conversion to a perturbation problem may be the only way to make progress.

The thematic approach of perturbation theory is to decompose a tough problem into an infinite number of relatively easy ones. Hence, perturbation theory is most useful when the first few steps reveal the important features of the solution and the remaining ones give small corrections.

In perturbation theory it is convenient to have an asymptotic order relation that expresses the relative magnitudes of two functions more precisely than $<<$ but less precisely than $\sim$. We define

$$f(x) = 0[g(x)], \qquad x \to x_0$$

and say "$f(x)$ is at most of order $g(x)$ as $x \to x_0$" or "$f(x)$ is big oh of $g(x)$ as $x \to x_0$" if $f(x)/g(x)$ is bounded for x near x_0; that is $|f(x)/g(x)| < M$, for some constant M, if x is sufficiently close to x_0 [2].

In perturbation theory one may calculate just a few terms in a perturbation series. Whether or not this series is convergent, the notation "0" is very useful for expressing the order of magnitude of the first neglected term when that term has not been calculated explicitly.

3.2 Regular and Singular Perturbation Theory

The formal techniques of perturbation theory are a natural generalization of the ideas of local analysis of differential equations. Local analysis involves approximating the solution to a differential equation near the point $x = a$ by developing a series solution about a in powers of a smal parameter, either $x - a$ for finite a or $\frac{1}{x}$ for $a = \infty$. Once the leading behaviour of the solution near $x = a$ (which we would now refer to as the zeroth-order solution) is known, the remaning coefficients in the series can be computed recursively.

The strong analogy between local analysis of differential equations and formal perturbation theory may be used to classify perturbation problems. Recall that there are two different types of series solutions to differential equations. A series solution about an ordinary point of a differential equation is always a Taylor series having a non-vanishing radius of convergence. A series solution about a singular point does not have this form. Instead, it may either be a convergent series not in Taylor series form (such as a Frobenius series) or it may be a divergent series. Series solutions about singular points often have the remakable property of being meaningful near a singular point yet not existing at the singular point.

Perturbation series also occur in two variaties. We define a "regular" perturbation problem as one whose perturbation series is a power series in ϵ having a non-vanishing radius of convergence. A basic feature of all regular perturbation problems is that the exact solution for small but nonzero $|\epsilon|$ smoothly approaches the unperturbed or zeroth-order solution as $\epsilon \to 0$.

We define a "singular" perturbation problem [2] as one whose perturbation series either does not take the form of a power series or, if it does, the power series has a vanishing radius of convergence. In singular perturbation theory there is sometimes no solution to the unperturbed problem; when a solution to the unperturbed problem does exist, its qualitative features are distincly different from those of the exact solution for arbitrarily small but non-zero ϵ. In either case, the exact solution for $\epsilon = 0$ is fundamentally different in character from the "neighbouring" solutions obtained in the limit $\epsilon \to 0$. If there is no such abrupt change in character, then we would have to classify the problem as a regular perturbation problem.

When dealing with a singular perturbation problem, one must take care to distinguish between the "zeroth - order" solution and the solution of the unperturbed problem, since the latter may not even exist. There is no difference between these two in a regular perturbation theory, but in a singular perturbation theory the zeroth-order solution may depend on ϵ and may exist only for nonzero ϵ. Here is an example of singular perturbation problem:

Example 1: (Roots of a polynomial.) How does one determine the approximate root of

$$\epsilon^2 x^6 - \epsilon x^4 - x^3 + 8 = 0? \tag{3.2.1}$$

We may begin by setting $\epsilon = 0$ to obtain the unperturbed problem $-x^3 + 8 = 0$, which is easily solved:

$$x = 2, 2w, 2w^2 \tag{3.2.2}$$

where $w = e^{2\pi i/3}$ is a complex root of unity. Note that the unperturbed equation has only three roots while the original equation has six roots. This abrupt change in the character of the solution, namely the disappearence of three roots when $\epsilon = 0$ implies that (3.2.1) is a "singular perturbation" problem. Part of the exact solution ceases to exist when $\epsilon = 0$.

The explanation for this behaviour is that the three missing roots tend to ∞ as $\epsilon \to 0$. Thus, for those roots it is no longer valid to neglect $\epsilon^2 x^6 - \epsilon x^4$ compared with $-x^3 + 8$ in the limit $\epsilon \to 0$. Of course, for the three roots near $2, 2w$ and $2w^2$, the terms $\epsilon^2 x^6$ and ϵx^4 are indeed small as $\epsilon \to 0$ and we may assume a regular perturbation expansion for these roots of the form

$$x_k(\epsilon) = 2e^{2\pi i k/3} + \sum_{n=1}^{\infty} a_{n,k} \epsilon^n, \quad k = 1, 2, 3. \tag{3.2.3}$$

Substituting (3.2.3) into (3.2.1) and comparing powers of ϵ gives a sequence of equations which determine the coefficients $a_{n,k}$.

To track down the three missing roots we first estimate their orders of magnitude as $\epsilon \to 0$. We do this by considering all possible dominant balances between pairs of terms in (3.2.1). There are four terms in (3.2.1) so there are six pairs to consider:

(a) Suppose $\epsilon^2 x^6 \sim \epsilon x^4 (\epsilon \to 0)$ is the dominant balance. Then $x = 0(\epsilon^{-1/2})(\epsilon \to 0)$. It follows that the terms $\epsilon^2 x^6$ and ϵx^4 are both $0(\epsilon^{-1})$. But $\epsilon x^4 << x^3 = 0(\epsilon^{-3/2})$ as $(\epsilon \to 0)$, so x^3 is the biggest term in the equation and is not balanced by any other term. Thus, the assumption that $\epsilon^2 x^6$ and ϵx^4 are the dominant terms as $(\epsilon \to 0)$ is inconsistent.

(b) Suppose $\epsilon x^4 \sim x^3$ as $(\epsilon \to 0)$. Then $x = 0(\epsilon^{-1})$. It follows that $\epsilon x^4 \sim x^3 = 0(\epsilon^{-3})$. But $x^3 << \epsilon^2 x^6 = 0(\epsilon^{-4})$ as $(\epsilon \to 0)$. Thus $\epsilon^2 x^6$ is the largest term in the equation. Hence, the original assumption is again inconsistent.

(c) Suppose $\epsilon^2 x^6 \sim 8$ so that $x = 0(\epsilon^{-1/3})$ $(\epsilon \to 0)$. Hence $x^3 = 0(\epsilon^{-1})$ is the largest term, which is again inconsistent.

(d) Suppose $\epsilon x^4 \sim 8$ so that $x = 0(\epsilon^{-1/4})(\epsilon \to 0)$. Then $x^3 = 0(\epsilon^{-3/4})$ is the biggest term, which is also inconsistent.

(e) Suppose $x^3 \sim 8$. Then $x = 0(1)$. This is a consistent assumption because the other two terms in the equation, $\epsilon^2 x^6$ and ϵx^4, are negligible compared with x^3 and 8, and we recover the three roots of the unperturbed equation $x = 2, 2w$ and $2w^2$.

