

# **PERTURBATIVE AND EXACT ANALYSIS OF POINT INTERACTIONS**

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**by  
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# **ABSTRACT**

## **PERTURBATIVE AND EXACT ANALYSIS OF POINT INTERACTIONS**

In this thesis, a general formulation for the bound state energies of a finite number of attractive Dirac delta potentials is given in terms of a finite dimensional matrix. The stationary scattering problem is also studied using the distributional solutions of algebraic equations in momentum space. Finally, the energy gap and splitting for the bound state energies when the distance between the delta potentials is large is approximately calculated using a kind of perturbation theory.

# ÖZET

## NOKTASAL ETKİLEŞİMLERİN PERTÜRBATİF VE TAM ANALİZİ

Bu tezde, sonlu sayıda çekici Dirac delta potansiyellerinin bağlı durum enerjileri için genel bir formülasyon sonlu boyutlu bir matris cinsinden ifade edilmiştir. Ayrıca, durağan saçılma problemi momentum uzayında yazılmış cebirsel denklemlerin dağılımsal çözümleri kullanılarak çalışılmıştır. Son olarak delta potansiyelleri arasındaki mesafe büyük olduğunda bağlı durum enerjilerindeki değişim ve ayrışma, bir çeşit pertürbasyon teorisi kullanılarak yaklaşıkça hesaplanmıştır.

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## LIST OF SYMBOLS

$\hbar$ : Planck's constant

$\mathcal{H}$ : Hilbert space

$\langle \cdot, \cdot \rangle$ : Inner product

$z$ : Complex number

$P.V$  : The Cauchy principal value

$\text{Im}(z)$ : Imaginary part of  $z$

$\mathbb{P}$ : Projection operator

The end of a proof is shown by the symbol  $\square$ .

$C^\infty$  : The set of infinitely many differential functions



# CHAPTER 1

## INTRODUCTION

Exact analytical solutions are not in general available for many practical problems in quantum mechanics. In such cases, we usually consult some approximation methods, such as time-dependent/ time-independent perturbation theory, semi-classical approximation (also called WKB approximation, which stands for the initials of the physicists Wentzel-Kramers-Brillouin and other names can also be included in this list), adiabatic approximation, sudden approximation, etc. (Landau and Lifshitz, 2013; Shankar, 2012; Bransden and Joachain, 2000), or we try to find numerical solutions. Each method has its own advantage in solving the problems. For instance, it is well-known that WKB method (Landau and Lifshitz, 2013) or instanton calculations (Coleman, 1988), are particularly useful in studying the formation of bound state or penetration through potential barrier problems in quantum mechanics. One-dimensional anharmonic potential  $V(x) = \frac{\lambda^2}{8}(x^2 - a^2)^2$  is a classic example (see e.g., §50 in (Landau and Lifshitz, 2013)), where the barrier penetration by tunnelling can be analysed through the WKB approximation.

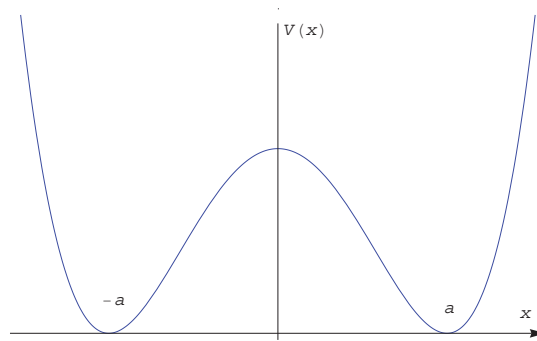


Figure 1.1. Symmetric Anharmonic Double Well Potential

When the energy scale determined by the natural length scale  $a$  of the system is much smaller than the binding energy of the system, i.e.,  $\frac{\hbar^2}{2ma^2} \ll E_B$ , the potential separates

into two symmetrical wells with a very high barrier (see Fig. 1.1). In this extreme limiting case, as a first approximation, each well (on the right part or left) has separately the same energy levels and these energy levels are degenerate due to the parity symmetry. However, if the coupling constant  $\lambda$  is large but finite, the particle initially confined to one well can tunnel to the other well so that the degeneracy in the energy levels disappears. The splitting in the resulting energy levels (between the true ground state and the first excited level due to the tunneling) can be estimated using WKB approximation, see Landau and Lifshitz (2013). Rigorous bounds for the splitting in the bound state energies of double well potentials are studied in Harrell (1980). Moreover, the formal aspects of the problem of calculating the quantum mechanical tunnel splittings in a smooth, symmetric, one dimensional double-well potential are discussed in (Garg, 2000).

In this thesis, we study the estimation of the energy splitting for a particular singular potential, namely Dirac delta potentials separated by large distances by using a kind of perturbation theory, which was first introduced in (Erman and Turgut, 2010, 2019). We start with finitely many Dirac delta potentials and develop the bound state analysis of this problem by expressing the problem in terms of a finite dimensional matrix, called principal matrix. This formulation allows us to analyze the bound state energies qualitatively or numerically. Indeed, the subject of Dirac delta potentials in one dimension is very old and there is a large amount of literature, see e.g., the books (Demkov and Ostrovskii, 1988; Albeverio et al., 1988; Albeverio and Kurasov, 2000). The heuristic approach for a single Dirac delta potentials is even discussed in many elementary quantum mechanics textbooks, see e.g., (Griffiths and Schroeter, 2018). Such a singular potential is an idealized potential where the de-Broglie wavelength of the particle is much larger than the range of the potential. There are many applications of the above type of singular potential in atomic physics, molecular physics and nuclear physics, and solid state physics (Demkov and Ostrovskii, 1988; Uncu et al., 2005; Cacciapuoti, 2005; Kronig and Penney, 1931). The model in higher dimensions is also interesting since it is considered to be a simple model where the idea of renormalization in quantum field theory is used (Bethe and Peierls, 1935; Thomas, 1935; Gosdzinsky and Tarrach, 1991; Manuel and Tarrach, 1994; Mead and Godines, 1991; Perez and Coutinho, 1991; Thorn, 1979; Huang, 1992; Jackiw, 1991; Phillips et al., 1998; Mitra et al., 1998; Nyeo, 2000; Adhikari and Frederico, 1995).

From a purely mathematical point of view, the formal Hamiltonian operator as-

sociated with delta potentials is not a well defined operator in  $L^2(\mathbb{R}^n)$  due to the fact that  $\delta$  does not map square integrable functions to the square integrable functions. A detailed exposition of the subject (in terms of quadratic forms, nonstandard analysis, Von Neumann's approach to self-adjoint extensions of symmetric operators are some of the rigorous approaches to the problem) has been extensively discussed in the monographs (Albeverio and Kurasov, 2000; Albeverio et al., 1988). There are several thesis about such singular interactions, e.g., see (Cacciapuoti, 2005; Altunkaynak, 2005; Gopalakrishnan, 2006; Erman, 2010; Surace, 2010; Tunalı, 2014; Kızılkaya, 2020), and they summarize the subject in very detail, so we shall not review all the aspects of such singular potentials.

Another result in this paper is about the stationary scattering solutions for finitely many Dirac delta potentials in one dimension. This is achieved in momentum space by using the distributional solutions (Lieber, 1975; Schmalz et al., 2010) in contrast to the well-known method, known as  $i\epsilon$  prescription (Shankar, 2012). The boundary conditions for the scattering, namely outgoing boundary conditions, are explicitly used within this method, whereas the boundary conditions are implicit in the  $i\epsilon$  prescription.

The thesis is organized as follows. In Chapter 2, we shortly review the necessary concepts, important theorems about the distribution theory. Chapter 3 introduces the methodology for the finite number of Dirac delta potentials and the problem is expressed in terms of a finite dimensional matrix. Then, the bound state and stationary scattering problem using the distribution theory is studied. In Chapter 4, we give a brief exposition of the perturbation theory for symmetric matrices in order to make the thesis self-contained. Chapter 5 is the main topic of the thesis, where we derive the energy splitting formula as the distance between the supports of delta potential is large by developing a kind of perturbation theory applied to the finite dimensional matrix instead of Hamiltonian.

## CHAPTER 2

### SOME ELEMENTARY RESULTS IN DISTRIBUTION THEORY

The Dirac delta function, usually denoted by  $\delta(x)$  is a very useful and convenient tool in Quantum mechanics. It was first described as an ordinary function, where its value is infinite at  $x = 0$  and zero everywhere else. After its heuristic description, its rigorous formulation was given by Schwartz in terms of so-called distributions. Another advantage of distributions is the availability of derivatives and this makes them useful in the theory of partial differential equations. Distributions are defined by the linear functionals of a suitable space of test functions. This section introduces some elementary concepts and some useful theorems that we are going to use in this thesis.

The basic idea of the definition of Dirac delta distribution is not difficult. Its motivation is based on the following question: Can we find a kind of mathematical “filter” for a given sufficiently smooth function  $f(x)$  such that the result of filtering is the value of the function at any prescribed point  $x_0$  ? (Balakrishnan, 2003) For simplicity, let us choose  $x_0 = 0$ . In other words, we are looking for this mathematical filter  $\delta$  such that the expression below is satisfied:

$$\langle \delta, f \rangle = f(0) . \quad (2.1)$$

In order to give a precise definition of delta function, we need to give some definitions from the theory of distributions (Appel, 2007).

**Definition 2.1** (*Gustafson and Sigal, 2011*)

*The support of a function  $f : \mathbb{R} \rightarrow \mathbb{R}$  is the closure of the set where it is non-zero :*

$$\text{supp}(f) := \overline{\{x \in \mathbb{R} : f(x) \neq 0\}} . \quad (2.2)$$

**Definition 2.2** (Appel, 2007)

The test function space, denoted by  $\mathcal{D}(\mathbb{R})$ , is the vector space of functions  $\phi$  from  $\mathbb{R}$  into  $\mathbb{R}$ , which are class of  $C^\infty(\mathbb{R})$  and have bounded support. A test function is any function  $\phi \in \mathcal{D}(\mathbb{R})$ .

**Definition 2.3** (Debnath et al., 2005)

A linear functional  $T$  on the space  $\mathcal{D}(\mathbb{R})$  is a rule that we assign to every test function  $\phi$  a real number denoted by  $\langle T, \phi \rangle$  such that

$$\langle T, c_1\phi_1 + c_2\phi_2 \rangle = c_1\langle T, \phi_1 \rangle + c_2\langle T, \phi_2 \rangle, \quad (2.3)$$

for arbitrary test functions  $\phi_1$  and  $\phi_2$ .

Convergence of the sequence of the test function is rather technical since we need to define a topology on this vector space. The natural definition of convergence in the space of test functions is given by

**Definition 2.4** (Appel, 2007)

A sequence of test functions  $(\phi_n)_{n \in \mathbb{N}} \in \mathcal{D}$  converges to a function  $\phi \in \mathcal{D}$  if

- the supports of the functions  $\phi_n$  are contained in a fixed bounded subset, independent of  $n$ ,
- all the partial derivatives of all order of the  $\phi_n$  converge uniformly to the corresponding partial derivative of  $\phi$ .

**Definition 2.5** (Kanwal, 2012)

A linear functional on  $\mathcal{D}$  is continuous if and only if the sequence of complex numbers  $\langle T, \phi_n \rangle$  converges  $\langle T, \phi \rangle$  when the sequence of test functions  $\{\phi_n\}$  converges to the test function  $\phi$ .

Now we can give the definition of a distribution:

**Definition 2.6** (Appel, 2007)

A distribution on  $\mathbb{R}$  is any continuous linear functional defined on  $\mathcal{D}(\mathbb{R})$ . The distributions form a vector space called the space of distributions and denoted by  $\mathcal{D}'(\mathbb{R})$ .

The following theorem helps us that any locally integrable function defines a distribution.

**Theorem 2.1** (Appel, 2007)

*For any locally integrable function  $f : \mathbb{R} \rightarrow \mathbb{R}$ , there is an associated distribution  $T$ , defined by*

$$\langle T, \phi \rangle := \int_{\mathbb{R}} f(x) \phi(x) dx , \quad (2.4)$$

*for all  $\phi \in \mathcal{D}(\mathbb{R})$ . This is called a regular distribution associated with the locally integrable function  $f(x)$ .*

The proof of this theorem can be found in (Appel, 2007), where one must show that the above map is linear and continuous functional.

All the other distributions are called singular distributions. Dirac delta distribution is just a particular singular distribution, that is,

**Definition 2.7** (Appel, 2007)

*The Dirac delta distribution is a singular distribution which maps the test functions to the their values at  $x = 0$ , i.e.,*

$$\langle \delta, \phi \rangle := \phi(0) , \quad (2.5)$$

*for all  $\phi \in \mathcal{D}(\mathbb{R})$ .*

Most of the time in applications, it is convenient to write the above definition by treating Dirac delta distributions as if it is a regular distribution and we write the left hand side is expressed in terms of an integral as follows:

$$\int_{\mathbb{R}} \delta(x) \phi(x) dx = \phi(0) . \quad (2.6)$$

Alternatively, Dirac delta distributions can be defined as the limit of some certain se-

quence of ordinary functions  $\delta_n(x)$  in the sense that

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}} \delta_n(x) \phi(x) dx = \phi(0) . \quad (2.7)$$

This formula is known as shifting property or reproducing property of the Dirac delta distributions (Kanwal, 2012). There are several examples for such sequences and their general properties are summarized in (Kanwal, 2012).

The motivation for defining some algebraic and analytical operations on distributions is based on the idea that we somehow convert the expressions that we do not know to the expressions that we know how to deal with it. Therefore, one can define the product of distributions by some smooth functions in the following way:

**Definition 2.8** (Appel, 2007)

Let  $T \in \mathcal{D}'(\mathbb{R})$  be a distribution and let  $\psi$  be a function in  $C^\infty(\mathbb{R})$ . The product  $\psi T \in \mathcal{D}'(\mathbb{R})$  is defined by

$$\langle \psi T, \phi \rangle := \langle T, \psi \phi \rangle , \quad (2.8)$$

for any  $\phi \in \mathcal{D}(\mathbb{R})$ .

Notice that the right hand side is well-defined since the product of infinitely differentiable functions with test functions gives again test functions. That is the reason that we define the product of distributions with smooth functions. In particular, we have an explicit and useful formula for the product of Dirac delta distribution with smooth functions:

**Lemma 2.1** (Appel, 2007)

Let  $\psi$  be a  $C^\infty(\mathbb{R})$  function. Then

$$\psi(x) \delta(x) = \psi(0) \delta(x) , \quad (2.9)$$

in the distributional sense.

The above equation (2.9) should be understood in the distributional sense, i. e. , it makes

sense only if they act on some test functions space:

$$\langle \psi(x)\delta(x), \phi(x) \rangle = \langle \psi(0)\delta(x), \phi(x) \rangle , \quad (2.10)$$

for any test functions  $\phi$ .

*Proof:*

$$\langle \psi\delta, \phi \rangle := \langle \delta, \psi\phi \rangle = \psi(0)\phi(0) = \psi(0)\langle \delta, \phi \rangle = \langle \psi(0)\delta, \phi \rangle . \quad \square \quad (2.11)$$

In particular, if  $\psi(x) = x \in C^\infty(\mathbb{R})$ ,

$$x\delta(x) = 0 . \quad (2.12)$$

**Theorem 2.2** *The equation*

$$xT(x) = 0 \quad (2.13)$$

*with an unknown distribution  $T$ , admits the multiples of the Dirac Delta distribution as solutions, and these are the non-trivial only solutions*

$$x T(x) = 0 \iff T = \alpha\delta , \text{ with } \alpha \in \mathbb{C} . \quad (2.14)$$

*Proof:* ( $\Leftarrow$ ): If  $T = \alpha\delta$ , then from (2.12) we obtain the equation (2.13).

( $\Rightarrow$ ) : Suppose  $xT(x) = 0$  for some regular distribution  $T$  associated with a locally integrable function  $f(x)$ . It means that

$$\langle xT(x), \phi(x) \rangle = \langle T(x), x\phi(x) \rangle = \int_{\mathbb{R}} f(x)x\phi(x)dx = 0 , \quad (2.15)$$



for all test functions  $\phi(x)$ . Since  $x\phi(x)$  is a test function as well, call it as  $\psi(x)$ , we have

$$\int_{\mathbb{R}} f(x)\psi(x)dx = 0 \text{ for all } \psi(x) \text{ in test functions .} \quad (2.16)$$

It implies that  $f(x) \equiv 0$ . Actually, there will be no other singular distributions and this is given in (Appel, 2007), which we are not going to show it here explicitly. In fact, one can think that there could be other distributional solutions of the equation (2.13). For instance,  $T(x) = x^2\delta(x)$ . But this is a trivial solution.  $\square$

Similarly, one can define the derivative of distributions within the same philosophy mentioned above. Consider first a regular distribution  $T$ . Then, we have

$$\langle T', \phi \rangle = \int_{\mathbb{R}} f'(x)\phi(x)dx = - \int_{\mathbb{R}} f(x)\phi'(x)dx = -\langle T, \phi' \rangle , \quad (2.17)$$

where we have used the integration by parts thanks to the compact support of the test functions. This motivates us to define

**Definition 2.9** (Kanwal, 2012)

*The distributional derivative of a distribution  $T$  is defined by*

$$\langle T', \phi \rangle = -\langle T, \phi' \rangle , \quad (2.18)$$

*for all test functions  $\phi$ .*

As an explicit example, let us consider the regular distribution associated with Heaviside step function (which is 1 when  $x > 0$  and zero otherwise) defined by  $\langle H, \phi \rangle := \int_0^\infty \phi(x)dx$ . Then, the derivative (in the sense of distributions) of  $H$  becomes

$$\langle H', \phi \rangle = -\langle H, \phi' \rangle = - \int_0^\infty \phi'(x)dx = \phi(0) = \langle \delta, \phi \rangle , \quad (2.19)$$

for all test functions  $\phi$ . This means that  $H' = \delta$ .

