

POINT INTERACTIONS IN QUANTUM MECHANICS

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ABSTRACT

POINT INTERACTIONS IN QUANTUM MECHANICS

In this thesis, the point interactions in quantum mechanics in the context of renormalization are reviewed. Some spectral properties for special configuration of the centers of point interactions are given in detail. Also, the isotropic harmonic oscillator with point interaction in one dimension and in two dimensions are discussed shortly.

ÖZET

KUANTUM MEKANİĞİNDE NOKTA ETKİLEŞİMLER

Bu tezde, renormalizasyon çerçevesi içerisinde kuantum mekaniğindeki noktasal etkileşimler gözden geçirilmiştir. Noktasal etkileşimlerin merkezlerinin özel konfigürasyonları için, bazı spektral özellikleri detaylı biçimde verilmiştir. Ayrıca, bir ve iki boyuttaki noktasal etkileşim içeren izotropik harmonik salınıcı kısaca tartışılmıştır.

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LIST OF SYMBOLS

Δ : Laplacian

\hbar : Reduced Planck's constant

$\delta^{(D)}(\mathbf{x})$: Dirac delta function in \mathbb{R}^D

Φ_{ij} : The (renormalized) principal matrix

A_i : Eigenvector of the (renormalized) principal matrix

$\mathcal{D}(H_0)$: Domain of H_0

$\Theta_\Lambda(\mathbf{p})$: The characteristic function

$Ran(H)$: Range of the operator H

$Ker(H)$: Kernel of the operator H

$R(\mathbf{x}, \mathbf{y}; E)$: Resolvent kernel in coordinate representation

$R(\mathbf{p}, \mathbf{q}; E)$: Resolvent kernel in momentum representation

$K_t(\mathbf{x}, \mathbf{y})$: Heat kernel

$J_0(x)$: Bessel function of the first kind

$K_\nu(x)$: Modified Bessel function of the third kind

$H_0^{(1)}(z)$: Hankel function of the first kind of order zero

$\Gamma(z)$: Gamma function

$B(x, y)$: Beta function

$\Psi(x)$: Digamma function

${}_1F_1(a; b; c)$: Confluent hypergeometric functions of the first kind

CHAPTER 1

INTRODUCTION

In this thesis, we present an elementary study of point interactions in quantum mechanics (especially in two dimensions) from a non-perturbative renormalization point of view. The point interactions are formally described by the following Schrödinger operator with potential energy term (delta function) supported on discrete set of points (sometimes called centers)

$$-\frac{\hbar^2}{2m}\Delta - \sum_{i=1}^N \lambda_i \delta^{(D)}(\mathbf{x} - \mathbf{a}_i) , \quad (1.1)$$

where Δ is the self-adjoint Laplacian in $L^2(\mathbb{R}^D)$ and $D = 1, 2, 3$ is the dimension of the underlying space, λ_i 's are called the coupling constant or strength of the potential (assumed to be positive throughout the thesis unless otherwise stated), $\delta^{(D)}(\mathbf{x} - \mathbf{a}_i)$ is the Dirac delta function centered at \mathbf{a}_i ($\delta_{\mathbf{a}_i}(\cdot)$ is another notation which is also commonly used). Such point interactions are considered to represent many physical systems quantitatively if the de-Broglie wavelength of the particle is much larger than the range of the potential. The studies on the applications of the above model Hamiltonian or its various modifications are well-known in wide range of areas of physics from atomic physics, to molecular physics and nuclear physics (Demkov & Ostrovskii, 1988) (Uncu, 2007) (Cacciapuoti, 2005). One of the most well-known example to such models is Kronig-Penney model in solid state physics (Kronig & Penney, 1931) (Kittel, 2005). It is essentially based on a Hamiltonian with infinitely many periodic point interactions in one dimension, which describes a non-relativistic electron moving in a fixed crystal lattice. What makes this model very interesting is the fact that it explains the energy band structure of solids very well and it is exactly solvable.