(f) Suppose $\epsilon^2 x^6 \sim x^3 (\epsilon \to 0)$. Then $x = 0(\epsilon^{-2/3})$. This is consistent because $\epsilon^2 x^6 \sim x^3 = 0(\epsilon^{-2})$ is bigger than $\epsilon x^4 = 0(\epsilon^{-5/3})$ and $8 = 0(1)$ as $\epsilon \to 0$.

Thus, the magnitudes of the three missing roots are $0(\epsilon^{-2/3})$ as $\epsilon \to 0$. This result is a clue to the structure of the perturbation series for the missing roots. In particular, it suggests a scale transformation for the variable x:

$$x = \epsilon^{-2/3} y. \tag{3.2.4}$$

Substituting (3.2.4) into (3.2.1) gives

$$y^6 - y^3 + 8\epsilon^2 - \epsilon^{1/3} y^4 = 0. \tag{3.2.5}$$

This is now a "regular perturbation" problem for y in the parameter $\epsilon^{1/3}$ because the unperturbed problem $y^6 - y^3 = 0$ has six roots $y = 1, w, w^2, 0, 0, 0$. Now, no roots disappear in the limit $\epsilon^{1/3} \to 0$. The perturbative corrections to these roots may be found by assuming a regular perturbation expansion in powers of $\epsilon^{1/3}$:

$$y = \sum_{n=0}^{\infty} y_n (\epsilon^{1/3})^n \tag{3.2.6}$$

Nevertheless, when $y_0 = 0$ we find that $y_1 = 0$ and $y_2 = 2, 2w, 2w^2$. Thus, since the first two terms in the series vanish, $x = \epsilon^{-2/3} y$ is not really $0(\epsilon^{-2/3})$ but rather $0(1)$ and we have reproduced the three finite roots near $x = 2, 2w, 2w^2$.

We may also apply perturbation theory to a differential equation [22]. Here is an example of this kind:

Example 2:

The initial - value problem

$$y'' + (1 + \epsilon x) y = 0, \qquad y(0) = 1, \qquad y'(0) = 0 \tag{3.2.7}$$

is a regular perturbation problem in ϵ over the finite interval $0 \leq x \leq L$.

We may begin by setting $\epsilon = 0$ to obtain the "unperturbed problem"

$$y'' + y = 0$$

with the boundary conditions $y(0) = 1, y'(0) = 0$. The solution is easily found that,

$$y(x, 0) = A \cos x + B \sin x.$$

Substituting the associated boundary conditions , the exact solution is just $y(x, \epsilon) = y(x, 0) = \cos x$.

Propose a perturbation series,

$$y(x, \epsilon) = \sum_{n=0}^{\infty} y_n(x) \epsilon^n \quad \text{at} \quad \epsilon = 0$$

$$y(x, \epsilon) = y_0(x) + y_1(x)\epsilon + y_2(x)\epsilon^2 + \cdots$$

The value at $\epsilon = 0$ is $y(x, 0) = y_0(x) = \cos x$. If we take the first and second derivatives of the perturbation series and substitute into the equation (3.2.7), we find that,

$$
\begin{aligned}
\sum_{n=0}^{\infty} y_n''(x)\epsilon \quad &+ \quad (1+\epsilon x)\sum_{n=0}^{\infty} y_n(x)\epsilon^n = 0 \\
y_0''(x) + y_0(x) \quad &+ \quad \sum_{n=0}^{\infty}[y_{n+1}''(x) + y_{n+1}(x) + xy_n(x)]\epsilon^{n+1} = 0 \\
[y_0''(x) + y_0(x)]\epsilon^0 \quad &+ \quad [y_1''(x) + y_1(x) + xy_0(x)]\epsilon^1 \\
+[y_2''(x) \quad &+ \quad y_2(x) + xy_1(x)]\epsilon^2 + \cdots = 0
\end{aligned}
$$

Then, equating each power of ϵ to zero, we get,

$$
\begin{array}{lllrcl}
\epsilon^0 & : & y_0'' + y_0 = 0; \quad y_0(x) = \cos x; & y_0(0) & = & 1, \\
 & & & y_0'(0) & = & 0 \\
\epsilon^1 & : & y_1''(x) + y_1(x) = -xy_0(x); \quad y_1(0) = 0, & y_1'(0) & = & 0 \\
\epsilon^2 & : & y_2''(x) + y_2(x) = -xy_1(x); \quad y_2(0) = 0, & y_2'(0) & = & 0
\end{array}
$$

and so on.

First, examine the first-order perturbation problem,

$$y_1'' + y_1 = -x\cos x, \qquad y_1(0) = y_1'(0) = 0.$$

We may solve the problem by the method of variation of parameters. Define $y_1(x)$ as folows;

$$y_1(x) = A\cos x + B\sin x + f_1(x).$$

Propose a particular solution of the form,

$$f_1(x) = u_1(x)\cos x + u_2(x)\sin x.$$

We find the values of u_1 and u_2 by imposing the necessary conditions as follows:

$$u_1(x) = -\frac{1}{4}x\cos 2x + \frac{1}{8}\sin 2x$$

and

$$u_2(x) = -\frac{1}{4}x^2 - \frac{1}{4}x\sin 2x - \frac{1}{8}\cos 2x.$$

So, we write $y_1(x)$ such that,

$$y_1(x) = A\cos x + B\sin x + \frac{1}{4}\cos x\{\frac{1}{2}\sin 2x - x\cos 2x\}$$

$$-\frac{1}{4}\sin x\{x^2 + x\sin 2x + \frac{1}{2}\cos 2x\}.$$

By substituting the conditions, we find $A = 0$ and $B = \frac{1}{8}$. Then, $y_1(x)$ is written in the form,

$$y_1(x) = -\frac{1}{4}[x^2\sin x - \sin x + x\cos x].$$

The solution of the differential equation (3.2.7) becomes,

$$y(x,\epsilon) = \cos x - \frac{1}{4}[x^2\sin x - \sin x + x\cos x]\epsilon + 0(\epsilon^2).$$

In the same way, we may solve the second - order perturbation problem,

$$y_2^{''} + y_2(x) = -xy_1(x), \qquad y_2(0) = y_2^{'}(0) = 0.$$

Again using the method of variation of parameters, we write

$$y_2(x) = A\cos x + B\sin x + f_2(x).$$

Then, propose a particular solution in the form,

$$f_2(x) = u_1(x)\cos x + u_2(x)\sin x.$$

We find the values of u_1 and u_2 such that,

$$u_1(x) = -\frac{1}{4}\left\{\frac{1}{16}\cos 2x(-10x^2 + 7) - \frac{1}{4}\sin 2x(x^3 - \frac{7}{2}x) + \frac{x^4}{8} - \frac{x^2}{4}\right\}$$

and

$$u_2(x) = \frac{1}{4}\left\{\frac{1}{4}x\cos 2x\left(-x^2+\frac{7}{2}\right) - \frac{1}{8}\sin 2x\left(-5x^2+\frac{7}{2}\right) + \frac{x^3}{6}\right\}.$$

So, we write $y_2(x)$ as follows:

$$y_2(x) = \frac{1}{32}x^4\cos x - \frac{5}{48}x^3\sin x - \frac{7}{16}x^2\cos x + \frac{7}{16}x\sin x.$$

We obtain the perturbation solution in the form,

$$\begin{aligned} y(x) &= \cos x + \epsilon\left(-\frac{1}{4}x^2\sin x - \frac{1}{4}x\cos x + \frac{1}{4}\sin x\right) \\ &+ \epsilon^2\left(\frac{1}{32}x^4\cos x - \frac{5}{48}x^3\sin x - \frac{7}{16}x^2\cos x + \frac{7}{16}x\sin x\right) + \cdots, \end{aligned}$$

$y(x)$ converges for all x and ϵ, with increasing rapidity as $\epsilon \to 0+$ for fixed x.