## 2.1. Principal Value as a Distribution

Consider the following function  $\frac{1}{x}$ . It is easy to see that it does not define a regular distribution since it is not integrable around  $x = 0$ . On the other hand, it is well-known that (Kanwal, 2012) its Cauchy Principal Value is well-defined, that is,

$$P.V \int_{-\infty}^{\infty} \frac{\phi(x)}{x} dx := \lim_{\epsilon \rightarrow 0^+} \left[ \int_{-\infty}^{-\epsilon} \frac{\phi(x)}{x} dx + \int_{\epsilon}^{\infty} \frac{\phi(x)}{x} dx \right], \quad (2.20)$$

the limit on the right hand side always exists. This suggests to define the principal value as a distribution:

$$\langle P.V (1/x), \phi \rangle := P.V \int_{-\infty}^{\infty} \frac{1}{x} \phi(x) dx. \quad (2.21)$$

Let us now show that  $P.V(1/x)$  is a distribution. This can be shown by using the definition of distribution check that it is continuous linear functional. Alternatively, one can directly show that it is a distributional derivative of the regular distribution associated with the function  $\log |x|$ . This can be done by using the integration by parts formula as follows (Dijk, 2013):

$$\langle P.V(1/x), \phi \rangle = - \lim_{\epsilon \rightarrow 0^+} \int_{|x| \geq \epsilon} \log |x| \phi'(x) dx = - \int_{-\infty}^{\infty} \log |x| \phi'(x) dx, \quad (2.22)$$

or equivalently  $P.V(1/x) = (\log |x|)'$ .

**Theorem 2.3** *The principal value of  $1/x$  satisfies*

$$x P.V(1/x) = 1. \quad (2.23)$$

*Proof:* For any test function  $\phi \in \mathcal{D}(\mathbb{R})$ , we have by definition of product of a distribution  $P.V.(1/x)$  by a  $C^\infty(\mathbb{R})$  function :

$$\begin{aligned}\langle x P.V.(1/x), \phi \rangle &= \langle P.V.(1/x), x\phi \rangle = \lim_{\epsilon \rightarrow 0^+} \int_{|x| > \epsilon} \frac{x\phi(x)}{x} dx \\ &= \int_{-\infty}^{\infty} \phi(x) dx = \langle 1, \phi \rangle ,\end{aligned}\tag{2.24}$$

for all  $\phi \in \mathcal{D}(\mathbb{R})$ .  $\square$

**Theorem 2.4** *The solutions in the space of distributions of the equation*

$$xT(x) = 1\tag{2.25}$$

*are given by*

$$T(x) = P.V.(1/x) + \alpha\delta(x) \text{ where } \alpha \in \mathbb{C} .\tag{2.26}$$

*Proof:* If  $T$  satisfies  $xT(x) = 1$ , then if we define  $S(x) := T(x) - P.V.(1/x)$  satisfies

$$xS(x) = 0 .\tag{2.27}$$

from the theorem (2.3). Then, by the Theorem (2.2) , we get

$$S(x) = \alpha\delta(x) \Rightarrow T(x) = P.V.(1/x) + \alpha\delta .\tag{2.28}$$

As a consequence of the previous results, one can easily prove the below theorem (Appel, 2007), which will be used in our calculations later on:

**Theorem 2.5** *The distributional solutions of  $(x^2 - a^2)T(x) = 1$  are given by*

$$T(x) = A\delta(x - a) + B\delta(x + a) + P.V \left( \frac{1}{x^2 - a^2} \right) , \quad (2.29)$$

where  $a > 0$ ,  $A, B$  are arbitrary complex numbers, and

$$P.V \left( \frac{1}{x^2 - a^2} \right) := \frac{1}{2a} \left( P.V. \left( \frac{1}{x - a} \right) - P.V \left( \frac{1}{x + a} \right) \right) . \quad (2.30)$$

## 2.2. Fourier Transform of Distributions

Let us also give the definition of the Fourier transform of distributions, in particular, Dirac delta distribution. This is the extension of the definition of Fourier transform of square integrable function  $\psi(x)$ , given by

$$(\mathcal{F}(\psi))(p) : \widehat{\psi}(p) = \int_{\mathbb{R}} e^{-ipx} \psi(x) dx , \quad (2.31)$$

to the larger class “functions”. This can be achieved if we restrict the class of distributions to the so-called tempered distributions. Let  $\mathcal{S}$  be the set of infinitely differentiable and “rapidly decaying functions” together with their derivatives.  $\mathcal{S}$  is called Schwartz space. The space of continuous linear functionals on  $\mathcal{S}$  is known as the tempered distributions. Here we skip some technical details, such as the convergence of the sequence of functions in Schwartz space and the technical definition of rapid decays. One can consult for all these technical details to (Kanwal, 2012; Dijk, 2013; Appel, 2007). Once we define the tempered distributions, we can define their Fourier transform by following the same spirit of the above definitions for differentiation and multiplication, that is,

**Definition 2.6** *The Fourier transform of a tempered distribution  $T$  is defined by*

$$\langle \mathcal{F}(T), \phi \rangle := \langle T, \mathcal{F}(\phi) \rangle , \quad (2.32)$$

for any  $\phi \in \mathcal{S}(\mathbb{R}^D)$ .

Using the above definition, we can find the Fourier transform of Dirac delta distribution  $\delta(x)$  as

$$\langle \mathcal{F}(\delta), \phi \rangle = \langle \delta, \mathcal{F}\phi \rangle = \langle \delta, \hat{\phi} \rangle := \hat{\phi}(0) . \quad (2.33)$$

From the Fourier transform of  $\phi(x)$

$$\hat{\phi}(0) = \int_{\mathbb{R}} e^{-ipx} \phi(x) dx \Big|_{p=0} = \int_{\mathbb{R}} \phi(x) dx = \langle 1, \phi \rangle . \quad (2.34)$$

Hence we get  $\langle \mathcal{F}(\delta), \phi \rangle = \langle 1, \phi \rangle$  for all  $\phi$ , i.e., formally

$$\mathcal{F}(\delta) = 1 . \quad (2.35)$$

As a final remark, the reason why we have to restrict the class of test functions lies in the fact that the Fourier transform of a compactly supported function is not necessarily compactly supported. However, the Fourier transform of a Schwartz function is always Schwartz function (Appel, 2007). All the above definitions and results can be extended to the higher dimensions.

## CHAPTER 3

### FINITELY MANY DIRAC DELTA POTENTIALS IN ONE DIMENSION

In this thesis, there are two main problems which are bound state problem and stationary scattering problem.

#### 3.1. Bound State Problem

In one dimension, the time-independent *Schrödinger equation* with  $N$  Dirac delta potential is formally given by

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \sum_{i=1}^N \lambda_i \delta(x - a_i) \psi(x) = E\psi(x) , \quad (3.1)$$

where  $a_i$  is the location of support of the Dirac delta function. We assume that  $a_i \neq a_j$  for  $i \neq j$  and  $\lambda_i > 0$  for all  $i$ , which means that the supports of Dirac delta potentials do not coincide and they are given fixed points. Since  $E < 0$  for bound states, it is useful to parametrize the energy as follows

$$E = -\nu^2 , \quad (3.2)$$

where  $\nu > 0$ . Then, by applying the formal Fourier transform to Equation (3.1), we find the Fourier transformed wave function:

$$\hat{\psi}(p) = \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \sum_{i=1}^N \lambda_i \psi(a_i) e^{-\frac{ipa_i}{\hbar}} . \quad (3.3)$$

This formula includes the unknown quantities  $\nu^2$  and  $\psi(a_i)$ . Therefore, we first need to find them. Let us define

$$B_i := \psi(a_i) = \int_{-\infty}^{\infty} \widehat{\psi}(p) e^{\frac{ipa_i}{\hbar}} \frac{dp}{2\pi\hbar}, \quad (3.4)$$

where we have used the formal inverse Fourier transformation given by

$$\psi(x) := \int_{-\infty}^{\infty} \widehat{\psi}(p) e^{\frac{ipx}{\hbar}} \frac{dp}{2\pi\hbar}. \quad (3.5)$$

Substituting the equation (3.3) into the equation (3.4), we get

$$B_i = \int_{-\infty}^{\infty} \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \sum_{j=1}^N \lambda_j B_j e^{-\frac{ipa_j}{\hbar}} e^{\frac{ipa_i}{\hbar}} \frac{dp}{2\pi\hbar}. \quad (3.6)$$

Let us split the  $j = i$ -th term in the summation

$$B_i = \int_{-\infty}^{\infty} \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \lambda_i B_i \frac{dp}{2\pi\hbar} + \int_{-\infty}^{\infty} \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \sum_{j \neq i}^N \lambda_j B_j e^{\frac{ip(a_i - a_j)}{\hbar}} \frac{dp}{2\pi\hbar}, \quad (3.7)$$

or we can rewrite the equation (3.7) as

$$\begin{aligned} & \left( 1 - \lambda_i \int_{-\infty}^{\infty} \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \frac{dp}{2\pi\hbar} \right) B_i \\ & - \sum_{\substack{j=1 \\ (j \neq i)}}^N \left( \lambda_j \int_{-\infty}^{\infty} e^{-\frac{ip(a_i - a_j)}{\hbar}} \frac{1}{\left(\frac{p^2}{2m} + \nu^2\right)} \frac{dp}{2\pi\hbar} \right) B_j = 0. \end{aligned} \quad (3.8)$$

This equation can be written in a more compact way

$$\sum_{j=1}^N \Gamma_{ij} B_j = 0, \quad (3.9)$$

by defining the following matrix

$$\Gamma_{ij} = \begin{cases} 1 - \lambda_i \int_{-\infty}^{\infty} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{dp}{(2\pi\hbar)} & \text{if } i = j , \\ -\lambda_j \int_{-\infty}^{\infty} \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{\frac{p^2}{2m} + \nu^2} \frac{dp}{(2\pi\hbar)} & \text{if } i \neq j , \end{cases} \quad (3.10)$$

where  $i = j$  part is diagonal part and  $i \neq j$  part is non-diagonal part.

Since we would like to formulate our problem in terms of a symmetric matrix, let us scale  $B_j$  by

$$B_j = \frac{1}{\lambda_j} A_j , \quad (3.11)$$

so that the equation (3.9) becomes

$$\sum_{j=1}^N \Phi_{ij} A_j = 0 , \quad (3.12)$$

where

$$\Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda_i} - \int_{-\infty}^{\infty} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{dp}{(2\pi\hbar)} & \text{if } i = j , \\ - \int_{-\infty}^{\infty} \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{\frac{p^2}{2m} + \nu^2} \frac{dp}{(2\pi\hbar)} & \text{if } i \neq j . \end{cases} \quad (3.13)$$

All the nontrivial solutions to the equation (3.12) give us the bound state energies of the system. Firstly, let us calculate the integrals in the definition of the matrix  $\Phi$ . Let us call the indefinite integral in the diagonal part of  $\Phi$  by  $I_1$  :

$$I_1 := \int_{-\infty}^{\infty} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{dp}{2\pi\hbar} = \frac{2m}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{dp}{p^2 + 2m\nu^2} . \quad (3.14)$$



By making a change of variables,  $p = \nu \sqrt{2m} \tan(\theta)$ , it is easy to find

$$I_1 = \sqrt{\frac{m}{2}} \frac{1}{\hbar \nu} . \quad (3.15)$$

Let us also define the improper integral in the off-diagonal part of  $\Phi$  as  $I_2$  :

$$\begin{aligned} I_2 &:= \left( \frac{m}{\pi \hbar} \right) \int_{-\infty}^{\infty} \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp \\ &= \frac{m}{\pi \hbar} \int_{-\infty}^{\infty} \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp = \left( \frac{m}{\pi \hbar} \right) \lim_{R \rightarrow \infty} \int_{-R}^R \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp . \end{aligned} \quad (3.16)$$

Since the above improper integral is convergent which is easy to check, we have considered the *Cauchy principal value (P.V)* of the integral  $I_2$ , see e.g.; (Brown et al., 2009). Notice that the poles appear on the imaginary axis given by  $p = \pm i\sqrt{2m}\nu$ , so that we can easily evaluate the integral by *Residue theorem*, (Brown et al., 2009). By choosing the

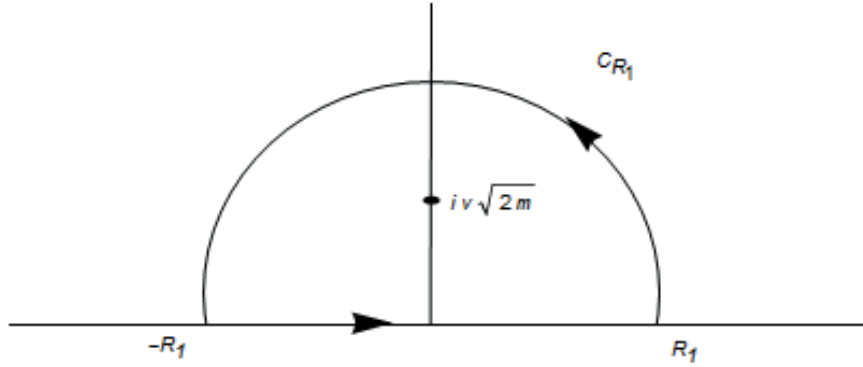


Figure 3.1. The choice of the contour for  $I_2$  for  $(a_i - a_j) > 0$ .

contour as shown in Figure (3.1) for  $(a_i - a_j) > 0$ , the *Residue theorem* tells us

$$\frac{m}{\pi \hbar} \oint \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp = 2\pi i \left( \frac{m}{\pi \hbar} \right) \text{Res}_{(p=i\nu\sqrt{2m})} \left[ \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} \right] . \quad (3.17)$$

The left-hand side can be decomposed as

$$\left(\frac{m}{\pi\hbar}\right) \left[ \int_{-R_1}^{R_1} \frac{e^{\frac{ip(a_i-a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp + \int_{C_{R_1}} \frac{e^{\frac{ip(a_i-a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp \right]. \quad (3.18)$$

As  $R_1 \rightarrow \infty$ , the first integral is the one we are looking for and the second one goes to zero thanks to the *Jordan lemma*. The right-hand side of the equation (3.17) becomes

$$\sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} e^{-\frac{\sqrt{2m\nu}(a_i-a_j)}{\hbar}}. \quad (3.19)$$

On  $C_{R_1}$ ,  $p = R_1 e^{i\theta}$  where  $0 \leq \theta \leq \frac{\pi}{2}$  and  $dp = R_1 i e^{i\theta} d\theta$ . Then ,

$$\begin{aligned} & \left| \int_0^{\pi/2} \left(\frac{m}{\hbar\pi}\right) \frac{e^{\frac{iR_1 e^{i\theta}(a_i-a_j)}{\hbar}}}{R_1^2 e^{2i\theta} + 2m\nu^2} R_1 i e^{i\theta} d\theta \right| \\ & \leq \left(\frac{m}{\hbar\pi}\right) \int_0^{\pi/2} \left| e^{\frac{-R_1 \sin(\theta)(a_i-a_j)}{\hbar}} \right| \frac{|R_1|}{|R_1^2 e^{2i\theta} + 2m\nu^2|} d\theta \end{aligned} \quad (3.20)$$

as  $R_1 \rightarrow \infty$ .

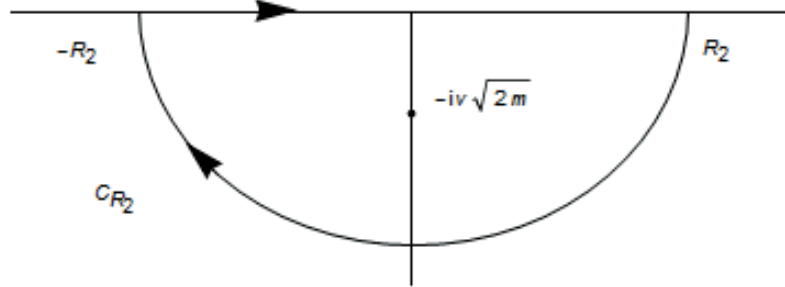


Figure 3.2. The choice of the contour for  $I_2$  for  $(a_i - a_j) < 0$ .