The higher-dimensional extensions were first studied by Bethe and Peierls (Bethe & Peierls, 1935) and separately by Thomas (Thomas, 1935) to describe the interaction between proton and neutron in the nucleus by a zero range potential in three dimensions. Bethe and Peierls gave a boundary condition on the wave function which corresponds to delta potential in three dimensions. But it was Thomas who realized the necessity of the renormalization of the coupling constant and he approximated the Hamiltonian (1.1) by short range scaled potentials. Then, starting from 1930's these two works and Fermi's work which describes the motion of neutrons in hydrogenous substances (Fermi, 1962) in nuclear physics stimulated tremendous developments in this field and the extension of the many-body versions of the model started

to develop in 1950's. An extensive discussion on the historical development and its various applications of the subject with a long list of references is given in the introduction to the monograph (Albeverio & Gesztesy & Høegh-Krohn & Holden & Exner, 1988).

The generalization of Kronig-Penney model into two and three dimensions is also possible and studied in (Maleev, 1966) (Berezin, 1986) after the above developments.

Let us first explain why the above model Hamiltonian is problematic from the physical point of view in two dimensions by using a simple scaling argument. For simplicity, we consider only one center and choose its center as the origin. Then, the time-independent Schrödinger equation for the above Hamiltonian reads

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x}) - \lambda\delta^{(2)}(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}) , \quad (1.2)$$

where $E = -\nu^2$ for bound states ($\nu > 0$). One can show that under the formal scaling transformation $\mathbf{x} \rightarrow \eta\mathbf{x}$ by some positive constant η , that the left hand side is scaled by a factor $1/\eta^2$ and using the scaling properties of delta functions and wave function in two dimensions (from the normalization). This give rises to the conclusion that we have formally the same Schrödinger equation except for the bound state energy is scaled by a factor η^2 . However, if you suppose that there exists a ground state with energy $-\nu_{gr}^2$, there should also exist another ground state energy $-\eta^2\nu_{gr}^2$. Since the scaling parameter η is arbitrary, the bound state energy can be lowered as much as we like, which essentially says that the ground state is unbounded from below, i.e., $E_{gr} \rightarrow -\infty$. This is completely unacceptable from physical point of view. Though one dimensional problem is completely well understood, the two-dimensional problem becomes ill-defined in this perspective. Actually, the problem still exists in higher dimensions as well although the nature of the problem is quite different from its two-dimensional counterpart. In higher dimensions, if the potential term is more singular than the kinetic term, the Hamiltonian is not self-adjoint any more and ill-defined so the formal Hamiltonian has to be modified to make it meaningful since dynamics in quantum mechanics is generated by the self-adjoint Hamiltonian. Therefore, point interactions in more than one dimension that are as singular as kinetic term or more singular than that in higher dimensions leads to infinite expressions as we shall see in the thesis. In order to be able to cure the above-mentioned problem, one may consult the resolution of a similar problem appeared in quantum field theory, namely renormalization.

First step to cure the above trouble is to smooth out the singularity at short distances by assuming that the the form of the potential is only valid down to a scale which we can not access physically. That scale is called cut-off. This part of the procedure is known as regularization. Then we have to deduce the physics of the problem in shorter distances by

assuming the every physical quantity is finite or make sense from some experimentally measured quantity (e.g., bound state energy or phase shift in the scattering process). Once we have the experimentally measured result and the long distance behavior of the problem, the short distance behavior (or equivalently high energy behavior) can be predicted uniquely, which makes the renormalization procedure remarkable (For example, the magnetic dipole moment of the electron calculated from the renormalization procedure in quantum electrodynamics confirmed the experimental result within 14 significant digits!, see (Kraus & Griffiths, 1992) for a rather pedagogical introduction to renormalization in quantum field theory).