This initial - value problem must be reclassified as a singular perturbation problem over the semi-infinite interval $0 \le x < \infty$. While the exact solution does approach the solution to the unperturbed problem as $\epsilon \to 0+$ for fixed x, it does not do so uniformly for all x.

Example 2 shows that the interval itself can determine whether a perturbation problem is regular or singular. The feature that is common to all such examples is that on *nth*-order perturbative approximation bears less and less resemblance to the exact solution as x increases.

3.3 Perturbation methods for Linear Eigenvalue problems

3.3.1 Introduction

Perturbation methods attempt to solve a given problem by approximating it by simpler problems whose solutions are more or less explicitly known.

In eigenvalue problems the perturbation method [10], [28] yields numerical results comparatively quickly provided you are satisfied with approximations of low order. However, even in problems which appear to be very simple, it might be difficult to ascertain whether or not the method applied would converge or to estimate the error incurred by stopping at a certain order of approximation. Sometimes the method obviously does not converge-at least not in the usual sense; then there is the problem of trying to interpret the results computed, if they have any significance at all.

3.3.2 Perturbation of Schrödinger Equation

In this section, we shall show how the perturbation theory [39] can be used to approximate the eigenvalues and eigenfunctions of the Schrödinger equation of the form,

$$(-H_0 + \epsilon H_1)\psi = E\psi \tag{3.3.8}$$

where H_0 and H_1 are operators and ϵ is the perturbation parameter. We remark, at this point, that if the Hamiltonian can be written as a convergent power series in a certain parameter ϵ, or particularly, as in equation (3.3.8) with H_1 being a bounded operator, then the perturbed eigenvalues and eigenfunctions are analytic functions of ϵ, and their power series are convergent power series in a neighbourhood of $\epsilon = 0$. Theorem (2.3.1) of Rellich [28].

Therefore, let λ_n, for a fixed index n, is a simple discrete eigenvalue of the Hamiltonian operator H_0, associated to the eigenfunction ϕ_n, namely,

$$-H_0\phi_n = \lambda_n\phi_n \tag{3.3.9}$$

is the unperturbed quantum mechanical system, the solutions of which are assumed to be known completely. Since H_0 is Hermitian, the set of eigenfunctions $\{\phi_i\}_{i=0}^{\infty}$ forms a complete orthogonal set. Let $\lambda_i, (i = 0, 1, 2, \cdots)$, be the corresponding eigenvalues of the system. So, λ_n is just one of them, which is assumed to be discrete and simple.

Hence, we formally expand the eigenfunctions and the energy eigenvalues in the form of power series in ϵ, for small, but nonzero $|\epsilon|$,

$$\psi_n(\xi,\epsilon)=\sum_{k=0}^{\infty}F_n^{(k)}(\xi)\epsilon^k \tag{3.3.10}$$

and

$$E_n(\epsilon)=\sum_{k=0}^{\infty}w_k(n)\epsilon^k,\quad n=0,1,2,\cdots. \tag{3.3.11}$$

Substituting the equations (3.3.10) and (3.3.11) into the perturbed Schrödinger equation (3.3.8) it follows that,

$$-H_0F_n^{(0)}=w_0(n)F_n^{(0)} \tag{3.3.12}$$

and

$$-H_0F_n^{(k)}+H_1F_n^{(k-1)}=\sum_{s=0}^{k}w_s(n)F_n^{(k-s)},\quad k=1,2,\cdots. \tag{3.3.13}$$

Here, we know the solutions of the eigenvalue problem defined in (3.3.12), and they are the eigenfunctions ϕ_j and associated eigenvalues λ_j for $j=0,1,2,\cdots$, where the set $\{\phi_j\}_{j=0}^{\infty}$ forms a complete orthogonal set of eigenfunctions. We assume that the normalization condition,

$$\left\langle F_n^{(s)},F_n^{(0)}\right\rangle=\delta_{so},\quad s=0,1,\cdots,k. \tag{3.3.14}$$

Multiplying equation (3.3.13) through by $F_n^{(0)}(\xi)$, integrating at the associated boundary conditions, we find

$$\sum_{s=0}^{k}w_s(n)\left\langle F_n^{(k-s)},F_n^{(0)}\right\rangle=-\left\langle H_0F_n^{(k)},F_n^{(0)}\right\rangle+\left\langle H_1F_n^{(k-1)}F_n^{(0)}\right\rangle. \tag{3.3.15}$$

Since a global normalization is possible when (3.3.15) is solved for $F_n^{(k)}$ and from our assumption that the normalization condition (3.3.14) holds, we get

$$w_k(n)=\left\langle H_1F_n^{(k-1)},F_n^{(0)}\right\rangle,\quad k=1,2,\cdots. \tag{3.3.16}$$

Thus, it is possible to define $F_n^{(k)}$ and $w_k(n)$ from (3.3.15) and (3.3.16) which give an iterative procedure for calculating the coefficients in the perturbation series.

3.3.3 Enclosed Quantum Mechanical Systems

Consider the enclosed Schrödinger equation in one dimension,

$$H\psi = E\psi, \quad H = -\frac{d^2}{dx^2} + V(x), \quad x \in [-L, L], \quad \psi(\mp L) = 0 \tag{3.3.17}$$

where the potential is in the form

$$V(x) = \sum_{i=1}^{K} v_{2i} x^{2i}, \quad v_{2K} > 0. \tag{3.3.18}$$

Making use of the scaling transformation

$$\xi = \frac{\pi}{L} x, \quad \xi \in [-\pi, \pi] \tag{3.3.19}$$

the problem is altered to

$$\left[-\frac{d^2}{d\xi^2} + \left(\frac{L}{\pi}\right)^2 V(\xi) \right] \psi(\xi) = \Omega \psi(\xi), \; \psi(\mp\pi) = 0 \tag{3.3.20}$$

where

$$\Omega = \left(\frac{L}{\pi}\right)^2 E, \quad V(\xi) = \sum_{i=1}^{K} c_{2i} \xi^{2i}, \quad c_{2i} = \left(\frac{L}{\pi}\right)^{2i} v_{2i}. \tag{3.3.21}$$

Therefore the formulation in the previous section (3.3.2) can be considered with

$$H_0 = \frac{d^2}{d\xi^2} = D^2, \quad H_1 = V(\xi), \quad \epsilon = \left(\frac{L}{\pi}\right)^2, \quad E = \frac{\Omega}{\epsilon} \tag{3.3.22}$$

We may rewrite equation (3.3.20) as

$$(-H_0 + \epsilon H_1)\psi(\xi,\epsilon) = \Omega(\epsilon)\psi(\xi,\epsilon), \quad \psi(\mp\pi,\epsilon) = 0. \tag{3.3.23}$$