Similarly, for  $(a_i - a_j) < 0$ , we choose the contour as shown in the figure (3.2)

$$\left(\frac{m}{\pi\hbar}\right) \oint \frac{e^{\frac{ip(a_i - a_j)}{\hbar}}}{p^2 + 2m\nu^2} dp = \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} e^{\frac{\sqrt{2m}\nu(a_i - a_j)}{\hbar}} . \quad (3.21)$$

Combining all these results (3.15), (3.19) and (3.21), we finally obtain

$$\Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda_i} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & \text{if } i = j , \\ -\sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} e^{-\frac{\sqrt{2m}\nu|a_i - a_j|}{\hbar}} & \text{if } i \neq j . \end{cases} \quad (3.22)$$

The matrix  $\Phi$  is called *principal matrix*. This terminology is first introduced by S. G. Rajeev when he discussed the many-body version of these potentials, (Rajeev, 1999). We have non-trivial solution of

$$\sum_j \Phi_{ij} A_j = 0 , \quad (3.23)$$

if and only if

$$\det(\Phi_{ij}(\nu)) = 0 . \quad (3.24)$$

If we solve (3.24), we will find bound state energies from  $E = -\nu^2$ .

Let us summarize our results by the following theorem:

**Theorem 3.1** *Bound state energies  $E = -\nu^2$  of  $N$  attractive Dirac delta potentials in one dimension are given by the solutions of  $\det(\Phi_{ij}(\nu)) = 0$ , where  $\Phi$  is the  $N \times N$  matrix given by (3.22).*

In general, this equation is difficult to solve analytically since it is a transcendental equation. For this reason, we consider particular cases.

### 3.1.1. One Center Case

For  $N = 1$  and  $a = 0$  we have always one bound state and the bound state energy can be found from the solution of

$$\frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} = 0 . \quad (3.25)$$

Hence, we obtain the well-known result in the literature (Griffiths and Schroeter, 2018)

$$E = -\frac{m\lambda^2}{2\hbar^2} . \quad (3.26)$$

One can also find the bound state wave function by taking the inverse Fourier transformation of the solution (3.3),

$$\psi(x) = \sqrt{\frac{m\lambda}{\hbar^2}} e^{-\frac{m\lambda}{\hbar^2}|x|} , \quad (3.27)$$

which is also consistent with the result in (Griffiths and Schroeter, 2018). The most common approach for this single Dirac delta potential is to solve the Schrödinger equation in coordinate space separately for the regions  $x < 0$  and  $x > 0$ , and then apply the continuity and jump discontinuity conditions for the wave function at  $x = 0$ . This will give exactly the same result given above.

### 3.1.2. Two Center Case

**Theorem 3.2** *For  $N = 2$ , we have at most two bound states. In order to have exactly two bound states, then the distance  $d = |a_1 - a_2|$  between the delta centers must satisfy*

$$d > \frac{\hbar^2}{2m} \left( \frac{1}{\lambda_1} + \frac{1}{\lambda_2} \right) = d_{critical} . \quad (3.28)$$

*Proof:* For  $N = 2$ , the equation (3.22) is reduced to

$$\Phi(\nu) = \begin{pmatrix} \frac{1}{\lambda_1} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m\nu}|a_1-a_2|}{\hbar}}}{\hbar\nu} \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m\nu}|a_1-a_2|}{\hbar}}}{\hbar\nu} & \frac{1}{\lambda_2} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \end{pmatrix}. \quad (3.29)$$

Then, the bound state condition (3.24) turns out to be

$$\left( \frac{1}{\lambda_1} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \right) \left( \frac{1}{\lambda_2} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \right) = \left( \frac{m}{2\hbar^2\nu^2} e^{-\frac{2\sqrt{2m\nu}|a_1-a_2|}{\hbar}} \right). \quad (3.30)$$

By multiplying both sides with  $\lambda_1\lambda_2\nu^2$ , we obtain

$$\left( \nu - \sqrt{\frac{m}{2}} \frac{\lambda_1}{\hbar} \right) \left( \nu - \sqrt{\frac{m}{2}} \frac{\lambda_2}{\hbar} \right) = \frac{m\lambda_1\lambda_2}{2\hbar^2} e^{-\frac{2\sqrt{2m\nu}|a_1-a_2|}{\hbar}}. \quad (3.31)$$

Let us denote  $\nu = x > 0$ ,  $\sqrt{\frac{m}{2}} \frac{\lambda_1}{\hbar} = c_1$ ,  $\sqrt{\frac{m}{2}} \frac{\lambda_2}{\hbar} = c_2$  and  $\frac{2\sqrt{2m}|a_1-a_2|}{\hbar} = \beta$ , then the above equation (3.31) reads

$$(x - c_1)(x - c_2) = c_1c_2e^{-\beta x}, \quad (3.32)$$

which is a transcendental equation and it is hard to solve analytically. Instead of finding explicit analytical solutions, let us analyze whether there exist solutions or not by simply plotting the graph of functions in both sides of the equation (3.32). We have always at least one root. First, let us analyze the number of positive roots of the equation (3.32). Since the right-hand side is a positive monotonically decreasing function of  $x$  whereas the parabola in the left-hand side is increasing function of  $x$  when  $x$  is sufficiently large, as shown in the figure (3.3). Now, as it is easy to see from the figure (3.3), we may not have the 2nd root always. However, we have the 2nd root if the slope of the left hand side exceeds the slope of the left hand side near the origin in magnitude:

$$c_1 + c_2 < \beta c_1c_2. \quad (3.33)$$

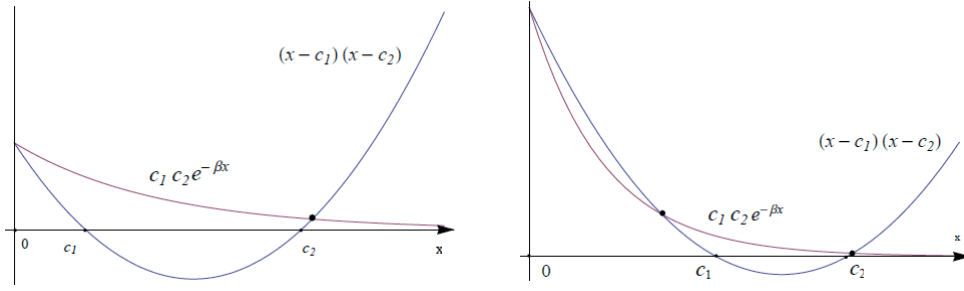


Figure 3.3. (a) Graph of  $(x - c_1)(x - c_2)$  and  $c_1 c_2 e^{-\beta x}$  for  $c_1 = 5$ ,  $c_2 = 20$  and  $\beta = 0.1$   
(b) Graph of  $(x - c_1)(x - c_2)$  and  $c_1 c_2 e^{-\beta x}$  for  $c_1 = 1$ ,  $c_2 = 1.7$  and  $\beta = 2.5$

By going back to the original variables, we obtain the desired condition. The meaning of the equations is that if the distance between centers is larger than the above mentioned critical distance, then we have exactly two bound states.  $\square$

Let us consider the following particular case, where the strengths of each Dirac delta potential are the same :

**Theorem 3.3** *For  $N = 2$  and  $c_1 = c_2 = c$ , the bound state energies of the system in the presence of two point interactions are explicitly given by*

$$E_{\pm} = - \left[ \sqrt{\frac{m}{2}} \frac{\lambda}{\hbar} + \frac{\hbar}{\sqrt{2m}|a_1 - a_2|} W \left( \pm \frac{m\lambda|a_1 - a_2|}{\hbar^2} e^{-\frac{m\lambda|a_1 - a_2|}{\hbar^2}} \right) \right]^2, \quad (3.34)$$

where  $W(z)$  is the Lambert  $W$  function.

*Proof:* For  $c_1 = c_2 = c$  ( $\lambda_1 = \lambda_2 = \lambda$ ), equation (3.32) becomes

$$(x - c) e^{\frac{\beta x}{2}} = \pm c. \quad (3.35)$$

Rewriting this equation in the following form

$$\frac{\beta}{2} (x - c) e^{\frac{\beta(x-c)}{2}} = \pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}}. \quad (3.36)$$

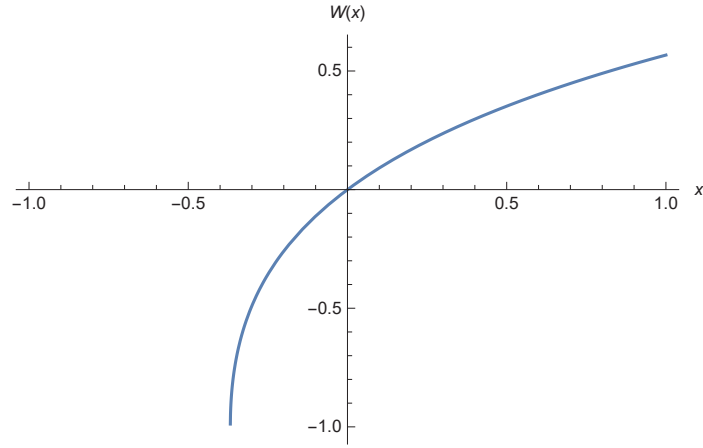


Figure 3.4. The graph of Lambert  $W(x)$  function

Solutions of this equation can be expressed in terms of the Lambert  $W$  function. There are many applications about the Lambert  $W$  function such as enumeration of trees in combinatorics, in the solution of iterated exponentiation, a jet fuel problem and an enzyme kinetics problem, capacitor fields, conformal mapping, and also in Wien's displacement law, (Corless et al., 1996) (Valluri et al., 2000). The definition of the function is given by the solution of the transcendental equation below :

$$y e^y = x \Rightarrow y \equiv W(x) . \quad (3.37)$$

Therefore, the solution to equation (3.36) becomes

$$\frac{\beta}{2}(x_{\pm} - c) = W\left(\pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}}\right) , \quad (3.38)$$

and

$$x_{\pm} = c + \frac{2}{\beta} W\left(\pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}}\right) . \quad (3.39)$$

Back to our original variables, we have

$$\nu = \sqrt{\frac{m}{2}} \frac{\lambda}{\hbar} + \frac{\hbar}{\sqrt{2m}|a_1 - a_2|} W \left( \pm \frac{m\lambda|a_1 - a_2|}{\hbar^2} e^{-\frac{m\lambda|a_1 - a_2|}{\hbar^2}} \right) . \quad (3.40)$$

Since  $E = -\nu^2$ , we can easily find the desired result.  $\square$

**Corollary 3.4** (*Special Case*)

For  $N = 2$ ,  $\lambda_1 = \lambda_2 = \lambda$  and also  $a_1 = -a$  and  $a_2 = a$ , we have at most two bound states. The critical distance is

$$d = 2a > \frac{\hbar^2}{m\lambda} = d_{critical} . \quad (3.41)$$

### 3.2. Stationary Scattering Problem

Actual time-dependent physical scattering problem can be described in the context of stationary *Schrödinger equation* if the wave function of the incoming particle to the potential center is sharply peaked around  $p = k$  (Faddeev and Yakubovskii, 2009). For this reason, it is sufficient to study the time-independent *Schrödinger equation* where  $E = \frac{\hbar^2 k^2}{2m}$ :

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} - \sum_{j=1}^N \lambda_j \delta(x - a_j) \psi(x) = \frac{\hbar^2 k^2}{2m} \psi(x) . \quad (3.42)$$

Suppose that  $a_1 < a_2 < \dots < a_N$  without loss of generality. Here  $\lambda_j$  are real numbers. As we did for the bound states, let us solve the scattering problem in momentum space in the same spirit discussed in (Lieber, 1975) for the single delta center.

Let us first rewrite the above equation in the following form :

$$\psi''(x) + k^2 \psi(x) = -\frac{2m}{\hbar^2} \sum_{j=1}^N \lambda_j \delta(x - a_j) \psi(x) . \quad (3.43)$$



The solution of the inhomogeneous equation (3.43) can be written in terms of Green's function :

$$\psi_k(x) = e^{ikx} + \int_{-\infty}^{\infty} G_0(x - x', E_k) \rho(x') dx' , \quad (3.44)$$

where  $\rho(x) = -\frac{2m}{\hbar^2} \sum_{j=1}^N \lambda_j \delta(x - a_j) \psi(x)$ , and  $e^{ikx}$  is the solution of the homogeneous part and (which physically represent wave function of the incoming particle), and  $G_0$  satisfies the following differential equation together with the outgoing boundary condition  $G_0(y; E_k) \sim e^{ik|y|}$  as  $y \rightarrow \pm\infty$  (also called Sommerfeld radiation condition in one dimension):

$$\left( \frac{d^2}{dy^2} + k^2 \right) G_0(y, E_k) = \delta(y) . \quad (3.45)$$

This is indeed the Green's function for the Helmholtz equation under the outgoing boundary condition in one dimension. By taking formal Fourier transformation of this equation, we get

$$\left( -\frac{p^2}{\hbar^2} + k^2 \right) \widehat{G}_0(p; E_k) = 1 . \quad (3.46)$$

Our goal is to solve the equation (3.46). The solution is

$$\widehat{G}_0(p) = \frac{1}{k^2 - \frac{p^2}{\hbar^2}} = \frac{\hbar^2}{\hbar^2 k^2 - p^2} , \quad (3.47)$$

if we are looking for solution in function space that are square integrable. Here we require the distributional solutions for scattering problem, so we need to include them. The distributional solutions to algebraic equations was discussed in previous Chapter. Therefore, using the Theorem (2.5), we have the following general solution

$$\widehat{G}_0(p) = A\delta(p - \hbar k) + B\delta(p + \hbar k) - \hbar^2 P.V \left( \frac{1}{p^2 - \hbar^2 k^2} \right) . \quad (3.48)$$

One can also solve this using  $i\epsilon$  prescription method (Shankar, 2012), where the boundary conditions are implicitly used. With this distributional solution approach, we will explicitly impose the boundary conditions. This was also discussed in (Lieber, 1975; Schmalz et al., 2010). The formal inverse Fourier transformation is then

$$\widehat{G}_0(y) = \int_{-\infty}^{\infty} e^{\frac{ipy}{\hbar}} \widehat{G}_0(p) \frac{dp}{2\pi\hbar} . \quad (3.49)$$

Substituting the equation (3.48) into the equation (3.49) , we have

$$G_0(y) = \int_{-\infty}^{\infty} e^{\frac{ipy}{\hbar}} \left[ A\delta(p - \hbar k) + B\delta(p + \hbar k) \right] \frac{dp}{2\pi\hbar} - \hbar^2 P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p^2 - \hbar^2 k^2} \frac{dp}{2\pi\hbar} . \quad (3.50)$$

Firstly, we need to compute the principal values

$$\begin{aligned} & P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p^2 - \hbar^2 k^2} \frac{dp}{2\pi\hbar} \\ &= \frac{1}{4\pi\hbar^2 k} \left( P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p - \hbar k} dp - P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p + \hbar k} dp \right) , \end{aligned} \quad (3.51)$$

for  $y > 0$ . Consider the first principal value

$$I(k) := P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p - \hbar k} dp . \quad (3.52)$$

It has a simple pole at  $p = \hbar k$  on the real axis. Let us choose the contour  $C$  on the complex  $p$  plane, consisting of 3 pieces:

- $C_1$ : The clockwise semi-circle contour around the pole  $p = \hbar k$
- $C_2$ : The contour along real axis with removed  $\epsilon$  neighborhood of the poles.
- $C_R$ : The counterclockwise semi-circle contour with radius  $R$  on the upper half plane .

Then, we have

$$\int_{C_1} \frac{e^{\frac{ipy}{\hbar}}}{p - \hbar k} dp + \int_{C_2} \frac{e^{\frac{ipy}{\hbar}}}{p - \hbar k} dp + \int_{C_R} \frac{e^{\frac{ipy}{\hbar}}}{p - \hbar k} dp = 0 , \quad (3.53)$$

where we have used the Residue theorem (Brown et al., 2009) and the fact that integrand is analytic inside the closed contour  $C = C_1 \cup C_2 \cup C_R$ . The following theorem will be useful in evaluating the contour integral over  $C_1$  and  $C_2$ :

**Theorem 3.5** (Ablowitz et al., 2003) Consider the following contour shown in Figure 3.5 below and suppose  $f(z)$  has a simple pole at  $z = z_0$  with residue  $\text{Res}(f(z); z_0) = c$ .