Hence, our task will be the determination of the serial expansions of $\Omega(\epsilon)$ and $\psi(\xi,\epsilon)$ in nonnegative powers of ϵ, i.e.

$$\Omega_n(\epsilon) = \sum_{k=0}^{\infty} w_k(n)\epsilon^k, \quad \psi_n(\xi,\epsilon) = \sum_{k=0}^{\infty} F_n^{(k)}(\xi)\epsilon^k, \quad n = 0, 1, 2, \cdots . \tag{3.3.24}$$

Since the perturbation potential H_1 can be made bounded, the perturbation theory of linear operators dictates us that the resulting energy eigenvalue series for $\Omega(\epsilon)$ will be valid in some non-zero region of Ω complex plane. The radius of such a convergence region depends clearly on L, and covers all Ω-complex plane as L approaches zero, since perturbation series terminates at the zeroth order term. As a result, we may expect that (3.3.24) are convergent as long as L remains smaller than a finite number, $\rho(L)$ say. Substitution of (3.3.24) into (3.3.23),

$$-\sum_{k=0}^{\infty} H_0 F_n^{(k)}(\xi)\epsilon^k + \sum_{k=0}^{\infty} H_1 F_n^{(k)}(\xi)\epsilon^{k+1} = \sum_{k=0}^{\infty} w_k(n)\epsilon^k \sum_{k=0}^{\infty} F_n^{(k)}(\xi)\epsilon^k$$

we find that

$$\sum_{k=0}^{\infty}[-H_0 F_n^{(k)}(\xi) + H_1 F_n^{(k-1)}(\xi)]\epsilon^k = \sum_{k=0}^{\infty}\left[\sum_{s=0}^{k} w_{k-s}(n) F_n^{(s)}(\xi)\right]\epsilon^k, F_n^{(-1)}(\xi) \equiv 0$$

so that

$$-H_0 F_n^{(k)}(\xi) + H_1 F_n^{(k-1)}(\xi) = \sum_{s=0}^{k} w_{k-s}(n) F_n^{(s)}(\xi), \quad k = 0, 1, \cdots .$$

Then we obtain,

$$\left[H_0 + w_0(n)I\right]F_n^{(0)}(\xi) = 0 \tag{3.3.25}$$

$$\left[H_0 + w_0(n)I\right]F_n^{(1)}(\xi) = \left[H_1 - w_1(n)I\right]F_n^{(0)}(\xi) \tag{3.3.26}$$

$$\big[H_0+w_0(n)I\big]F_n^{(k)}(\xi)=\big[H_1-w_1(n)I\big]F_n^{(k-1)}(\xi)-\sum_{s=0}^{k-2}w_{k-s}(n)F_n^{(s)}(\xi),\, k\geq 2 \tag{3.3.27}$$

where I is unit operator in the operator space to which H_0 and H_1 belong. On the other hand, the boundary conditions in (3.3.23) imply that

$$F_n^{(k)}(\mp\pi)=0, \quad k=0,1,\cdots. \tag{3.3.28}$$

As is shown, the original problem (3.3.20) has been reduced to solving $F_n^{(k)}(\xi)$ and $w_k(n)$ in (3.3.24) recursively. From (3.3.25), we see that the zeroth-order wave functions $F_n^{(0)}(\xi)$ satisfy the differential equation

$$\frac{d^2F_n^{(0)}}{d\xi^2}+w_0(n)F_n^{(0)}=0$$

whose solutions are given in terms of circular functions

$$F_n^{(0)}(\xi)=a_0\cos\sqrt{w_0(n)}\xi+b_0\sin\sqrt{w_0(n)}\xi, \quad a_0,b_0: \quad \text{constants.}$$

Using (3.3.28), we have,

$$a_0\cos\sqrt{w_0(n)}\pi+b_0\sin\sqrt{w_0(n)}\pi=0$$

$$a_0\cos\sqrt{w_0(n)}\pi-b_0\sin\sqrt{w_0(n)}\pi=0.$$

For non-trivial solutions for a_0 and b_0, we must have

$$\begin{vmatrix}\cos\sqrt{w_0(n)}\pi & \sin\sqrt{w_0(n)}\pi \\ \cos\sqrt{w_0(n)}\pi & -\sin\sqrt{w_0(n)}\pi\end{vmatrix}=0$$

which implies that either

$$w_0(n)=\left(n+\frac{1}{2}\right)^2 \text{ or } w_0(n)=(n+1)^2,\; n=0,1,2,\cdots \tag{3.3.29}$$

corresponding to two different solutions

$$F_n^{(0)}(\xi) = a_0 \cos\left(n + \frac{1}{2}\right)\xi \text{ and } F_n^{(0)}(\xi) = b_0 \sin(n+1)\xi$$

respectively. These solutions represent symmetric and anti-symmetric states of the problem owing to the fact that $V(-\xi) = V(\xi)$. Therefore we have

$$F_n^{(0)}(\xi) = \begin{cases} \phi_{2n}(\xi) = \frac{1}{\sqrt{\pi}} \cos\left(n + \frac{1}{2}\right)\xi \quad , \quad \text{for symmetric states} \\ \\ \phi_{2n+1}(\xi) = \frac{1}{\sqrt{\pi}} \sin\left(n+1\right)\xi \quad , \quad \text{for anti-symmetric states} \end{cases} \tag{3.3.30}$$

where we have taken $a_0 = b_0 = \frac{1}{\sqrt{\pi}}$ for normalization, i.e.

$$\int_{-\pi}^{\pi} \left[F_n^{(0)}(\xi)\right]^2 d\xi = 1.$$

Multiplying equation (3.3.27) through by $F_n^{(0)}(\xi)$, integrating from $-\pi$ to π,

$$\begin{aligned} \left\langle [H_0 + w_0(n)I]F_n^{(k)}, F_n^{(0)} \right\rangle &= \left\langle [H_1 - w_1(n)I]F_n^{(k-1)}, F_n^{(0)} \right\rangle - \\ &- \sum_{s=0}^{k-2} w_{k-s}(n) \left\langle F_n^{(s)}, F_n^{(0)} \right\rangle \end{aligned}$$

and using the self -adjointness of $H_0 + w_0(n)I$, we find that

$$\sum_{s=0}^{k-2} w_{k-s}(n) \left\langle F_n^{(s)}, F_n^{(0)} \right\rangle = \left\langle H_1 F_n^{(k-1)}, F_n^{(0)} \right\rangle - w_1(n) \left\langle F_n^{(k-1)}, F_n^{(0)} \right\rangle.$$

Since a global normalization is always possible when the differential equation (3.3.27) is solved for $F_n^{(k)}(\xi)$, we assume that the normalization condition

$$< F_n^{(s)}, F_n^{(0)} >= \delta_{s0}, \ s = 0, 1, \cdots, k \tag{3.3.31}$$

holds, and hence obtain the formula

$$w_k(n) =< H_1 F_n^{(k-1)}, F_n^{(0)} >, \quad k = 1, 2, \cdots . \tag{3.3.32}$$

for the coefficients of the energy series in (3.3.24). The equation in (3.3.26) has the same homogeneous part as (3.3.25) so that its complementary solutions is of form $F_n^{(0)}(\xi)$. Therefore, we should find a particular solution only. By the method of the variation of parameters, we obtain

$$\begin{aligned} F_n^{(1)}(\xi) &= a_1 \cos\sqrt{w_0(n)}\xi + b_1 \sin\sqrt{w_0(n)}\xi - \frac{1}{\sqrt{w_0(n)}} \cos\sqrt{w_0(n)}\xi \\ & \int_{-\pi}^{\xi} \sin\sqrt{w_0(n)}u[V(u) - w_1(n)]F_n^{(0)}(u)du + \\ &+ \frac{1}{\sqrt{w_0(n)}} \sin\sqrt{w_0(n)}\xi \int_{-\pi}^{\xi} \cos\sqrt{w_0(n)}u[V(u) - w_1(n)]F_n^{(0)}(u)du \end{aligned}$$

or

$$F_n^{(1)}(\xi) = [a_1 + A_0(\xi)] \cos\sqrt{w_0(n)}\xi + [b_1 + B_0(\xi)] \sin\sqrt{w_0(n)}\xi \tag{3.3.33}$$

where

$$A_0(\xi) = -\frac{1}{\sqrt{w_0(n)}} \int_{-\pi}^{\xi} \sin\sqrt{w_0(n)}u[V(u) - w_1(n)]F_n^{(0)}(u)du, \;\; A_0(-\pi) = 0 \tag{3.3.34}$$

and

$$B_0(\xi) = \frac{1}{\sqrt{w_0(n)}} \int_{-\pi}^{\xi} \cos\sqrt{w_0(n)}u[V(u) - w_1(n)]F_n^{(0)}(u)du, \;\; B_0(-\pi) = 0 \tag{3.3.35}$$

a_1 and b_1 being some arbitrary constants. From the conditions (3.3.28), we have

$$a_1 \cos\sqrt{w_0(n)}\pi - b_1 \sin\sqrt{w_0(n)}\pi = 0 \tag{3.3.36}$$

$$a_1 \cos\sqrt{w_0(n)}\pi + b_1 \sin\sqrt{w_0(n)}\pi = -A_0(\pi)\cos\sqrt{w_0(n)}\pi - B_0(\pi)\sin\sqrt{w_0(n)}\pi. \tag{3.3.37}$$

For the symmetric states;

$$F_n^{(0)}(\xi) = F_n^{(0)}(-\xi) = \phi_{2n}(\xi) = \frac{1}{\sqrt{\pi}}\cos\left(n+\frac{1}{2}\right)\xi \text{ and } w_0(n) = \left(n+\frac{1}{2}\right)^2.$$

It can be easily shown that

$$A_0(\pi) = B_0(\pi) = 0.$$

Now, equations (3.3.36) and (3.3.37) give the results

$$a_1 \cos\left(n+\frac{1}{2}\right)\pi - b_1 \sin\left(n+\frac{1}{2}\right)\pi = 0$$

$$\Rightarrow -b_1(-1)^n = 0 \quad \Rightarrow b_1 = 0 \quad \text{and}$$

a_1 remains arbitrary. Therefore,

$$F_n^{(1)}(\xi) = \sqrt{\pi}[a_1 + A_0(\xi)]F_n^{(0)}(\xi) + B_0(\xi)\sin\left(n+\frac{1}{2}\right)\xi \tag{3.3.38}$$

in which a_1 may be determined according to the normalization condition (3.3.31).

CHAPTER 4

NUMERICAL APPLICATIONS

4.1 The Confined Harmonic Oscillator

We shall show how perturbation theory can be used to approximate the eigenvalues and eigenfunctions of the Confined Harmonic Oscillator, that is, we may solve (3.3.17) for $V(x) = x^2$,

$$\left[-\frac{d^2}{dx^2} + x^2\right]\psi(x) = E\psi(x), \quad \psi(\mp L) = 0, \quad x \in [-L, L]. \tag{4.1.1}$$

Following the same procedure in (3.3.3) the problem is altered to

$$\left[-\frac{d^2}{d\xi^2} + \epsilon V(\xi)\right]\psi(\xi) = \Omega\psi(\xi), \quad V(\xi) = H_1 = \epsilon\xi^2 \tag{4.1.2}$$

where $\epsilon = (\frac{L}{\pi})^2$. From (3.3.30), we know the zeroth-order wave functions $F_n^{(0)}(\xi)$ and we will only consider the symmetric states, thus we take only the eigenfunctions,

$$F_n^{(0)}(\xi) = \frac{1}{\sqrt{\pi}}\cos(n + \frac{1}{2})\xi, \quad n = 0, 1, 2, ... \tag{4.1.3}$$

and the corresponding eigenvalues,

$$w_0(n) = (n + \frac{1}{2})^2, \quad n = 0, 1, 2, ... \quad . \tag{4.1.4}$$

Since we know the formula in (3.3.32) for the coefficients of the energy series in (3.3.24), we may calculate $w_1(n)$ as follows:

$$w_1(n) = \langle H_1 F_n^{(0)}, F_n^{(0)} \rangle = \frac{\epsilon}{\pi} \int_{-\pi}^{\pi} \xi^2 \cos^2(n+\frac{1}{2})\xi d\xi = \epsilon \Big[\frac{\pi^2}{3} - \frac{1}{2w_0(n)}\Big]. \quad (4.1.5)$$

From (3.3.38), we may calculate $F_n^{(1)}(\xi)$ such that

$$F_n^{(1)}(\xi) = \Bigg[a_1 - \frac{4\epsilon}{16\sqrt{\pi}w_0^2(n)} + \frac{\epsilon(\xi^2+\pi^2) - 2w_1(n)}{4\sqrt{\pi}w_0(n)}\Bigg] \cos(n+\frac{1}{2})\xi$$

$$+\frac{1}{2\sqrt{\pi w_0(n)}}\Bigg[\frac{\epsilon}{3}(\xi^3+\pi^3) - (\xi+\pi)(w_1(n) + \frac{2\epsilon}{4w_0(n)})\Bigg] \sin(n+\frac{1}{2})\xi. \quad (4.1.6)$$

The constant a_1 may be determined from the normalization condition as follows

$$a_1 = \frac{L^2}{2w_0(n)}\Big[-\frac{1}{3} + \frac{1}{2\pi^2 w_0(n)}\Big] - \frac{3}{\pi}. \quad (4.1.7)$$

When we use the formula in (3.3.32), we find the following value for the coefficient $w_2(n)$;

$$w_2(n) = \langle H_1 F_n^{(1)}, F_n^{(0)} \rangle = \langle \epsilon\xi^2 F_n^{(1)}, F_n^{(0)} \rangle$$

$$= \frac{L^2}{4w_0(n)}\Bigg[\frac{1}{4w_0(n)\pi^2}\Big[-16L^2 + 10w_1(n)\Big]$$

$$+\frac{1}{15}\Big[13L^2 - 25w_1(n) + 10a_1\sqrt{\pi}(2w_0(n) - \frac{3}{\pi^2})\Big] + \frac{21L^2}{4w_0^2(n)\pi^4}\Bigg]. \quad (4.1.8)$$

We may write

$$\Omega_n^{(N)}(\epsilon) = \sum_{k=0}^{N} w_k(n)\epsilon^k$$

here N denotes the order perturbative contribution to the energy, where

$$E_n^{(N)} = \frac{1}{\epsilon}\Omega_n^{(N)}(\epsilon)$$

may be written from (3.3.22).