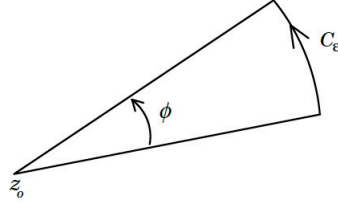


Figure 3.5. Small Contour arc  $C_\epsilon$

Then, we have

$$\lim_{\epsilon \rightarrow 0} \int_{C_\epsilon} f(z) dz = i\phi c . \quad (3.54)$$

*Proof:* If  $f(z)$  has a simple pole with  $\text{Res}(f(z); z_0) = c$ , then from the Laurent expansion of  $f(z)$  in the neighborhood of  $z = z_0$

$$f(z) = \frac{c}{z - z_0} + g(z) , \quad (3.55)$$

where  $g(z)$  is analytic in the neighborhood of  $z = z_0$ . Thus,

$$\lim_{\epsilon \rightarrow 0} \int_{C_\epsilon} f(z) dz = \lim_{\epsilon \rightarrow 0} c \int_{C_\epsilon} \frac{dz}{z - z_0} + \lim_{\epsilon \rightarrow 0} \int_{C_\epsilon} g(z) dz . \quad (3.56)$$

Along the contour  $C_\epsilon$ , we have  $z = z_0 + \epsilon e^{i\theta}$ . Hence, the first integral on the right-hand side gives

$$\int_{C_\epsilon} \frac{dz}{z - z_0} = \int_0^\phi \frac{i\epsilon e^{i\theta} d\theta}{\epsilon e^{i\theta}} = i\phi. \quad (3.57)$$

As for the second integral,  $|g(z)| \leq \text{constant}$  around the neighborhood of  $z = z_0$  since  $g(z)$  is analytic function there. This implies that the second integral vanishes in the limit of  $\epsilon \rightarrow 0$  and we obtain the desired result (3.54).  $\square$

The contour integration over  $C_R$  in the equation (3.53) vanishes as  $R \rightarrow \infty$  thanks to the *Jordan Lemma* (Brown et al., 2009). Then, as  $\epsilon \rightarrow 0^+$  and  $R \rightarrow \infty$ , we obtain the expression for the principal value

$$I(k) = i\pi \lim_{p \rightarrow \hbar k} \frac{(p - \hbar k) e^{\frac{ipy}{\hbar}}}{(p - \hbar k)} = i\pi e^{iky}, \quad (3.58)$$

for  $y > 0$ . Similarly, for  $y < 0$  we must choose the contour  $C_R$  on the lower half plane, and  $C_1$  as the counterclockwise small contour around the pole. In this case, we have no simple poles inside the closed contour so we get

$$I(k) = -i\pi \lim_{p \rightarrow \hbar k} \frac{(p - \hbar k) e^{\frac{ipy}{\hbar}}}{(p - \hbar k)} = -i\pi e^{iky}, \quad (3.59)$$

for  $y < 0$ . Hence, we obtain the expression for the principal value

$$\begin{aligned} P.V \int_{-\infty}^{\infty} \frac{e^{\frac{ipy}{\hbar}}}{p^2 - \hbar^2 k^2} \frac{dp}{2\pi\hbar} &= \frac{1}{4\pi\hbar^2 k} (I(k) - I(-k)) \\ &= \frac{i}{4\hbar^2 k} \begin{cases} (-e^{iky} + e^{-iky}) & y < 0, \\ (e^{iky} - e^{-iky}) & y > 0. \end{cases} \end{aligned} \quad (3.60)$$

Consequently, the equation (3.50) for  $y > 0$  becomes

$$G_0(y) = e^{iky} \left( \frac{A}{2\pi\hbar} - \frac{i}{4k} \right) + e^{-iky} \left( \frac{B}{2\pi\hbar} + \frac{i}{4k} \right). \quad (3.61)$$

By applying the boundary conditions for Green's functions (we do not expect reflections in the positive axis if we assume that the particle is sent from the far left region), we have

$$\frac{B}{2\pi\hbar} = -\frac{i}{4k} . \quad (3.62)$$

For  $y < 0$ ,

$$G_0(y) = e^{iky} \left( \frac{A}{2\pi\hbar} + \frac{i}{4k} \right) + e^{-iky} \left( \frac{B}{2\pi\hbar} - \frac{i}{4k} \right) . \quad (3.63)$$

By the outgoing boundary condition mentioned before, the first term on the right hand side of above equation must be zero. Then, we have

$$G_0(y) = e^{-iky} \left( \frac{B}{2\pi\hbar} - \frac{i}{4k} \right) . \quad (3.64)$$

Since  $\frac{B}{2\pi\hbar} = -\frac{i}{4k}$ , we find

$$G_0(y) = - \left( \frac{i}{2k} \right) e^{ik|y|} . \quad (3.65)$$

Finally, we can find the scattering wave function  $\psi_k^+(x)$  satisfying outgoing boundary condition after inserting  $G_0(y)$  obtained above:

$$\psi_k^+(x) = e^{ikx} + \frac{im}{\hbar^2 k} \sum_{j=1}^N \lambda_j e^{ik|x-a_j|} \psi_k^+(a_j) . \quad (3.66)$$

Actually, this is not the final result since we have an unknown expression  $\psi_k(a_j)$  on the right hand side of the equation. To find this, let us consider the consistency conditions.

For  $x = a_i$  :

$$\psi_k^+(a_i) = e^{ika_i} + \frac{im}{k\hbar^2} \lambda_i \psi_k^+(a_i) + \frac{im}{k\hbar^2} \sum_{\substack{j=1 \\ (j \neq i)}}^N \lambda_j e^{ik|a_i - a_j|} \psi_k^+(a_j) , \quad (3.67)$$

where we have splitted the  $j = i$ th term in the summation. Then, we arrange the equation (3.67) as

$$\left(1 - \frac{im}{k\hbar^2} \lambda_i\right) \psi_k^+(a_i) - \frac{im}{k\hbar^2} \sum_{\substack{j=1 \\ (j \neq i)}}^N \lambda_j e^{ik|a_i - a_j|} \psi_k^+(a_j) = e^{ika_i} . \quad (3.68)$$

If we define the following matrix,

$$\Gamma_{ij}(k) := \begin{cases} 1 - \frac{im}{k\hbar^2} \lambda_i & \text{if } i = j , \\ -\frac{im}{k\hbar^2} \lambda_j e^{ik|a_i - a_j|} & \text{if } i \neq j . \end{cases} \quad (3.69)$$

The above consistency condition can be reexpressed in a matrix form :

$$\sum_{j=1}^N \Gamma_{ij} \psi_k^+(a_j) = e^{ika_i} . \quad (3.70)$$

Let us scale the functions as  $\psi_k^+(a_j) := \frac{\phi_k^+(a_j)}{\lambda_j}$ . Then,

$$\sum_{j=1}^N \Gamma_{ij} \psi_k^+(a_j) = \Gamma_{ii} \frac{\phi_k^+(a_i)}{\lambda_i} + \sum_{\substack{j=1 \\ (i \neq j)}}^N \Gamma_{ij} \frac{\phi_k^+(a_j)}{\lambda_j} = e^{ika_i} . \quad (3.71)$$

Let

$$\Phi_{ij} := \begin{cases} \frac{\Gamma_{ii}}{\lambda_i} & \text{if } i = j \\ \frac{\Gamma_{ij}}{\lambda_j} & \text{if } i \neq j \end{cases} = \begin{cases} \frac{1}{\lambda_i} - \frac{im}{k\hbar^2} & \text{if } i = j , \\ -\frac{im}{k\hbar^2} e^{ik|a_i - a_j|} & \text{if } i \neq j . \end{cases} \quad (3.72)$$

Hence, we get

$$\sum_{j=1}^N \Phi_{ij} \phi_k^+(a_j) = e^{ika_i} , \quad (3.73)$$

or

$$\phi_k^+(a_j) = \sum_{l=1}^N (\Phi^{-1})_{jl} e^{ika_l} . \quad (3.74)$$

Substituting this into the solution of (3.66), we prove that

**Theorem 3.6** *The scattering wave function in the presence of  $N$  attractive Dirac delta potentials is given by*

$$\psi_k^+ = e^{ikx} + \sum_{j,l=1}^N \frac{im}{k\hbar^2} e^{ik|x-a_j|} (\Phi^{-1})_{jl} e^{ika_l} . \quad (3.75)$$

where the matrix  $\Phi_{jl}$  is given by (3.73).

### 3.2.1. Reflection and Transmission Coefficients

Assume that the incoming particles are sent from the left. Then, the coefficient of  $e^{-ikx}$  in the solution of  $\psi_k^+(x)$  when  $x < a_j$  for all  $j$  gives us the reflection coefficient:

$$r(k) = \sum_{j,l=1}^N \frac{im}{k\hbar^2} e^{ika_j} (\Phi^{-1})_{jl} e^{ika_l} . \quad (3.76)$$

Similarly, the coefficient of  $e^{ikx}$  in the solution of  $\psi_k^+$  when  $x > a_j$  for all  $j$  gives us the transmission coefficient :

$$t(k) = 1 + \sum_{j,l=1}^N \frac{im}{k\hbar^2} e^{-ika_j} (\Phi^{-1})_{jl} e^{ika_l} . \quad (3.77)$$

For  $N = 1$  and  $\lambda_1 = \lambda$ , we get the well-known results, (Griffiths and Schroeter, 2018) :

$$R(k) = |r(k)|^2 = \frac{m^2 \lambda^2}{\hbar^4 k^2 + m^2 \lambda^2} , \quad (3.78)$$

and

$$T(k) = |t(k)|^2 = \frac{\hbar^4 k^2}{\hbar^4 k^2 + m^2 \lambda^2} . \quad (3.79)$$

It is easy to see that  $T \rightarrow 1$  as  $k \rightarrow \infty$ . We plot the transmission coefficient as a function of  $k$  for different values of  $\lambda$  in Fig. 3.6.

For  $N = 2$  and if we choose  $\lambda_1 = \lambda_2 = \lambda$ ,  $a_1 = -a$  and  $a_2 = a$  without loss of generality, we find

$$\Phi_{ij}(k) = \begin{pmatrix} \frac{1}{\lambda} - \frac{im}{k\hbar^2} & -\frac{im}{k\hbar^2} e^{2ika} \\ -\frac{im}{k\hbar^2} e^{2ika} & \frac{1}{\lambda} - \frac{im}{k\hbar^2} \end{pmatrix} , \quad (3.80)$$



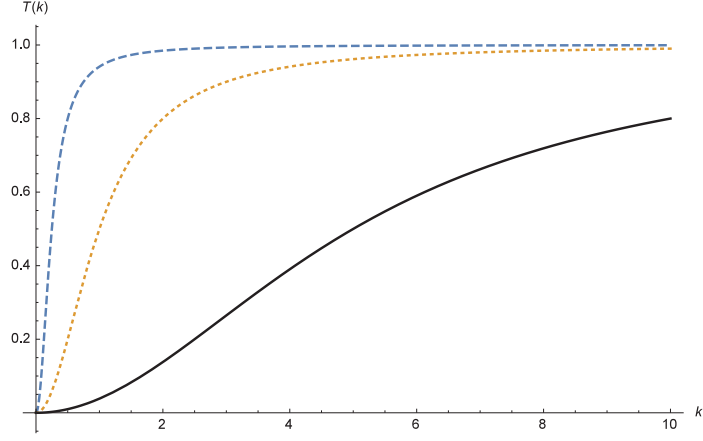


Figure 3.6. Transmission coefficients  $T(k)$  versus  $k$  for  $\lambda = 0.5$  (Dashed curve),  $\lambda = 2$  (Dotted curve), and  $\lambda = 10$  (Black curve).

and its inverse is given by

$$\Phi_{ij}^{-1}(k) = \frac{1}{\det \Phi} \begin{pmatrix} \frac{1}{\lambda} - \frac{im}{k\hbar^2} & -\frac{im}{k\hbar^2} e^{2ika} \\ -\frac{im}{k\hbar^2} e^{2ika} & \frac{1}{\lambda} - \frac{im}{k\hbar^2} \end{pmatrix}, \quad (3.81)$$

where

$$\det(\Phi) = \left( \frac{1}{\lambda} - \frac{im}{k\hbar^2} \right)^2 + \frac{m^2}{k^2 \hbar^4} e^{4ika}. \quad (3.82)$$

Then, from the formula for the reflection coefficient (3.76) we have

$$r(k) = \frac{im}{k\hbar^2} \left[ e^{ika_1} \Phi_{11}^{-1} e^{ika_1} + e^{ika_1} \Phi_{12}^{-1} e^{ika_2} + e^{ika_2} \Phi_{21}^{-1} e^{ika_1} + e^{ika_2} \Phi_{22}^{-1} e^{ika_2} \right]. \quad (3.83)$$

Since  $a_1 = -a$ ,  $a_2 = a$ , we obtain the explicit formula of the reflection coefficient as

$$\begin{aligned} r(k) &= \frac{1}{\det \Phi} \frac{im}{k\hbar^2} \left[ e^{-2ika} \left( \frac{1}{\lambda} - \frac{im}{k\hbar^2} \right) + \frac{2im}{k\hbar^2} e^{2ika} + e^{2ika} \left( \frac{1}{\lambda} - \frac{im}{k\hbar^2} \right) \right] \\ &= \frac{1}{\det \Phi} \frac{im}{k\hbar^2} \left[ \left( \frac{1}{\lambda} - \frac{im}{k\hbar^2} \right) \left( e^{2ika} + e^{-2ika} \right) + \frac{2im\lambda}{k\hbar^2} e^{2ika} \right]. \end{aligned} \quad (3.84)$$

Then, one can find  $R(k) = |r(k)|^2$  and similarly  $T(k) = 1 - R(k)$ . One can also plot

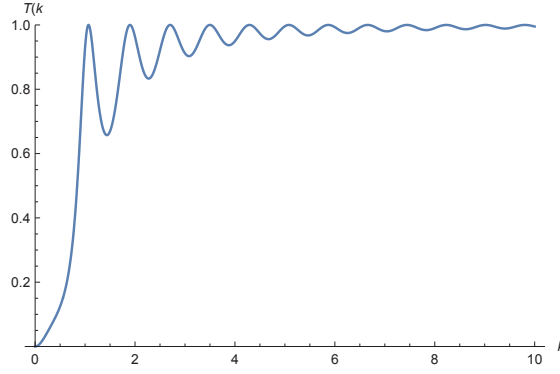


Figure 3.7. Transmission coefficient versus  $k$  for particular values of the parameters  $a = 2$  and  $\lambda = 1$  units.

the transmission coefficients as a function of  $k$  for larger number of delta potentials, see Fig. 3.8. It is interesting to notice that the transmission coefficients form zero bands as we increase the number of Dirac delta potentials periodically. This is one way to show the energy band gaps for a periodic delta lattice (Rorres, 1974). The values of  $k$  for which  $T(k) = 1$  are known as the transmission resonances (Erman et al., 2018).

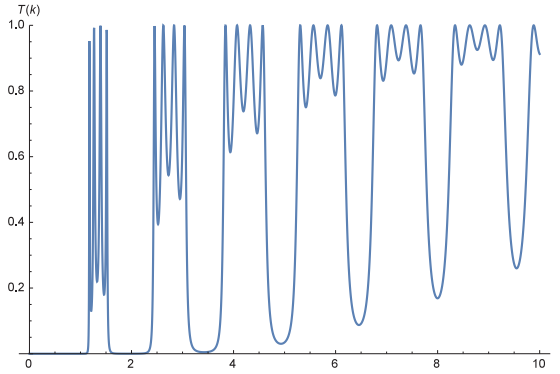


Figure 3.8. Transmission coefficient for  $N = 5$  versus  $k$  for particular values of the parameters  $a = 2$  and  $\lambda = 1$  units.

## CHAPTER 4

### PERTURBATION THEORY

We would like to review very basic results in perturbation theory in this chapter so that we can use them in the next chapter.

#### 4.1. Basic Idea of Perturbation Theory in a Simple Example

Perturbation theory was first introduced for studying the motion of planets in celestial mechanics originally studied by Poincaré (Poincaré, 1893). In order to give the motivation of the method, let us consider the simplest situation, where we are looking for a solution to some polynomial equations. Suppose the problem is to find the roots of

$$x^2 - 3.99x + 3.02 = 0 . \quad (4.1)$$

Certainly, it can be solved by the quadratic formula. However, suppose that we can not obtain an analytical formula (which could be the case for transcendental or higher order polynomial equations). Let us illustrate the idea of the perturbation theory within this simple example (Murdock, 1999). There are essentially four steps:

1. Since  $-3.99 = -4 + 0.01$  and  $3.02 = 3 + 0.02$ , the above equation (4.1) can be approximated by  $x^2 - 4x + 3 = 0$  and this can be solved easily (or we sometimes obtain exact solutions) by factorizing it as  $(x - 1)(x - 3) = 0$ . We have two roots:  $x_1 = 1, x_2 = 3$ .
2. In the second step, we define a family of problems depending on a small parameter  $\epsilon$ . For instance, if we choose  $\epsilon = 0.01$ , then (4.1) can be rewritten as

$$x^2 + (\epsilon - 4)x + (3 + 2\epsilon) = 0 . \quad (4.2)$$

The above equation (4.2) is an example of a perturbation family, a family of problems depending on the small parameter  $\epsilon$  which is solvable when  $\epsilon = 0$ , that is, When  $\epsilon = 0.01$ , the above equation becomes the target equation.

3. In the third step, we will look for approximate solutions of (4.2), in the form of polynomials (truncated power series) in the small parameter  $\epsilon$ , that is,

$$x_1 = 1 + \epsilon x_1^{(1)} + \epsilon^2 x_1^{(2)} + O(\epsilon^3) , \quad (4.3)$$

$$x_2 = 3 + \epsilon x_2^{(1)} + \epsilon^2 x_2^{(2)} + O(\epsilon^3) . \quad (4.4)$$

Substituting these into equation (4.2) and multiplying the terms out and arranging it in the same powers of  $\epsilon$ , the resulting equation must be true for all  $\epsilon$ . By keeping only terms of the order  $O(\epsilon^3)$ , we obtain

$$x_1 = 1 + \frac{3}{2}\epsilon + \frac{15}{8}\epsilon^2 + O(\epsilon^3) , \quad (4.5)$$

$$x_2 = 3 - \frac{5}{2}\epsilon - \frac{15}{8}\epsilon^2 + O(\epsilon^3) . \quad (4.6)$$

Evaluating of these solutions for  $\epsilon = 0.01$  up to order  $O(\epsilon^3)$  gives an approximate solution of our original problem (4.1):

$$x_1 \approx 1.0121875 , \quad (4.7)$$

$$x_2 \approx 2.9748125 . \quad (4.8)$$

4. The last step is to check the amount of error in these approximations. In this example,  $x_1 = 1.0151913452107089$  and  $x_2 = 2.974808654789291$ .

This example already reveals a lot about perturbation theory. The scope of perturbation theory is in general much broader, but the main idea is the same, (Murdock, 1999). They can include more complicated functions and even differential equations. If the small

parameter is in front of the term with the highest power or order, then the method fails, and one must extend the method in this case, see singular perturbation theory in (Murdock, 1999; Bender and Orszag, 2013). The perturbation theory in finite dimensional matrices is extensively studied in the book (Kato, 2013) and the extension of the method to operators in Hilbert spaces is much complicated due to the domain issues of unbounded operators (Reed and Simon, 1978).

## 4.2. Perturbation Theory for Hermitian Matrices

Since we shall later consider the Dirac delta potentials in a perturbative way, and their spectral properties are described by some  $N \times N$  Hermitian matrix, we would like to first review the subject of perturbation theory for Hermitian matrices. There are several interesting problems in quantum mechanics that is exactly solvable. However, the number of such exactly solvable cases are limited. For this reason, approximation methods are key for understanding physical systems. Approximation theories are frequently more understandable for physical phenomena rather than solving them based on exact numerical solutions of the corresponding equations. One of the main approximation methods used in quantum mechanics is the so-called *perturbation theory*. We will review the subject from the textbook (Faddeev and Yakubovskii, 2009) in order to be self-contained.

Assume that  $\Phi_0$  is a given self-adjoint operator defined on complete finite dimensional Hilbert space  $\mathbb{C}^n$  whose spectrum (its eigenvalues) is known. Suppose that  $\delta\Phi$  is another self-adjoint operator on  $\mathbb{C}^n$  which is “small” in some sense and consider the sum

$$\Phi = \Phi_0 + \delta\Phi . \quad (4.9)$$

Here, we do not specify what is meant by the smallness of  $\delta\Phi$  in general. Since we are going to study the perturbation theory of matrices, we will assume that all the terms of  $\delta\Phi$  are much smaller than the terms of  $\Phi_0$ . In general, the perturbation theory in infinite dimensional spaces is rather technical and the detailed analysis is more difficult (see e. g., (Rellich and Berkowitz, 1969; Reed and Simon, 1978; Kato, 2013)).

### 4.2.1. Non-Degenerate Case (Simple Eigenvalues)

We begin with the problem of perturbation of a simple eigenvalue (No degeneracy or no geometric/algebraic multiplicity). Consider the one-parameter family of operators

$$\Phi(\epsilon) = \Phi_0 + \epsilon \delta \Phi. \quad (4.10)$$

Clearly, we see  $\Phi(0) = \Phi_0$  and  $\Phi(1) = \Phi$ . Suppose that the eigenvectors and the eigenvalues of  $\Phi_0$  are  $A^{(0)}$  and  $\omega^{(0)}$ , respectively, i.e. ,

$$\Phi_0 A^{(0)} = \omega^{(0)} A^{(0)} . \quad (4.11)$$

The spectrum of  $\Phi_0$  is simple which means that to each  $\omega^{(0)}$  there corresponds only one eigenvector  $A^{(0)}$ . The eigenvalue equation for the operator  $\Phi(\epsilon)$  is

$$\Phi(\epsilon) A(\epsilon) = \omega(\epsilon) A(\epsilon) . \quad (4.12)$$

Our aim is to solve the above eigenvalue problem. Suppose that  $A(\epsilon)$  and  $\omega(\epsilon)$  are analytic functions of  $\epsilon$ , that is, they can be represented in the following form:

$$\omega(\epsilon) = \omega^{(0)} + \epsilon \omega^{(1)} + \epsilon^2 \omega^{(2)} + \dots \quad (4.13)$$

$$A(\epsilon) = A^{(0)} + \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \dots \quad (4.14)$$

Actually, one can show that the eigenvalues and the eigenvectors of an analytic regular matrix as a function of  $\epsilon$  are analytic for small  $\epsilon$ .

**Theorem 4.1** *Suppose that a Hermitian matrix  $\Phi_{ij}(\epsilon)$  for real  $\epsilon$  ( $\Phi_{ij}(\epsilon) = \overline{\Phi_{ji}(\epsilon)}$ ) has a convergent power series expansion for small  $\epsilon$ . Then, its eigenvalues are analytic function of  $\epsilon$  for small  $\epsilon$ .*

*Proof:* Since the eigenvalues of  $\Phi$  are just the roots of the characteristic equation

$$\det \begin{pmatrix} \Phi_{11} - \omega & \Phi_{12} & \cdots & \Phi_{1n} \\ \Phi_{21} & \Phi_{21} - \omega & \cdots & \Phi_{2n} \\ \vdots & \ddots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \Phi_{nn} - \omega \end{pmatrix} = 0 . \quad (4.15)$$

This determinant is a polynomial of degree  $n$  in  $\omega$ , that is,

$$\omega^n + c_1\omega^{n-1} + c_2\omega^{n-2} + \dots + c_{n-1}\omega + c_n = 0 , \quad (4.16)$$

where the coefficients  $c_i$  are functions of the matrix elements  $\Phi_{ij} = \Phi_{0(ij)} + \epsilon\delta\Phi_{ij}$ . Given the matrix  $\Phi$ , they are considered to be polynomial in  $\epsilon$ . According to The Newton-Puiseux Theorem (Puiseux, 1850), which states that, if  $f(x, y)$  is a polynomial in two variables with complex coefficients, then the solutions  $y$  as functions of  $x$  for the equation  $f(x, y) = 0$  can be expanded as a Puiseux series  $y = \sum_{k=k_0}^{\infty} d_k x^{k/n}$  where  $n$  is a positive integer and  $k_0$  is an integer. This series is convergent in a neighbourhood of the origin  $x = 0$ , we may now write the solution of (4.16) as

$$\omega(\epsilon) = \omega + \beta_1\epsilon^{\frac{1}{h}} + \beta_2\epsilon^{\frac{2}{h}} + \dots \quad (4.17)$$

Here  $h$  is not Planck constant. This series is known as *Puiseux's expansion* and it is convergent for small  $|\epsilon|$ . Let  $\beta_n$  denote the first non-zero coefficient, i.e.,

$$\beta_1 = \dots = \beta_{n-1} = 0 , \beta_n \neq 0 . \quad (4.18)$$

Let's rewrite the equation (4.17) in the following way :

$$\omega(\epsilon) = \omega + \beta_1\epsilon^{\frac{1}{h}} + \beta_2\epsilon^{\frac{2}{h}} + \dots + \beta_{n-1}\epsilon^{\frac{n-1}{h}} + \beta_n\epsilon^{\frac{n}{h}} + \beta_{n+1}\epsilon^{\frac{n+1}{h}} + \dots \quad (4.19)$$

The above equation is lined up as

$$\begin{aligned}\beta_n &= \frac{\omega(\epsilon) - \omega - \epsilon^{\frac{n}{h}} \left[ \beta_{n+1} \epsilon^{\frac{1}{h}} + \beta_{n+2} \epsilon^{\frac{2}{h}} + \dots \right]}{\epsilon^{\frac{n}{h}}} \\ &= \frac{\omega(\epsilon) - \omega}{\epsilon^{\frac{n}{h}}} - \left[ \beta_{n+1} \epsilon^{\frac{1}{h}} + \beta_{n+2} \epsilon^{\frac{2}{h}} + \dots \right].\end{aligned}\quad (4.20)$$

When we take the limit as  $\epsilon \rightarrow 0^+$ , then we find

$$\lim_{\epsilon \rightarrow 0^+} \frac{\omega(\epsilon) - \omega}{\epsilon^{\frac{n}{h}}} \quad (4.21)$$

is real since all eigenvalues of Hermitian matrix  $\Phi$  are real. On the other hand, letting  $\epsilon \rightarrow 0^-$ .

$$\beta_n = \lim_{\epsilon \rightarrow 0^-} \frac{\omega(\epsilon) - \omega}{\epsilon^{\frac{n}{h}}} = \frac{\omega(\epsilon) - \omega}{((-1)(-1)\epsilon)^{\frac{n}{h}}} = \lim_{\epsilon \rightarrow 0^-} \frac{1}{(-1)^{\frac{n}{h}}} \frac{\omega(\epsilon) - \omega}{(-\epsilon)^{\frac{n}{h}}}. \quad (4.22)$$

Hence,  $(-1)^{\frac{n}{h}}$  must be real, therefore  $n$  must be a multiple of  $h$  as

$$n = kh, \quad k \in \mathbb{Z}. \quad (4.23)$$

We can continue this argument to show that only integer powers of  $\epsilon$  can have nonzero coefficients.  $\square$

Similarly, one can also prove that eigenvectors can be expanded as integer power series of  $\epsilon$  but the proof is more complicated, see e.g., (Rellich and Berkowitz, 1969) for the details.

Now, substituting (4.13) and (4.14) into (4.12), we obtain

$$\begin{aligned}(\Phi_0 + \epsilon \delta \Phi)(A^{(0)} + \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \dots) \\ = (\omega^{(0)} + \epsilon \omega^{(1)} + \epsilon^2 \omega^{(2)} + \dots)(A^{(0)} + \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \dots),\end{aligned}\quad (4.24)$$



for all  $\epsilon$ . Since all the terms with the same powers of  $\epsilon$  should be equal, we get the system of equations

$$\begin{aligned}
\epsilon^0 : \quad \Phi_0 A^{(0)} &= \omega^{(0)} A^{(0)} , \\
\epsilon^1 : \quad \Phi_0 A^{(1)} + \delta\Phi A^{(0)} &= \omega^{(0)} A^{(1)} + \omega^{(1)} A^{(0)} , \\
&\vdots \\
\epsilon^k : \quad \Phi_0 A^{(k)} + \delta\Phi A^{(k-1)} &= \omega^{(0)} A^{(k)} + \omega^{(1)} A^{(k-1)} + \dots + \omega^{(k)} A^{(0)} . \quad (4.25)
\end{aligned}$$

These equations can be written in a more convenient way :

$$\begin{aligned}
\Phi_0 A^{(0)} &= \omega^{(0)} A^{(0)} \\
(\Phi_0 - \omega^{(0)}) A^{(1)} &= (\omega^{(1)} - \delta\Phi) A^{(0)} , \\
(\Phi_0 - \omega^{(0)}) A^{(2)} &= (\omega^{(1)} - \delta\Phi) A^{(1)} + \omega^{(2)} A^{(0)} , \\
&\vdots \\
(\Phi_0 - \omega^{(0)}) A^{(k)} &= (\omega^{(1)} - \delta\Phi) A^{(k-1)} + \dots + \omega^{(k)} A^{(0)} , \quad (4.26)
\end{aligned}$$

where the expressions of the form  $\Phi_0 - \omega^{(0)}$  refer to  $\Phi_0 - \omega^{(0)} I$  for simplicity. By the first equation (4.26),  $A^{(0)}$  is an eigenvector of  $\Phi_0$ , and from the assumption about non-degeneracy of the spectrum, let

$$A^{(0)} = A_n \quad \text{and} \quad \omega^{(0)} = \omega_n , \quad (4.27)$$

where we use the index  $n$  to label the  $n$  th eigenvalue/eigenvector of  $\Phi_0$ . Before returning to the subsequent equations in (4.26), we select a normalization condition for the vector  $A(\epsilon)$ . The following normalization condition

$$\langle A(\epsilon), A^{(0)} \rangle = 1 \quad (4.28)$$

is the most convenient choice and we have used the inner product of two vectors  $A$  and  $B$  on  $\mathbb{C}^N$   $\left(\langle A, B \rangle := \sum_{n=1}^N \overline{A_n} B_n\right)$ . Our assumption is that  $A^{(0)}$  is normalized in the sense that  $\left(\sum_{n=1}^N |A_n^{(0)}|^2\right)^{\frac{1}{2}} = 1$  and the condition (4.28) is equivalent to

$$\langle A^{(1)}, A^{(0)} \rangle = 0, \dots, \langle A^{(k)}, A^{(0)} \rangle = 0, \dots, \quad (4.29)$$

for all  $k$ . Therefore, we can find the corrections  $A^{(1)}, A^{(2)}, \dots, A^{(k)}, \dots$  in the subspace orthogonal to the vector  $A^{(0)} = A_n$ . Now, we consider the second equation in (4.26). This is an equation of the second kind with a Hermitian matrix  $\Phi_0$ , and  $\omega^{(0)}$  is an eigenvalue of  $\Phi_0$ . This equation

$$(\Phi_0 - \omega^{(0)})A^{(1)} = (\omega^{(1)} - \delta\Phi)A^{(0)} \quad (4.30)$$

has a solution if and only if the right-hand side is orthogonal to the vector  $A^{(0)}$ . Let us show this explicitly. For this, we take the inner product of both sides of the equation with  $A^{(0)}$  to get

$$\begin{aligned} \langle A^{(0)}, (\omega^{(1)} - \delta\Phi)A^{(0)} \rangle &= \langle A^{(0)}, (\Phi_0 - \omega^{(0)})A^{(1)} \rangle \\ &= \langle \Phi_0 A^{(0)}, A^{(1)} \rangle - \langle A^{(0)}, \omega^{(0)} A^{(1)} \rangle \\ &= \omega^{(0)} \langle A^{(0)}, A^{(1)} \rangle - \omega^{(0)} \langle A^{(0)}, A^{(1)} \rangle = 0, \end{aligned} \quad (4.31)$$

where we have used the equation  $\Phi_0 A^{(0)} = \omega^{(0)} A^{(0)}$  and Hermiticity of the matrix  $\Phi_0$  (in this case,  $\omega^{(0)}$  is real). Then, we obtain

$$(\omega^{(1)} - \delta\Phi)A^{(0)} \perp A^{(0)}. \quad (4.32)$$

Conversely, if the right-hand side of the equation (4.30) is orthogonal to  $A^{(0)}$

$$\langle A^{(0)}, (\omega^{(1)} - \delta\Phi)A^{(0)} \rangle = 0, \quad (4.33)$$

we get more explicitly the condition

$$\omega_n^{(1)} = \langle \delta\Phi A_n, A_n \rangle = \langle A_n, \delta\Phi A_n \rangle . \quad (4.34)$$

This result has a very simple interpretation. The first order correction  $\omega_n^{(1)}$  to the eigenvalue  $\omega_n$  is just the mean value of the perturbation  $\delta\Phi$  in the unperturbed state  $A_n$ .