We have given the necessary and sufficient information to find the analytic expressions for first three symmetric contributions to the perturbation series of energy, E_0, E_2, E_4. Here, we present some calculations based on these kinds of formula in Tables 1-6. We have calculated the values not for $E_n^{(N)}$ but for $\epsilon E_n^{(N)}$ in Tables $1, 3, 5$ for not to deal with the big numbers coming from small values of L. Hence it becomes possible to see that the convergence rate of the perturbation series decreases as L increases. In Tables $2, 4, 6$ we have given some values for $L \geq 1$. As can be easily seen, one can obtain quite high accuracy for sufficiently small L values. As a basic feature of a regular perturbation problem, the exact solution for small but nonzero ϵ smoothly approaches the unperturbed or zeroth order solution as $\epsilon \to 0$. These observations imply that the perturbation series presented in this example have limited convergence radius which depends on L and n.

Table 4.1: The comparison of cumulative scaled eigenvalues for $n = 0$, as a function of the boundary parameter L.

L	$\epsilon E_0^{(0)}$	$\epsilon E_0^{(1)}$	$\epsilon E_0^{(2)}$
0.001	0.2500000000	0.250000000000013	0.250000000000013
0.01	0.2500000000	0.250000000132476	0.250000000132474
0.1	0.2500000000	0.250001324	0.250001322
0.2	0.2500000000	0.2500211	0.2500210
0.3	0.2500000000	0.250107	0.250105
0.5	0.2500000000	0.2508	0.2507
0.7	0.2500000000	0.253	0.252
0.8	0.2500000000	0.255	0.254

Table 4.2: The comparison of cumulative perturbational energy eigenvalues for $n = 0$, as a function of the boundary parameter L, $L \geq 1$.

L	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$
1	2.4693	2.6002	2.5739
1.5	1.0975	1.3919	1.2339
2	0.6173	1.1407	0.5323
3	0.2743	1.4520	-3.2079

Table 4.3: The comparison of cumulative scaled eigenvalues for $n = 1$, as a function of the boundary parameter L.

L	$\epsilon E_2^{(0)}$	$\epsilon E_2^{(1)}$	$\epsilon E_2^{(2)}$
0.001	2.25000000	2.250000000000030	2.250000000000030
0.01	2.25000000	2.25000000031469	2.25000000031468
0.1	2.25000000	2.250003146	2.250003141
0.2	2.25000000	2.2500503	2.2500500
0.3	2.25000000	2.250254	2.250250
0.5	2.25000000	2.2519	2.2518
0.7	2.25000000	2.257	2.256
0.8	2.25000000	2.262	2.261

Table 4.4: The comparison of cumulative perturbational energy eigenvalues for $n = 1$, as a function of the boundary parameter L, $L \geq 1$.

L	$E_2^{(0)}$	$E_2^{(1)}$	$E_2^{(2)}$
1	22.2244	22.5353	22.4806
1.5	9.8775	10.5769	10.2908
2	5.5561	6.7994	5.8550
3	2.4693	5.2669	-0.0990

Table 4.5: The comparison of cumulative scaled eigenvalues for $n = 2$, as a function of the boundary parameter L.

L	$\epsilon E_4^{(0)}$	$\epsilon E_4^{(1)}$	$\epsilon E_4^{(2)}$
0.001	6.25000000	6.250000000000030	6.250000000000030
0.01	6.25000000	6.25000000032927	6.25000000032926
0.1	6.25000000	6.25000329	6.25000328
0.2	6.25000000	6.2500526	6.2500523
0.3	6.25000000	6.250266	6.250262
0.5	6.25000000	6.252	6.251
0.7	6.25000000	6.258	6.257
0.8	6.25000000	6.263	6.262

Table 4.6: The comparison of cumulative perturbational energy eigenvalues for $n = 2$, as a function of the boundary parameter L, $L \geq 1$.

L	$E_4^{(0)}$	$E_4^{(1)}$	$E_4^{(2)}$
1	61.7346	62.0599	62.0038
1.5	27.4376	28.1694	27.8826
2	15.4336	16.7346	15.8170
3	6.8594	9.7865	4.9760

4.2 The Quartic Anharmonic Oscillator

We shall find the eigenvalues and eigenfunctions of the Schrödinger equation,

$$\left[-\frac{d^2}{dx^2} + V(x) + \epsilon H_1(x)\right]\psi(x) = \Omega\psi(x), \quad x \in (-\infty, \infty) \tag{4.2.9}$$

where $V(x) = x^2$ and $H_1(x) = x^4$. So, the equation (4.2.9) becomes,

$$\left[-\frac{d^2}{dx^2} + x^2 + \epsilon x^4\right]\psi(x) = \Omega\psi(x), \quad x \in (-\infty, \infty). \tag{4.2.10}$$

We assume that removing the term H_1 from (4.2.9) makes the equation an exactly soluable eigenvalue problem. This suggests using perturbation theory to solve the family of eigenvalue problems in which H_1 is replaced by ϵH_1. We may seek a perturbative solution to (4.2.10) of the form,

$$\psi_n(x,\epsilon) = \sum_{k=0}^{\infty} F_n^{(k)}(x)\epsilon^k, \tag{4.2.11}$$

$$\Omega_n(\epsilon) = \sum_{k=0}^{\infty} w_k(n)\epsilon^k, \; n = 0, 1, 2, \cdots . \tag{4.2.12}$$

Substituting (4.2.11) and (4.2.12) into (4.2.10) and following the same procedure we used in the section 3.3.3, we have the resulting sequence of equations, by comparing the powers of ϵ, we get

$$\left[-\frac{d^2}{dx^2} + x^2 - w_0(n)\right] F_n^{(k)}(x) = -x^4 F_n^{(k-1)}(x) + \sum_{j=1}^{k} w_j(n) F_n^{(k-j)}(x), k = 1, 2, 3, \cdots , \tag{4.2.13}$$

whose solutions must satisfy the boundary conditions,

$$\lim_{|x|\to\infty} F_n^{(k)}(x) = 0, \quad k = 1, 2, 3, \cdots .$$

Equation (4.2.13) is linear and inhomogeneous. The associated homogeneous equation is just the unperturbed problem which is the Schrödinger equation for the quantum mechanical harmonic oscillator,

$$\frac{d^2}{dx^2}F_n^{(0)}(x) + [w_0(n) - x^2]F_n^{(0)}(x) = 0. \tag{4.2.14}$$

The solution of the equation (4.2.14), which has already been found in the Example (1) in section 2.3.1, is of the form,

$$F_n^{(0)}(x) = c_n e^{-x^2/2} H_n(x) \;\text{ where }\; w_0(n) = 2n + 1 \tag{4.2.15}$$

c_n can easily be determined using the normalization condition so that

$$c_n = \frac{1}{2^{n/2}\sqrt{n!}\pi^{1/4}}. \tag{4.2.16}$$

However, only one of the two linearly independent solutions of the unperturbed problem (the one that satisfies the boundary conditions) is assumed known. Therefore, we proceed by the method of reduction of order; to wit, we substitute