Since the solution of the second equation in (4.26) exists under the above condition, we can formally write the solution  $A^{(1)}$  as

$$A^{(1)} = (\Phi_0 - \omega^{(0)})^{-1}(\omega^{(1)} - \delta\Phi)A^{(0)}. \quad (4.35)$$

However, the above formal solution needs to be written in a more precise way. To understand the problem, we must study the matrices of the form  $(A - \lambda)^{-1}$ . This operator is called the *resolvent* of  $A$  at  $\lambda$  (Kreyszig, 1978). By the *spectral theorem* for self-adjoint operators  $A$  (Hermitian matrices in finite dimensional vector spaces), we have

$$A = \sum_m \lambda_m \mathbb{P}_m, \quad (4.36)$$

where  $\mathbb{P}_m$  is the orthogonal projection operator onto the  $m$  th eigenvector  $x_m$  associated with the eigenvalue  $\lambda_m$ , that is the action of the projection operator on any vector  $y \in \mathbb{C}^N$

$$\mathbb{P}_m y = \langle x_m, y \rangle x_m . \quad (4.37)$$

Then, since the functions of matrices  $(A - \lambda)^{-1}$  for real  $\lambda$  is defined via spectral theorem, we can write

$$(A - \lambda)^{-1} = \sum_m \frac{\mathbb{P}_m}{\lambda_m - \lambda} . \quad (4.38)$$

From equation (4.38), it is easy to see that the resolvent become singular when  $\lambda$  coincides with one of the eigenvalues of  $A$ , that is, when  $\lambda = \lambda_n$ . Let us recall that the right-hand side of the second equation in (4.26) is orthogonal to  $A^{(0)} = A_n$  and  $\langle A^{(0)}, A^{(1)} \rangle = 0$ . Therefore, we actually need not the operator  $(A - \lambda I)^{-1}$  itself, but instead  $(A - \lambda I)^{-1} \mathbb{P}$  acting in the subspace orthogonal to the vector  $A_n$ , where  $\mathbb{P}$  is the projection  $I - \mathbb{P}_n$  onto that subspace. Let us rewrite the operator  $(A - \lambda I)^{-1} \mathbb{P}$  in the following way now

$$(A - \lambda I)^{-1} \mathbb{P} = (A - \lambda I)^{-1} (I - \mathbb{P}_n) = (A - \lambda I)^{-1} - (A - \lambda I)^{-1} \mathbb{P}_n . \quad (4.39)$$

By the spectral theorem, we obtain

$$(A - \lambda I)^{-1} \mathbb{P} = \sum_m \frac{\mathbb{P}_m}{\lambda_m - \lambda} - \sum_m \frac{\mathbb{P}_m \mathbb{P}_n}{\lambda_m - \lambda} = \sum_{m \neq n} \frac{\mathbb{P}_m}{\lambda_m - \lambda} , \quad (4.40)$$

where we have used the orthogonality of the projection operators  $\mathbb{P}_n \mathbb{P}_m = \delta_{nm} \mathbb{P}_n$ . This expression now makes sense and it is well-defined for  $\lambda = \lambda_n$ . Therefore, the precise way of writing the solution 4.35 should be

$$A^{(1)} = (\Phi_0 - \omega^{(0)})^{-1} \mathbb{P} (\omega^{(1)} - \delta \Phi) A^{(0)} . \quad (4.41)$$

Substituting the first order correction result for the eigenvalues (4.34) into the above equation, we find

$$A^{(1)} = -(\Phi_0 - \omega_n)^{-1} \mathbb{P} (\mathbb{P}_n - I) \delta \Phi A_n . \quad (4.42)$$

Since  $\mathbb{P}$  acts on the subspace orthogonal to  $A_n$ , that is,  $\mathbb{P} \mathbb{P}_n = 0$ , so that

$$A^{(1)} = -(\Phi_0 - \omega_n)^{-1} \mathbb{P} \delta \Phi A_n . \quad (4.43)$$

Using the equation (4.40), we can express the first order correction to the eigenvectors  $A_n$  as

$$A^{(1)} = \sum_{\substack{m=1 \\ (m \neq n)}}^N \frac{\langle \delta \Phi A_n, A_m \rangle}{\omega_n - \omega_m} A_m . \quad (4.44)$$

We can similarly find all the corrections of subsequent orders. By the orthogonality to  $A^{(0)}$  of the right-hand side of the third equation in (4.26), we get

$$\langle (\Phi_0 - \omega^{(0)}) A^{(2)}, A^{(0)} \rangle = \langle (\omega^{(1)} - \delta \Phi) A^{(1)} + \omega^{(2)} A^{(0)}, A^{(0)} \rangle = 0 , \quad (4.45)$$

where we have used

$$\langle (\Phi_0 - \omega^{(0)}) A^{(2)}, A^{(0)} \rangle = \omega^{(0)} \langle A^{(2)}, A^{(0)} \rangle - \omega^{(0)} \langle A^{(2)}, A^{(0)} \rangle = 0 . \quad (4.46)$$

Therefore, we find

$$\omega^{(2)} = \langle \delta \Phi A^{(1)}, A^{(0)} \rangle . \quad (4.47)$$

Using the first order result for the eigenvector given by (4.44), we have an explicit formula for the second correction to the eigenvalue  $\omega_n$  :

$$\omega^{(2)} = \sum_{\substack{m=1 \\ (m \neq n)}}^N \frac{|\langle \delta \Phi A_n, A_m \rangle|^2}{(\omega_n - \omega_m)} . \quad (4.48)$$

The higher order corrections can be formally found by the repeated applications of the above procedure to the formulas  $\omega^{(k)} = \langle \delta \Phi A^{(k-1)}, A^{(0)} \rangle$  and  $A^{(k)} = (\Phi_0 - \omega^{(0)})^{-1} \mathbb{P} \times$  (the right-hand side of the corresponding equation in (4.26)). Let us summarize the results for the non-degenerate case as a theorem:

**Theorem 4.2** Suppose that a Hermitian matrix  $\Phi$  is decomposed as  $\Phi = \Phi_0 + \epsilon \delta \Phi$  and all the eigenvalues  $\omega^{(0)}$  of  $\Phi_0$  are explicitly known and non-degenerate (simple) and its eigenvector associated with this simple eigenvalue is  $A^{(0)}$ . Then, the first order and second order perturbation results of the  $n$ th eigenvalue and its associated eigenvector for  $\Phi$  are given by

$$\omega_n(\epsilon) = \omega_n^{(0)} + \epsilon \langle A_n, \delta \Phi A_n \rangle + \epsilon^2 \sum_{\substack{m=1 \\ (m \neq n)}}^N \frac{|\langle \delta \Phi A_n, A_m \rangle|^2}{(\omega_n - \omega_m)} + O(\epsilon^3), \quad (4.49)$$

$$A_n(\epsilon) = A_n + \epsilon \sum_{\substack{m=1 \\ (m \neq n)}}^N \frac{\langle \delta \Phi A_n, A_m \rangle}{\omega_n - \omega_m} A_m + O(\epsilon^2). \quad (4.50)$$

In general, we do not calculate all the terms in the perturbation theory and the series is actually a divergent one, and they are known as asymptotic series. Nevertheless, it is usually sufficient to truncate the series after a few terms.

The above formulation of the perturbation theory has the advantage that we can easily extend it to the case where there are multiple eigenvalues (with multiplicity greater than one) or also known as the degenerate case in the physics literature.

### 4.2.2. Degenerate Case

Now, we discuss the theory of perturbation of an eigenvalue with multiplicity greater than one (degenerate case), and restrict ourselves to the discussion of only the first order correction  $\omega^{(1)}$  to the eigenvalue  $\omega^{(0)}$  since it will be sufficient for our purposes. Let  $\omega_n = \omega$  be an eigenvalue of the matrix  $\Phi_0$  with multiplicity  $q$ , that is,

$$\Phi_0 A_i = \omega A_i, \quad (4.51)$$

where  $i = 1, 2, 3, \dots, q$ . Let us denote the eigenspace of  $\Phi_0$  corresponding to the eigenvalue  $\omega$  by  $\mathcal{H}_\omega$  and the projection operator onto this subspace spanned by the eigenvectors  $A_i$  by  $Q$ .

We did not assume anything about the degeneracy of the eigenvalues of  $\Phi_0$  until

the equations (4.26). Therefore we can safely go back to the system of equations (4.26), and conclude from first equation that  $\omega^{(0)} = \omega$  even in the degenerate case. However, we can not conclude the same for the eigenvector, i.e., we have  $A^{(0)} \neq A_i$ . Nevertheless, we can only deduce that  $A^{(0)} \in \mathcal{H}_\omega$ . Now, we illustrate that additional restrictions are imposed on the vector  $A^{(0)}$  so that they do not coincide with the eigenvectors  $A_i$  in the general case. Actually, the second equation in (4.26) has solutions if its right-hand side is orthogonal to the subspace  $\mathcal{H}_\omega$ :

$$Q(\omega^{(1)} - \delta\Phi)A^{(0)} = 0 . \quad (4.52)$$

Since  $QA^{(0)} = A^{(0)}$ , we can write this as

$$Q\delta\Phi QA^{(0)} = \omega^{(1)}A^{(0)} . \quad (4.53)$$

This equation tells us that  $A^{(0)}$  are eigenvectors of the matrix  $Q\delta\Phi Q$  on  $\mathbb{C}^q$ , and the  $\omega^{(1)}$  are eigenvalues of it. Practically, the problem reduces to the diagonalization of a matrix of order  $q$ . Substituting  $A^{(0)} = \sum_{i=1}^q c_i A_i$  in (4.53) and using  $QB = \sum_{j=1}^q \langle A_j, B \rangle A_j$ , we get

$$\begin{aligned} Q\delta\Phi QA^{(0)} &= Q\delta\Phi Q\left(\sum_{i=1}^q c_i A_i\right) \\ &= Q\delta\Phi \sum_{j=1}^q \sum_{i=1}^q c_i \langle A_j, A_i \rangle A_j \\ &= Q \sum_{i,j=1}^q c_i \langle A_j, A_i \rangle \delta\Phi A_j = Q \sum_{i=1}^q c_i \delta\Phi A_i = \sum_{i=1}^q \sum_{j=1}^q c_i \langle A_j, \delta\Phi A_i \rangle A_j . \end{aligned} \quad (4.54)$$

Hence, the equation (4.53) becomes

$$\sum_{j=1}^q \left( \sum_{i=1}^q c_i \langle A_j, \delta\Phi A_i \rangle - \omega^{(1)} c_j \right) A_j = 0 \quad (4.55)$$

so that

$$\sum_{i=1} \delta\Phi_{ji} c_i = \omega^{(1)} c_j , \quad (4.56)$$

where  $\delta\Phi_{ji} = \langle A_j, \delta\Phi A_i \rangle$  are the matrix elements of the perturbed matrix  $\delta\Phi$ . The matrix  $\delta\Phi_{ji}$  is Hermitian and thus can always be diagonalized (Meyer, 2000). The result (4.56) can be interpreted as

$$\sum_{j=1} (\delta\Phi_{ji} - \omega^{(1)} \delta_{ij}) c_j = 0 . \quad (4.57)$$

We have nontrivial solutions if and only if

$$\det (\delta\Phi_{ij} - \omega^{(1)} \delta_{ij}) = 0 , \quad (4.58)$$

from which we can find the first order corrections to the eigenvalue  $\omega$ .

If we list the eigenvalues of this matrix by  $\omega_j^{(1)}$ ,  $j = 1, 2, \dots, q$ , the first order perturbation theory gives the eigenvalues of the perturbed problem is given by  $\omega + \omega_j^{(1)}$ ,  $j = 1, 2, \dots, q$  by setting  $\epsilon = 1$ . Generally, one says that the perturbation removes the degeneracy, (Griffiths and Schroeter, 2018). The removal of the degeneracy can turn out to be incomplete if there are duplicates among the numbers  $\omega_j^{(1)}$ , i.e, if the operator  $Q\delta\Phi Q$  has still multiple eigenvalues.

The perturbation theory for unbounded operators in Hilbert spaces is, in general, a difficult subject and it is outside of the scope of this thesis. This is a generic situation in quantum mechanics, where we split the Hamiltonian operator  $H$  into two parts  $H_0$  (its eigenvalues and eigenvectors are assumed to be exactly solved) and the extra term  $V$ . However, due to the unboundedness of the Hamiltonian operator the analysis is rather involved. In this case, one must check all the technical issues about how the perturbation term deforms the spectrum of the operator that includes the discrete as well as continuous part. One can find all the details about the subject in (Kato, 2013; Reed and Simon, 1978). As a final remark in this chapter, one must be careful enough even in these finite



dimensional problems since the series that we find does not necessarily converge and they are not in general and they are known as asymptotic series. In this case, it would be sufficient to take a few terms in the expansion for practical problems, see (Bender and Orszag, 2013) for the details.

## CHAPTER 5

### THE GAP AND SPLITTING IN THE BOUND STATE ENERGIES THROUGH PERTURBATION THEORY

The main aim of this chapter is to find approximately the splitting in the bound state energy by applying the perturbation methods to the principal matrix rather than the Hamiltonian itself.

Let us first rewrite the principal matrix  $\Phi$  given by (3.22) as a function  $E = -\nu^2$  with  $\nu > 0$ , that is

$$\Phi_{ij}(E) = \begin{cases} \frac{1}{\lambda_i} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} & \text{if } i = j , \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\sqrt{-E}|a_i - a_j|}{\hbar}}}{\hbar\sqrt{-E}} & \text{if } i \neq j . \end{cases} \quad (5.1)$$

For  $N = 2$ , we have analytically found the bound state energies for  $\lambda_1 = \lambda_2$  in Chapter 2. Unfortunately, the bound state energies for an arbitrary number of delta potentials can not be found in terms of elementary functions. For this reason, we would like to develop a kind of approximation for which we can estimate the bound state energy. Let us consider the following family of matrices depending on the parameter  $\epsilon$ :

$$\Phi(E) = \Phi_0(E) + \epsilon\delta\Phi(E) , \quad (5.2)$$

where  $\Phi_0$  is the diagonal part of the principal matrix; it means that zeros of its eigenvalues can be exactly computed, and  $\delta\Phi$  is the off-diagonal part, this is assumed to be "small" perturbation to the diagonal part. We introduce a parameter  $\epsilon$  to keep track of the perturbation expansion. We will take  $\epsilon$  to be 1 at the end of our calculations.

## 5.1. Non-degenerate Case

Assume that  $\Phi_0$  is non-degenerate. We can interpret the original problem for which we look for nontrivial solutions of  $\Phi(E)A(E) = 0$  as an eigenvalue problem

$$\Phi(E)A(E) = w(E)A(E) , \quad (5.3)$$

where the zeros of  $w(E)$  corresponds to the nontrivial solution of  $\Phi(E)A(E) = 0$ . Since  $\Phi(E)$  is a symmetric matrix, we can apply the standard perturbation techniques to the principal matrix, developed in Chapter 3. In accordance with this purpose, assume that

$$w^k = w^{(0)k} + \epsilon w^{(1)k} + \epsilon^2 w^{(2)k} + \dots \quad (5.4)$$

$$A^k = A^{(0)k} + \epsilon A^{(1)k} + \epsilon^2 A^{(2)k} + \dots \quad (5.5)$$

Here we drop writing  $E$  dependence of the functions for simplicity. The solution to the related unperturbed eigenvalue problem

$$\Phi_0 A^{(0)k} = w^{(0)k} A^{(0)k} \quad (5.6)$$

is given by

$$w^{(0)k} = \frac{1}{\lambda_k} - \sqrt{\frac{m}{2}} \frac{1}{\hbar \sqrt{-E}} = [\Phi_0]_{kk} , \quad (5.7)$$

where  $[\Phi_0]_{kk}$  is the  $k$ th diagonal element of  $\Phi$ . It is easy to show that the eigenvectors associated with the eigenvalue  $w^{(0)k}$  is

$$A^{(0)k} = e^k = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (5.8)$$

where 1 is located in the  $k$ th position of the column and other elements of it are zero. In summary, we find

$$\Phi_0 A^{(0)k} = \Phi_0 e^k = \begin{pmatrix} 0 \\ \vdots \\ (\Phi_0)_{kk} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = (\Phi_0)_{kk} \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = (\Phi_0)_{kk} e^k = w^{(0)k} A^{(0)k}. \quad (5.9)$$

Notice that  $e_i^k$  forms a complete orthonormal set of basis :

$$\sum_{i=1} e_i^k e_i^l = \delta_{kl}. \quad (5.10)$$

Once we have found the eigenvalues and eigenvectors of the diagonal part of the principal matrix or unperturbed eigenvalue problem, we can perturbatively solve the full problem. Now, we will apply the first order  $w^{(1)k}$  perturbation results. Using the equation (4.34) in

Chapter 3, we get

$$\begin{aligned}
w^{(1)k} &= \langle \delta\Phi A^{(0)k}, A^{(0)k} \rangle = \langle \delta\Phi e^k, e^k \rangle = \langle e^k, \delta\Phi e^k \rangle \\
&= \sum_{i=1}^N \overline{(e^k)_i} (\delta\Phi e^k)_i = \sum_{i=1}^N (e^k)_i (\delta\Phi e^k)_i \\
&= \sum_{i,j=1}^N (e^k)_i \delta\Phi_{ij} (e^k)_j,
\end{aligned} \tag{5.11}$$

where we have used the self-adjointness of  $\delta\Phi$ . Then, we can simplify the above result as

$$w^{(1)k} = \sum_{i=1}^N \sum_{j=1}^N \delta_i^k (\delta\Phi)_{ij} \delta_j^k = (\delta\Phi)_{kk} = 0. \tag{5.12}$$