$$F_n^{(k)}(x) = F_n^{(0)}(x)G_n^{(k)}(x) \tag{4.2.17}$$

where $G_n^{(0)}(x) = 1$, into (4.2.13). Simplifying the result using (4.2.14) and multiplying by the integrating factor $F_n^{(0)}(x)$ gives,

$$2\Big[\frac{d}{dx}F_n^{(0)}(x)\Big]F_n^{(0)}(x)\Big[\frac{d}{dx}G_n^{(k)}(x)\Big] + \Big[F_n^{(0)}(x)\Big]^2\Big[\frac{d^2}{dx^2}G_n^{(k)}(x)\Big]$$
$$= \Big[F_n^{(0)}(x)\Big]^2\Big[x^4 G_n^{(k-1)}(x) - \sum_{j=1}^{k} w_j(n)F_n^{(k-j)}(x)\Big]$$

or

$$\frac{d}{dx}\left[\big[F_n^{(0)}(x)\big]^2\frac{d}{dx}G_n^{(k)}(x)\right] = \big[F_n^{(0)}(x)\big]^2\left[x^4 G_n^{(k-1)}(x) - \sum_{j=1}^{k} w_j(n)F_n^{(k-j)}(x)\right]. \tag{4.2.18}$$

If we integrate the equation (4.2.18) from $-\infty$ to ∞ and use

$$\left[F_n^{(0)}(x)\right]^2 \frac{d}{dx} G_n^{(k)}(x) = F_n^{(0)}(x) \frac{d}{dx} F_n^{(k)}(x) - \frac{d}{dx} F_n^{(0)}(x) F_n^{(k)}(x) \to 0$$

as $|x| \to \infty$, we obtain the formula for the coefficient $w_k(n)$:

$$w_k(n) = \frac{\displaystyle\int_{-\infty}^{\infty} F_n^{(0)}(x) \left[x^4 F_n^{(k-1)}(x) - \sum_{j=1}^{k-1} w_j(n) F_n^{(k-j)}(x) \right] dx}{\displaystyle\int_{-\infty}^{\infty} \left[F_n^{(0)}(x)\right]^2 dx}, k = 1, 2, 3, \cdots . \tag{4.2.19}$$

Integrating (4.2.19) twice gives the formula for $F_n^{(k)}(x)$:

$$F_n^{(k)}(x) = F_n^{(0)}(x) \int_a^x \frac{dt}{\left[F_n^{(0)}(t)\right]^2} \int_{-\infty}^t ds F_n^{(0)}(s) \left[s^4 F_n^{(k-1)}(s) - \sum_{j=1}^{k} w_j(n) F_n^{(k-j)}(s) \right],$$

$$k = 1, 2, 3, \cdots . \tag{4.2.20}$$

Observe that in (4.2.20), a is an arbitrary number at which we choose to impose $F_n^{(k)}(a) = 0$. This means we have fixed the overall normalization of $\psi(x)$ so that $F_n(a) = F_n^{(0)}(a)$. [Assuming that $F_n^{(0)}(a) \neq 0$]. If $F_n^{(0)}(t)$ vanishes between a and x, the integral in (4.2.20) seems formally divergent; however $F_n^{(k)}(x)$ satisfies a differential equation (4.2.13) which has no finite singular points. Thus, it is possible to define $F_n^{(k)}(x)$ everywhere as a finite expression.

For the ground state, i.e. $n = 0$, the differential equation (4.2.13) becomes,

$$\left(-\frac{d^2}{dx^2} + x^2 - 1 \right) F_0^{(k)}(x) = -x^4 F_0^{(k-1)}(x) + \sum_{j=1}^{k} w_j(0) F_0^{(k-j)}(x), \quad k = 1, 2. \tag{4.2.21}$$

Let $F_0^{(k)}(x) = F_0^{(0)}(x) G_0^{(k)}(x) = e^{-x^2/2} G_0^{(k)}(x)$ where $G_0^{(0)} \equiv 1$. Taking derivatives and substituting into the differential equation (4.2.21), we find

$$-\frac{d^2}{dx^2}G_0^{(k)}(x) + 2x\frac{d}{dx}G_0^{(k)}(x) = -x^4 G_0^{(k-1)}(x) + \sum_{j=1}^{k} w_j(0) G_0^{(k-j)}(x). \quad (4.2.22)$$

For $k = 1$, the equation (4.2.22) takes the form,

$$-\frac{d^2}{dx^2}G_0^{(1)}(x) + 2x\frac{d}{dx}G_0^{(1)}(x) = -x^4 + w_1(0).$$

If we take $\frac{d}{dx}G_0^{(1)} = g_0$ and substitute into above equation then we get,

$$-\frac{d}{dx}g_0(x) + 2xg_0(x) = -x^4 + w_1(0).$$

When we look for the series solutions of g_0, from the help of the value of $w_1(0)$ that we find from the equation (4.2.19), we see that g_0 contains a finite number of terms, namely we find polynomial solution and now it becomes possible to write $G_0^{(1)}$ then $F_0^{(1)}$. Therefore, we may find the value of $w_2(0)$ from (4.2.19) using the properties of Hermite polynomials; recurrence and orthogonality relations. Then following the same procedure, we find the value of $w_3(0)$ and all the values of $w_k(0)$ for $k = 1, 2, 3$ are found as follows:

$$w_1(0) = \frac{3}{4},\ w_2(0) = -\frac{21}{16},\ w_3(0) = \frac{333}{64}.$$

Observe that in (4.2.19), if we know $F_n^{(k-1)}$ it is possible to evaluate the value of $w_k(n)$. Now, it is possible to write the perturbation series for the smallest eigenvalue such that:

$$\Omega_0(\epsilon) \sim 1 + \frac{3}{4}\epsilon - \frac{21}{16}\epsilon^2 + \frac{333}{64}\epsilon^3 + \cdots . \quad (4.2.23)$$

For $n = 1$, the differential equation (4.2.13) becomes,

$$\left(-\frac{d^2}{dx^2} + x^2 - 3\right) F_1^{(k)}(x) = -x^4 F_1^{(k-1)}(x) + \sum_{j=1}^{k} w_j(1) F_1^{(k-j)}(x), k = 1, 2. \tag{4.2.24}$$

Let $F_1^{(k)}(x) = F_1^{(0)} G_1^{(k)}(x) = 2xe^{-x^2/2} G_1^{(k)}(x)$ where $G_1^{(0)} \equiv 1$. Then taking derivatives and substituting into the differential equation (4.2.24), we obtain,

$$-\frac{d^2}{dx^2} G_1^{(k)}(x) + 2(x - \frac{1}{x}) \frac{d}{dx} G_1^{(k)}(x) = -x^4 G_1^{(k-1)}(x) + \sum_{j=1}^{k} w_j(1) G_1^{(k-j)}(x). \tag{4.2.25}$$

Following the same procedure we used for $n = 0$, performing the necessary calculations for $k = 1, 2$ in (4.2.25) and by the help of the equation (4.2.19) for the coefficient $w_k(n)$, it is possible to evaluate the values of $w_k(1)$ for $k = 1, 2, 3$ as follows:

$$w_1(1) = \frac{15}{4}, \quad w_2(1) = -\frac{165}{16}, \quad w_3(1) = \frac{3915}{64}.$$

And now, we may write the perturbation series for $n = 1$ such that:

$$\Omega_1(\epsilon) \sim 3 + \frac{15}{14}\epsilon - \frac{165}{16}\epsilon^2 + \frac{3915}{64}\epsilon^3 + \cdots . \tag{4.2.26}$$

For $n = 2$, the differential equation (4.2.13) takes the form

$$(-\frac{d^2}{dx^2} + x^2 - 5) F_2^{(k)}(x) = -x^4 F_2^{(k-1)}(x) + \sum_{j=1}^{k} w_j(2) F_2^{(k-j)}(x), k = 1, 2. \tag{4.2.27}$$

Let $F_2^{(k)}(x) = F_2^{(0)}(x) G_2^{(k)}(x) = (4x^2 - 2)e^{-x^2/2} G_2^{(k)}(x)$ where $G_2^{(0)} \equiv 1$. Substituting into the differential equation (4.2.27), one can obtain

$$-\frac{d^2}{dx^2} G_2^{(k)}(x) + \frac{4x^3 - 10x}{2x^2 - 1} - \frac{d}{dx} G_2^{(k)}(x) = -x^4 G_2^{(k-1)}(x)$$
$$+ \sum_{j=1}^{k} w_j(2) G_2^{(k-j)}(x). \tag{4.2.28}$$

After performing the derivation for $k = 1, 2$ in equation (4.2.28), using the formula for the coefficient $w_k(n)$ and by the same procedure we used for the ground-state energy eigenvalue, we get the values for $w_k(2)$ for $k = 1, 2, 3$ as follows:

$$w_1(2) = 9.75, \quad w_2(2) = 10716.52875 \text{ and}$$

$$w_3(2) = 20217003.01769532.$$

Now, it is possible to write the perturbation series for $n = 2$ as follows:

$$\Omega_2(\epsilon) \sim 5 + 9.75\epsilon + 10716.52875\epsilon^2 + 20217003.01769532\epsilon^3 + \cdots . \qquad (4.2.29)$$

The terms in the perturbation series appear to be getting larger and series seem to be divergent for all ϵ. This divergence indicates that the perturbation problem is singular. There is an abrupt change in the nature of the solution when we pass to the limit $\epsilon \to 0$. This occurs because the perturbing term ϵx^4 is not small compared with x^2 when x is large.

In Tables $7-9$ we report the ground-state and the first two excited-state energy levels of the quartic anharmonic oscillator as a function of the anharmonicity constant, ϵ. And, in Tables $7 - 9$, some results from [33] are given for the comparison of our successive approximations. It is appearent that the perturbation method yields the most accurate numerical results for the ground-state eigenvalues. A slight slowing down of convergence is observed as the state number, n, increases.

Table 4.7: Ground-state energy eigenvalues of the quartic anharmonic oscillator as a function of the anharmonicity constant ϵ.

ϵ	$\Omega_0(\epsilon)$	$\Omega_0^\star(\epsilon)$
0.00001	1.000 007 499 868 755 203	1.000 007 499 868 755 202
0.0001	1.000 074 986 880 203	1.000 074 986 880 200
0.001	1.000 748 692 703	1.000 748 692 673
0.01	1.000 373 95	1.000 373 672
0.1	1.067	1.065 285 509
1	5.140	1.392 351 641

$\Omega_0^\star(\epsilon)$ are the exact values [33].

Table 4.8: $n = 1$ excited - state energy eigenvalues of the quartic anharmonic oscillator as a function of the anharmonicity constant ϵ.

ϵ	$\Omega_1(\epsilon)$	$\Omega_1^\star(\epsilon)$
0.00001	3.000 037 500	3.000 037 498
0.0001	3.000 374 897	3.000 374 896
0.001	3.003 739 749	3.003 739 748
0.01	3.036 529	3.036 525
0.1	3.333	3.306 872
1	57.609	4.648 812

$\Omega_1^\star(\epsilon)$ are the exact values [33].

Table 4.9: $n = 2$ excited - state energy eigenvalues of the quartic anharmonic oscillator as a function of the anharmonicity constant ϵ.

ϵ	$\Omega_2(\epsilon)$	$\Omega_2^\star(\epsilon)$
0.00001	5.000 098	5.000 097
0.0001	5.001 10	5.000 974
0.001	5.040	5.009 711
0.01	26.386	5.093 939

$\Omega_2^\star(\epsilon)$ are the exact values [33].

CHAPTER 5

Conclusion

In this thesis we deal with studies on the perturbation problems in quantum mechanics. In Chapter 1, we give a general information about perturbation theory as an introduction and some methods are presented to solve the Schrödinger equation.

In Chapter 2, we review of special functions and give some eigenvalue problems in quantum mechanics that can be solved by means of the classical orthogonal polynomials. We obtain the eigenvalues of the harmonic oscillator in the form of Hermite polynomials. The problem in the type of Pöschl-Teller potential has the solutions in the form of Jacobi polynomials. And we write the solutions of the problem in the type of Particle-in-a-box in terms of Chebyshev polynomials of the third and fourth kinds of degree n.

In Chapter 3, we deal with perturbation theory and its applications. First example is of singular perturbation problem to determine the approximate root of a polynomial. We also apply the perturbation theory to a differential equation.

In Chapter 4, we give two different types of perturbation problems; regular and singular. First, we deal with the confined harmonic oscillator. We give the necessary and sufficient information to find the analytic expressions for first three symmetric contributions to the perturbation series of energy, E_0, E_2, E_4 and we present some calculations based on these kinds of formula in Tables 1-6. As is seen that the convergence rate of the perturbation series decreases as L increases. One can obtain quite high accuracy for sufficiently small L values. As a basic feature of a regular perturbation problem, the exact solution for small but nonzero ϵ smoothly approaches the unperturbed or zeroth order solution as $\epsilon \to 0$. These observations imply that the perturbation series presented in that example have limited convergence radius which depends on L and n. Second, we give an example as a singular perturbative eigenvalue problem, the quartic anharmonic oscillator. In Tables $7-9$ we report the ground-state and the first two excited-state energy levels of the quartic anharmonic oscillator as a function of the anharmonicity constant, ϵ. And, in those tables, some results from [33] are given for the comparison of our successive approximations. It is appearent that the perturbation method yields the most accurate numerical results for the ground-state eigenvalues. A slight slowing down of convergence is observed as the state number, n, increases. We calculate the coefficients in the perturbation series in (4.2.23), (4.2.26), (4.2.29) and by the help of the formulas we find in those equations, we observe that the terms in those series appear to be getting larger and series seem to be divergent for all ϵ. This divergence indicates that the perturbation problem is singular. There is an abrupt change in the nature of the solution when we pass to the limit $\epsilon \to 0$. This occurs because the perturbing term ϵx^4 is not small compared with x^2 when x is large. If the functions $V(x)$ and $H_1(x)$ in this example were interchanged, then the resulting eigenvalue problem would be a regular perturbation problem because ϵx^2 is a small perturbation of x^4 for all $|x| < \infty$.

We conclude that the perturbation theory yields the most encouraging numerical results for the ground-state eigenvalues and for sufficiently small ϵ values.

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