Similarly, using the result given in the equation (4.48) in Chapter 3, the formula of the second order perturbation for the eigenvalues of the principal matrix  $\Phi$  is given by

$$w^{(2)k} = \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{|\langle \delta\Phi A^{(0)k}, A^{(0)l} \rangle|^2}{w^{(0)k} - w^{(0)l}}. \tag{5.13}$$

Then,

$$\begin{aligned}
|\langle \delta\Phi A^{(0)k}, A^{(0)l} \rangle|^2 &= |\langle A^{(0)k}, \delta\Phi A^{(0)l} \rangle|^2 = |\langle e^k, \delta\Phi e^l \rangle|^2 \\
&= \langle e^k, \delta\Phi e^l \rangle \langle \delta\Phi e^l, e^k \rangle = (\delta\Phi)_{kl} (\delta\Phi)_{lk}.
\end{aligned} \tag{5.14}$$

When using the symmetry of  $\delta\Phi$ , we find

$$w^{(2)k} = \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{(\delta\Phi)_{kl} (\delta\Phi)_{kl}}{w^{(0)k} - w^{(0)l}}. \tag{5.15}$$

Since  $\Phi_{kl} = (\delta\Phi)_{kl}$  for  $k \neq l$ ,

$$w^{(2)k} = \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{\Phi_{kl}^2}{w^{(0)k} - w^{(0)l}} . \quad (5.16)$$

The first order correction to the eigenvectors  $A^{(1)k}$  is given by

$$A^{(1)k} = \sum_{\substack{j=1 \\ (j \neq k)}}^N \frac{\delta\Phi_{jk}}{w^{(0)k} - w^{(0)j}} A^{(0)j} . \quad (5.17)$$

The bound state energies can be found from the solution of the equation  $w^k(E) = 0$ . The zeroth order approximation is the solution of

$$w^{(0)k}(E) = \frac{1}{\lambda_k} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} = 0 , \quad (5.18)$$

and the result is

$$E^{(0)k} = -\frac{m\lambda_k^2}{2\hbar^2} \quad (5.19)$$

is bound state energy of  $k$ th delta center where there is no other delta center. Furthermore, assume that

$$E^k = E^{(0)k} + \epsilon E^{(1)k} + \epsilon^2 E^{(2)k} + \dots \quad (5.20)$$

Let  $\delta E^k = \epsilon E^{(1)k} + \epsilon^2 E^{(2)k} + \dots$  for simplicity. Evaluating  $w^k(E)$  for  $E = E^k$  and using (5.20), we find

$$\begin{aligned} w^k(E) &= w^{(0)k}(E^{(0)k} + \delta E^k) + \epsilon w^{(1)k}(E^{(0)k} + \delta E^k) \\ &\quad + \epsilon^2 w^{(2)k}(E^{(0)k} + \delta E^k) + \dots \end{aligned} \quad (5.21)$$

Since  $w^{(1)k}(E) = (\delta\Phi)_{kk} = 0$  for any  $E$ , the equation (5.21) becomes

$$w^k(E) = w^{(0)k}(E^{(0)k} + \delta E^k) + \epsilon^2 w^{(2)k}(E^{(0)k} + \delta E^k) + \dots \quad (5.22)$$

Using Taylor expansion of  $w^{(0)k}$  around  $E^{(0)k}$ , and the fact  $w^{(0)k}(E^{(0)k}) = 0$ , we obtain

$$0 = \frac{\partial w^{(0)k}}{\partial E^{(0)k}}(\delta E^k) + \epsilon^2 \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{\Phi_{kl}^2(E^{(0)k} + \delta E^k)}{w^{(0)k}(E^{(0)k} + \delta E^k) - w^{(0)l}(E^{(0)k} + \delta E^k)} + \dots, \quad (5.23)$$

where we have substituted the second order perturbation result (5.16). Moreover, since  $\Phi$  is an analytic function for  $E < 0$  from explicit formula (5.1), we can use the Taylor expansion of the principal matrix  $\Phi$  around  $E = E_k^{(0)}$

$$\Phi_{kl}(E) = \Phi_{kl}(E^{(0)k} + \delta E^k) = \Phi_{kl}(E^{(0)k}) + \frac{\partial \Phi_{kl}}{\partial E^{(0)k}} \delta E^k + O((\delta E^k)^2), \quad (5.24)$$

where

$$\frac{\partial \Phi_{kk}}{\partial E^{(0)k}} = \left. \frac{\partial \Phi_{kk}}{\partial E} \right|_{E=E^{(0)k}}.$$

Using (5.24) in the numerator of the second term in (5.23) :

$$\Phi_{kl}^2(E^{(0)k} + \delta E^k) = \Phi_{kl}^2(E^{(0)k}) + 2\Phi_{kl}(E^{(0)k}) \frac{\partial \Phi_{kl}}{\partial E^{(0)k}} \delta E^k + O((\delta E^k)^2). \quad (5.25)$$

Similarly, using the Taylor expansion of the eigenvalues, the denominator of the second term in (5.23) gives rise to

$$\begin{aligned}
& w^{(0)k}(E^{(0)k} + \delta E^k) - w^{(0)l}(E^{(0)k} + \delta E^k) \\
&= w^{(0)k}(E^{(0)k}) + \frac{\partial w^{(0)k}}{\partial E^{(0)k}} \delta E^k - \left[ w^{(0)l}(E^{(0)k}) + \frac{\partial w^{(0)l}}{\partial E^{(0)k}} \delta E^k \right] + O((\delta E^k)^2) \quad (5.26) \\
&= \left[ \frac{\partial w^{(0)k}}{\partial E^{(0)k}} - \frac{\partial w^{(0)l}}{\partial E^{(0)k}} \right] \delta E^k - w^{(0)l}(E^{(0)k}) ,
\end{aligned}$$

or by equation (5.7)

$$w^{(0)k}(E^{(0)k} + \delta E^k) - w^{(0)l}(E^{(0)k} + \delta E^k) = \left( \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} - \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} \right) - \Phi_{ll}(E^{(0)k}) . \quad (5.27)$$

Substituting all the results in the equation (5.23), we get

$$\begin{aligned}
0 &= \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \delta E^k + \epsilon^2 \sum_{\substack{l=1 \\ (l \neq k)}}^N \left[ \Phi_{kl}^2(E^{(0)k}) + 2\Phi_{kl}(E^{(0)k}) \frac{\partial \Phi_{kl}}{\partial E^{(0)k}} \delta E^k \right] \\
&\quad \times \left[ \left( \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} - \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} \right) \delta E^k - \Phi_{ll}(E^{(0)k}) \right]^{-1} + O((\delta E^k)^2) . \quad (5.28)
\end{aligned}$$

Since we have assumed that  $|\Phi_{kl}| \ll \Phi_{ll}$ , we can rewrite the following term in the equation (5.28) as

$$\begin{aligned}
& \left[ \left( \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} - \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} \right) \delta E^k - \Phi_{ll}(E^{(0)k}) \right]^{-1} \\
&= -\frac{1}{\Phi_{ll}(E^{(0)k})} \left[ 1 + \frac{1}{\Phi_{ll}(E^{(0)k})} \left( \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} - \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} \right) \delta E^k \right] . \quad (5.29)
\end{aligned}$$



Substituting the equation (5.29) in the equation (5.28) and set  $\epsilon = 1$ , we obtain

$$\begin{aligned} \delta E^k \left[ \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \right] - \sum_{\substack{l=1 \\ (l \neq k)}}^N \left[ \Phi_{kl}^2(E^{(0)k}) + 2\Phi_{kl}(E^{(0)k}) \frac{\partial \Phi_{kl}}{\partial E^{(0)k}} \delta E^k \right] \\ \times \left[ \frac{1}{\Phi_{ll}(E^{(0)k})} \right] \left[ 1 + \frac{1}{\Phi_{ll}(E^{(0)k})} \left( \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} - \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} \right) \right] = 0 . \end{aligned} \quad (5.30)$$

Keeping only terms of up to the order  $\delta E^k$  :

$$\begin{aligned} \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{\Phi_{kl}^2(E^{(0)k})}{\Phi_{ll}^2(E^{(0)k})} \\ = \delta E^k \left[ \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} + \sum_{l \neq k} \frac{\Phi_{kl}^2}{\Phi_{ll}^2} \left( \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} - \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \right) - 2 \frac{\Phi_{kl}(E^{(0)k})}{\Phi_{ll}(E^{(0)k})} \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \right] . \end{aligned} \quad (5.31)$$

Then, we can solve  $\delta E_k$

$$\delta E^k = \frac{\sum_{\substack{l=1 \\ (l \neq k)}}^N \left( \frac{\Phi_{kl}^2}{\Phi_{ll}^2} \right)}{\left[ \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} + \sum_{l \neq k} \frac{\Phi_{kl}^2}{\Phi_{ll}^2} \left( \frac{\partial \Phi_{ll}}{\partial E^{(0)k}} - \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \right) - 2 \frac{\Phi_{kl}(E^{(0)k})}{\Phi_{ll}(E^{(0)k})} \frac{\partial \Phi_{kk}}{\partial E^{(0)k}} \right]} . \quad (5.32)$$

Since  $\Phi_{ll}$  is large, we may even ignore the second and third terms in the denominator so we get

$$\delta E^k \cong \frac{1}{\frac{\partial \Phi_{kk}}{\partial E^{(0)k}}} \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{\Phi_{kl}^2(E^{(0)k})}{\Phi_{ll}^2(E^{(0)k})} . \quad (5.33)$$

The equation (5.33) is our main result in this thesis. It is interesting that it contains information about the tunnelling regime.

The diagonal part is derivative with respect to  $E = E^{(0)k}$  :

$$\frac{\partial \Phi_{kk}}{\partial E} = -\sqrt{\frac{m}{2}} \frac{1}{2\hbar} (-E)^{-\frac{3}{2}} . \quad (5.34)$$

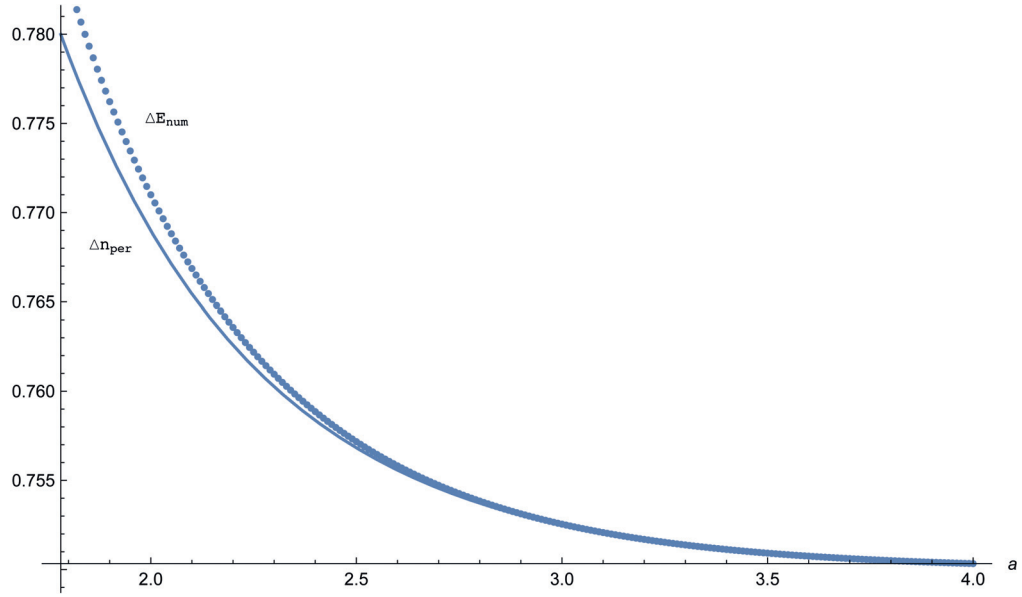


Figure 5.1. Energy Gap between the energy levels for  $N = 2$  as a function of  $a > 3/4$ .  
Here  $\hbar = 2m = 1$  and  $\lambda_1 = 1, \lambda_2 = 2$ .

Since  $E = -\frac{m\lambda_k^2}{2\hbar^2}$ , the equation (5.34) becomes ;

$$\frac{\partial \Phi_{kk}}{\partial E} = -\frac{\hbar^2}{m\lambda_k^3} . \quad (5.35)$$

Hence, substituting (5.35) and  $\Phi_{jk}$  into (5.33), we get

$$\delta E^k = -\frac{m\lambda_k}{\hbar^2} \sum_{\substack{l=1 \\ (l \neq k)}}^N \frac{\exp \left[ -\frac{2m}{\hbar^2} |a_k - a_l| \lambda_k \right]}{\frac{1}{\lambda_l} - \frac{1}{\lambda_k}} . \quad (5.36)$$

For  $N = 2$ , we can find the energy gaps between the two levels perturbatively and compare the results with the numerical computations by Mathematica. We plot the results as shown in Figure below.

## 5.2. Degenerate Case

For simplicity, let us consider  $N = 2$ ,  $\lambda_1 = \lambda_2 = \lambda$  and  $a_1 = -a$ ,  $a_2 = a$ . By the equation (5.1), we have

$$\Phi(E) = \begin{pmatrix} \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} & -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}}}{\hbar\sqrt{-E}} \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}}}{\hbar\sqrt{-E}} & \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} \end{pmatrix}. \quad (5.37)$$

Let us split the principal matrix as  $\Phi(E) = \Phi_0(E) + \delta\Phi(E)$ , where

$$\Phi_0(E) = \begin{pmatrix} \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} & 0 \\ 0 & \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}} \end{pmatrix}, \quad (5.38)$$

and

$$\delta\Phi(E) = \begin{pmatrix} 0 & -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}}}{\hbar\sqrt{-E}} \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}}}{\hbar\sqrt{-E}} & 0 \end{pmatrix}. \quad (5.39)$$

There is only one eigenvalue of  $\Phi_0$ , namely

$$w^{(0)}(E) = \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\sqrt{-E}}. \quad (5.40)$$

Recall that the bound states energies are the zeros of the eigenvalues of principal matrix  $\Phi$  so, we have

$$E^{(0)} = -\frac{m\lambda^2}{2\hbar^2}, \quad (5.41)$$

in other words  $w^{(0)}(E^{(0)}) = 0$ . We have two steps to find the corrections to the eigenvalue  $E^{(0)}$  when we add perturbation term  $\delta\Phi$ . We first need to find solve the equation (4.58)

$$\det \begin{pmatrix} -w^1 & \delta\Phi_{12} \\ \delta\Phi_{21} & -w^1 \end{pmatrix} = 0 . \quad (5.42)$$

After our calculation, we find

$$w^1(E) = \pm |\delta\Phi_{12}(E)| = \pm \sqrt{\frac{m}{2}} \frac{1}{\hbar \sqrt{-E}} e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}} , \quad (5.43)$$

where we have used  $\delta\Phi_{12} = \delta\Phi_{21}$ . Let us define

$$w_1^1(E) = -\sqrt{\frac{m}{2}} \frac{1}{\hbar \sqrt{-E}} e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}} , \quad (5.44)$$

and

$$w_2^1(E) = +\sqrt{\frac{m}{2}} \frac{1}{\hbar \sqrt{-E}} e^{-\frac{\sqrt{2m}\sqrt{-E}(2a)}{\hbar}} . \quad (5.45)$$

Next, our goal is to find how the bound state energies change under this perturbation. To do this, we need to find the zeros of eigenvalues of  $\Phi$ , that is

$$w(E) = w^{(0)} + \epsilon w^{(1)}(E) + \epsilon^2 w^{(2)}(E) + \dots = 0 . \quad (5.46)$$

Since the first order correction  $w^1 \neq 0$ , we expand  $w$  up to first order in  $\epsilon$ ,

$$w(E) = w^{(0)}(E) + \epsilon w^{(1)}(E) + O(\epsilon^2) . \quad (5.47)$$

Now, let us assume that

$$E = E^{(0)} + \epsilon E^{(1)} + \dots \quad (5.48)$$

Substituting this ansatz into above equation (5.48), we have

$$w^{(0)}(E^{(0)} + \epsilon E^{(1)} + O(\epsilon^2)) + \epsilon w^{(1)}(E^{(0)} + \epsilon E^{(1)} + O(\epsilon^2)) + O(\epsilon^2) = 0 . \quad (5.49)$$

Let us expand  $w^{(0)}$  and  $w^{(1)}$  around  $E^{(0)}$  :

$$w^{(0)}(E^{(0)} + \epsilon E^{(1)} + O(\epsilon^2)) = w^{(0)}(E^{(0)}) + (\epsilon E^{(1)} + O(\epsilon^2)) \frac{\partial w^{(0)}}{\partial E} \Big|_{E=E^{(0)}} + O(\epsilon^2) . \quad (5.50)$$

Similarly,

$$\begin{aligned} w^{(1)}(E^{(0)} + \epsilon E^{(1)} + O(\epsilon^2)) &= w^{(1)}(E^{(0)}) + (\epsilon E^{(1)} + O(\epsilon^2)) \frac{\partial w^{(1)}}{\partial E} \Big|_{E=E^{(0)}} + O(\epsilon^2) \\ &= w^{(1)}(E^{(0)}) \epsilon E^{(1)} \frac{\partial w^{(1)}}{\partial E} \Big|_{E=E^{(0)}} + O(\epsilon^2) . \end{aligned} \quad (5.51)$$

Putting equations (5.50) and (5.51) into (5.49), we get

$$\epsilon E^{(1)} \frac{\partial w^{(0)}}{\partial E} \Big|_{E=E^{(0)}} + \epsilon \left[ w^{(1)}(E^{(0)}) + \epsilon E^{(1)} \frac{\partial w^{(1)}}{\partial E} \Big|_{E=E^{(0)}} \right] + O(\epsilon^2) = 0 . \quad (5.52)$$

We only consider terms up to order  $O(\epsilon)$  :

$$E^1 = - \frac{w^{(1)}(E^{(0)})}{\frac{\partial w^{(0)}}{\partial E} \Big|_{E=E^{(0)}}} . \quad (5.53)$$

Since we have two eigenvalues  $w_1^{(1)}$  and  $w_2^{(1)}$ , we have

$$E_1^{(1)} = -\frac{w_1^{(1)}(E^{(0)})}{\left.\frac{\partial w^{(0)}}{\partial E}\right|_{E=E^{(0)}}} = -\left[\frac{\left(-\frac{1}{\lambda}\right)\exp\left(-\frac{2m\lambda a}{\hbar^2}\right)}{\frac{\hbar^2}{m\lambda^3}}\right], \quad (5.54)$$

and

$$E_2^{(1)} = -\frac{w_2^{(1)}(E^{(0)})}{\left.\frac{\partial w^{(0)}}{\partial E}\right|_{E=E^{(0)}}} = \left[\frac{\left(-\frac{1}{\lambda}\right)\exp\left(-\frac{2m\lambda a}{\hbar^2}\right)}{\frac{\hbar^2}{m\lambda^3}}\right]. \quad (5.55)$$

Hence, we can find the energy splitting using the perturbation theory

$$\delta E_{\text{perturbation}} = E_1^{(1)} - E_2^{(1)} = \frac{2m\lambda^2}{\hbar^2} e^{-\frac{2m\lambda a}{\hbar^2}}. \quad (5.56)$$

Using the exact explicit solutions for the bound state energies for this degenerate two center problem given in (3.34), the exact splitting in the bound state energies is given by

$$\begin{aligned} \delta E_{\text{exact}} = & -\left[\sqrt{\frac{m}{2}}\frac{\lambda}{\hbar} + \frac{\hbar}{\sqrt{2m}(2a)}W\left(\frac{m\lambda(2a)}{\hbar^2}e^{-\frac{m\lambda(2a)}{\hbar^2}}\right)\right]^2 \\ & + \left[\sqrt{\frac{m}{2}}\frac{\lambda}{\hbar} + \frac{\hbar}{\sqrt{2m}(2a)}W\left(-\frac{m\lambda(2a)}{\hbar^2}e^{-\frac{m\lambda(2a)}{\hbar^2}}\right)\right]^2. \end{aligned} \quad (5.57)$$

We are not going to study the general error analysis in a rigorous way but we can find show the error between the exact and the perturbative result for this special case. This can be illustrated by simply plotting the exact energy splitting formula and energy splitting formula obtained by perturbative approach as a function of  $a$  with fixed  $\lambda$  (See Fig. 5.2).

The error is getting smaller as the distance between the centers increases, as expected.

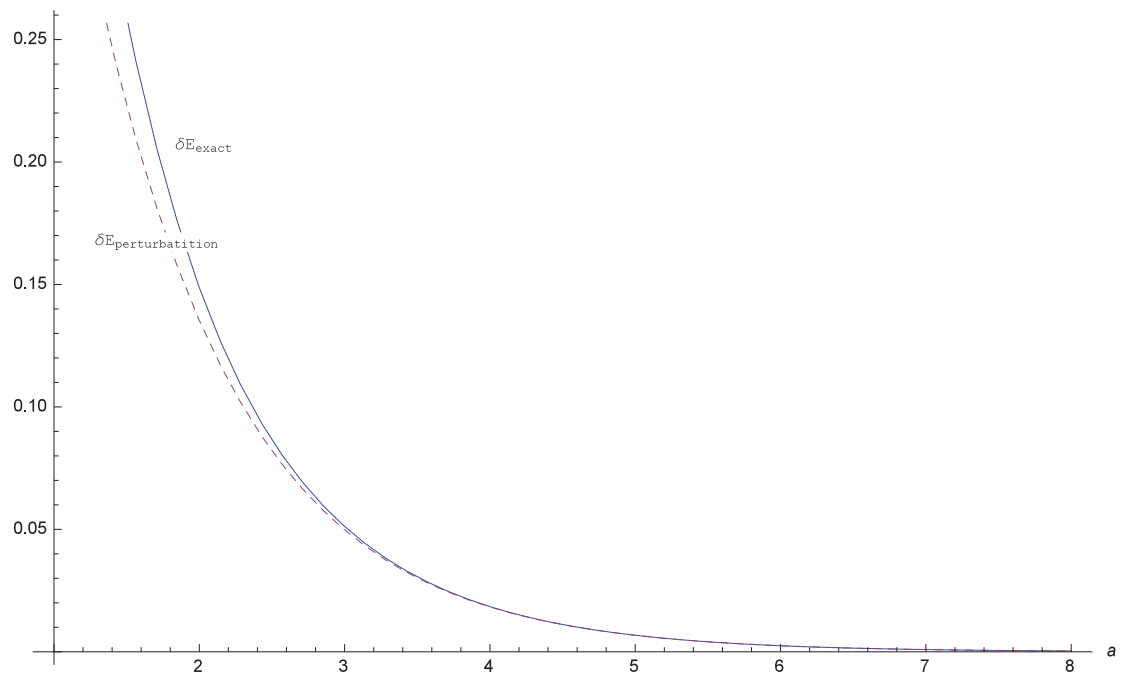


Figure 5.2. The comparison of exact and perturbative results for the energy splitting as a function of  $a$  for  $\lambda = 1$  in the units  $\hbar = 2m = 1$ .

## CHAPTER 6

### CONCLUSION

An estimate for the gap and the splitting in the bound state energies for the sufficiently separated multiple Dirac delta potentials is given by using the perturbation theory, which is applied to a finite dimensional matrix. Moreover, the solution to the stationary scattering problem for the same system is obtained using the distributional solution of the Schrödinger equation in momentum space. All the necessary tools, e.g., some elementary definitions and results in distribution theory, first order and second order perturbation formulas for symmetric matrices, are also summarized for the completeness of the thesis. The methodology discussed in this thesis can be generalized to the more general singular interactions, such as point interactions in higher dimensions, delta potentials supported by curves and surfaces.



## APPENDIX A

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 $\mathfrak{g}5[k_, \lambda_, a_] :=$ 
  Table[If[l  $\neq$  j,  $-\left(\frac{i}{2k}\right) \text{Exp}[-i k \text{Indexed}[\{0, 2 a, 4 a, 6 a, 8 a\}, \text{Abs}[l - j] + 1]]$ ,  $\frac{1}{\lambda} - \frac{i}{2k}$ ],
    {j, 5}, {l, 5}];
InvPh5[k_,  $\lambda$ _, a_] := Inverse[ $\mathfrak{g}5[k, \lambda, a]$ ];
t5[k_,  $\lambda$ _, a_] :=
  1 +
   $\sum_{l=1}^5 \sum_{j=1}^5 \left(\frac{i}{2k}\right) \text{Exp}[-i k \text{Indexed}[\{0, 2 a, 4 a, 6 a, 8 a\}, j]] (\text{InvPh5}[k, \lambda, a][[j, l]])$ 
  Exp[i k Indexed[{0, 2 a, 4 a, 6 a, 8 a}, l]];
Plot[Abs[t5[k, 5, 1]]2, {k, 0, 10}, PlotRange  $\rightarrow$  {0, 1}]

```

## REFERENCES

- Ablowitz, M. J., A. S. Fokas, and A. S. Fokas (2003). *Complex variables: introduction and applications*. Cambridge University Press.
- Adhikari, S. K. and T. Frederico (1995). Renormalization group in potential scattering. *Physical Review Letters* 74(23), 4572.
- Albeverio, S., F. Gesztesy, R. Hoegh-Krohn, and H. Holden (1988). *Solvable Models in Quantum Mechanics*. Springer.
- Albeverio, S. and P. Kurasov (2000). *Singular Perturbations of Differential Operators: Solvable Schrödinger-type Operators*, Volume 271. Cambridge University Press.
- Altunkaynak, I. B. (2005, 8). Spectral and scattering properties of point interactions. Master's thesis, Boğaziçi University.
- Appel, W. (2007). *Mathematics for Physics and Physicists*. Princeton University Press.
- Balakrishnan, V. (2003). All about the dirac delta function (?). *Resonance* 8(8), 48–58.
- Bender, C. M. and S. A. Orszag (2013). *Advanced mathematical methods for scientists and engineers I: Asymptotic methods and perturbation theory*. Springer Science & Business Media.
- Bethe, H. and R. Peierls (1935). Quantum theory of the dipton. *Proceedings of the Royal Society of London. Series A-Mathematical and Physical Sciences* 148(863), 146–156.
- Bransden, B. and C. Joachain (2000). *Quantum Mechanics* ,(Harlow, United Kingdom. Pearson Education),(Original work published 1989).
- Brown, J. W., R. V. Churchill, et al. (2009). *Complex Variables and Applications*. Boston: McGraw-Hill Higher Education.

- Cacciapuoti, C. (2005). *Point Interactions in Quantum Mechanics and Acoustics*. Ph. D. thesis, Ph. D. Thesis, Università Degli Studi Di Napoli Federico II.
- Coleman, S. (1988). *Aspects of symmetry: selected Erice lectures*. Cambridge University Press.
- Corless, R. M., G. H. Gonnet, D. E. Hare, D. J. Jeffrey, and D. E. Knuth (1996). On the lambert w function. *Advances in Computational mathematics* 5(1), 329–359.
- Debnath, L., P. Mikusinski, et al. (2005). *Introduction to Hilbert Spaces with Applications*. Academic Press.
- Demkov, Y. N. and V. Ostrovskii (1988). *Zero-Range Potentials and Their Applications in Atomic Physics*. Springer.
- Dijk, G. (2013). *Distribution theory*. de Gruyter.
- Erman, F. (2010, 7). *Heat Kernel Methods in Many Body Problems*. Ph. D. thesis, Boğaziçi University.
- Erman, F., M. Gadella, and H. Uncu (2018). On scattering from the one-dimensional multiple dirac delta potentials. *European Journal of Physics* 39(3), 035403.
- Erman, F. and O. T. Turgut (2010). Point interactions in two-and three-dimensional riemannian manifolds. *Journal of Physics A: Mathematical and Theoretical* 43(33), 335204.
- Erman, F. and O. T. Turgut (2019). A perturbative approach to the tunneling phenomena. *Frontiers in Physics* 7, 69.
- Faddeev, L. D. and O. A. Yakubovskii (2009). *Lectures on Quantum Mechanics for Mathematics Students*, Volume 47. American Mathematical Society.
- Garg, A. (2000). Tunnel splittings for one-dimensional potential wells revisited. *American Journal of Physics* 68(5), 430–437.

- Gopalakrishnan, S. (2006). *Self-adjointness and the Renormalization of Singular Potentials*. Ph. D. thesis, Amherst College.
- Gosdzinsky, P. and R. Tarrach (1991). Learning quantum field theory from elementary quantum mechanics. *American Journal of Physics* 59(1), 70–74.
- Griffiths, D. J. and D. F. Schroeter (2018). *Introduction to Quantum Mechanics*. Cambridge University Press.
- Gustafson, S. J. and I. M. Sigal (2011). *Mathematical Concepts of Quantum Mechanics*. Springer Science & Business Media.
- Harrell, E. M. (1980). Double wells. *Communications in Mathematical Physics* 75(3), 239–261.
- Huang, K. (1992). *Quarks, Leptons & Gauge Fields*. World Scientific.
- Jackiw, R. (1991). Delta-function potentials in two-and three-dimensional quantum mechanics. *MAB Bég memorial volume*, 25.
- Kanwal, R. P. (2012). *Generalized Functions, Theory and Applications*. Springer Science & Business Media.
- Kato, T. (2013). *Perturbation theory for linear operators*, Volume 132. Springer Science & Business Media.
- Kızılkaya, M. (2020). Two-particle schrodinger operators with point interactions. Master’s thesis, Izmir Institute of Technology.
- Kreyszig, E. (1978). *Introductory Functional Analysis with Applications*, Volume 1. Wiley New York.
- Kronig, R. d. L. and W. G. Penney (1931). Quantum mechanics of electrons in crystal lattices. *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character* 130(814), 499–513.

- Landau, L. D. and E. M. Lifshitz (2013). *Quantum mechanics: non-relativistic theory*, Volume 3. Elsevier.
- Lieber, M. (1975). Quantum mechanics in momentum space: An illustration. *American Journal of Physics* 43(6), 486–491.
- Manuel, C. and R. Tarrach (1994). Perturbative renormalization in quantum mechanics. *Physics Letters B* 328(1-2), 113–118.
- Mead, L. R. and J. Godines (1991). An analytical example of renormalization in two-dimensional quantum mechanics. *American Journal of Physics* 59(10), 935–937.
- Meyer, C. D. (2000). *Matrix analysis and applied linear algebra*, Volume 71. Siam.
- Mitra, I., A. DasGupta, and B. Dutta-Roy (1998). Regularization and renormalization in scattering from dirac delta potentials. *American Journal of Physics* 66(12), 1101–1109.
- Murdock, J. A. (1999). *Perturbations: theory and methods*. SIAM.
- Nyeo, S.-L. (2000). Regularization methods for delta-function potential in two-dimensional quantum mechanics. *American Journal of Physics* 68(6), 571–575.
- Perez, J. F. and F. A. B. Coutinho (1991). Schrödinger equation in two dimensions for a zero-range potential and a uniform magnetic field: An exactly solvable model. *American Journal of Physics* 59(1), 52–54.
- Phillips, D. R., S. R. Beane, and T. D. Cohen (1998). Nonperturbative regularization and renormalization: Simple examples from nonrelativistic quantum mechanics. *Annals of Physics* 263(2), 255–275.
- Poincaré, H. (1893). *Les méthodes nouvelles de la mécanique céleste: Méthodes de MM. Newcomb, Glydén, Lindstedt et Bohlin. 1893*, Volume 2. Gauthier-Villars it fils.
- Puiseux, V. (1850). *Recherches sur les fonctions algébriques*.

- Rajeev, S. G. (1999). Bound states in models of asymptotic freedom. *arXiv preprint hep-th/9902025*.
- Reed, M. and B. Simon (1978). *IV: Analysis of Operators*, Volume 4. Elsevier.
- Rellich, F. and J. Berkowitz (1969). *Perturbation theory of eigenvalue problems*. CRC Press.
- Rorres, C. (1974). Transmission coefficients and eigenvalues of a finite one-dimensional crystal. *SIAM Journal on Applied Mathematics* 27(2), 303–321.
- Schmalz, J. A., G. Schmalz, T. E. Gureyev, and K. M. Pavlov (2010). On the derivation of the green’s function for the helmholtz equation using generalized functions. *American Journal of Physics* 78(2), 181–186.
- Shankar, R. (2012). *Principles of Quantum Mechanics*. Springer Science & Business Media.
- Surace, S. C. (2010). Point interactions in nonrelativistic quantum mechanics. *Bachelor Thesis, Bern* 5.
- Thomas, L. H. (1935). The interaction between a neutron and a proton and the structure of  $h^3$ . *Physical Review* 47(12), 903.
- Thorn, C. (1979). Quark confinement in the infinite-momentum frame. *Physical Review D* 19(2), 639.
- Tunalı, S. (2014). Point interactions in quantum mechanics. Master’s thesis, Izmir Institute of Technology.
- Uncu, H., H. Erkol, E. Demiralp, and H. Beker (2005). Solutions of the schrödinger equation for dirac delta decorated linear potential. *Central European Journal of Physics* 3(2), 303–323.
- Valluri, S. R., D. J. Jeffrey, and R. M. Corless (2000). Some applications of the lambert

$w$  function to physics. *Canadian Journal of Physics* 78(9), 823–831.