There are various works on the renormalization of point interactions in physics literature from the several points of view. In (Gosdzinsky & Tarrach, 1991) (Manuel & Tarrach, 1994) (Mead & Godines, 1991) (Perez & Coutinho, 1991), different regularization schemes is performed in coordinate space or in momentum space (Thorn, 1979) (Huang, 1982) (Jackiw, 1991) (Philips & Beane & Cohen, 1998) (Mitra & DasGupta & Dutta-Roy, 1998) (Henderson & Rajeev, 1998) (Nyeo, 2000) (Adhikari & Frederico, 1995). The path integral approach of the two-dimensional case has been also discussed in (Camblong & Ordóñez, 2002). Moreover, the two-dimensional delta potentials is an explicit example of the dimensional transmutation and quantum mechanical symmetry breaking or anomaly. The renormalization inserts a scale into the problem by hand (by experimentally measured quantity), thus breaking the formal scale invariance of the Hamiltonian at the outset. This phenomenon is known as anomaly in quantum mechanics or quantum mechanical symmetry breaking (Holstein, 1993,J) and is an example of dimensional transmutation (Thorn, 1979) (Huang, 1982) (Coleman & Weinberg, 1973) (Camblong & Epele & Fanchiotti & Canal, 2001) (Camblong & Epele & Fanchiotti & Canal, 2001). It occurs when a dimensionless quantity (e.g.,coupling constant) is traded in for a quantity with a dimensional parameter (e.g., the experimentally measured bound state energy). A rather elementary problem in quantum mechanics provides an explicit example for several quantum field theoretical concepts such as regularization, renormalization, dimensional transmutation, quantum anomaly, exact non-perturbative solutions to renormalization group equations, etc. Therefore, working out the details of point interactions in quantum mechanics may help us to understand better the awkward renormalization procedure in a more elementary context rather than field theory, hoping to put the formalism in a mathematically rigorous setting. An another important-aspect of point interactions is that they can be exactly solvable, that is, the resolvent can be explicitly calculated in terms of the location and the strength of the centers (Albeverio & Gesztesy & Høegh-Krohn & Holden & Exner, 1988).

If we go back to the historical development for the point interactions, there were an another direction for their treatment in the rigorous mathematical setting, which was first studied by Berezin and Faddeev (Berezin & Faddeev, 1961) for three-dimensional case. In this

approach, the Hamiltonian which represents heuristic expression (1.1) is rigorously defined as a self-adjoint extension of Laplace operator in $L^2(\mathbb{R}^3)$ from the point of view of Krein's theory of self-adjoint extensions of symmetric operators (Albeverio & Kurasov, 2000), where a relation between the resolvent of the different self-adjoint extensions of a given symmetric operator is given. A detailed exposition of this subject from other points of view (in terms of quadratic forms, nonstandard analysis, and Von Neumann's approach to self-adjoint extensions of symmetric operators) has been extensively discussed in the monograph (Albeverio & Gesztesy & Høegh-Krohn & Holden & Exner, 1988). Actually, even in one dimension, the Hamiltonian given in (1.1) is ill-defined since the expression $\delta(x - a_i)$ is not even an operator in $L^2(\mathbb{R})$. One proper way to define point interactions in one dimension rigorously is by considering the Hamiltonian as a perturbation of a self-adjoint Laplace operator by a quadratic form. Then using the KLMN theorem, the meaning of $-\frac{\hbar^2}{2m}\Delta - \lambda_i\delta(x - a_i)$ is established (Reed & Simon, 1975). Dirac delta potential and the equivalent self-adjoint extension has been discussed in the context of point particle dynamics in (2+1)-dimensional gravity (Gerbert & Jackiw, 1989) and in Chern-Simons gauge theory (Aharonov-Bohm/Ehrenberg-Siday interaction) (Gerbert, 1989). There is yet another approach to give the expression (1.1) a well-defined meaning by constructing the resolvent by suitable limits of the regularized resolvents given by S.G. Rajeev (Rajeev, 1999).

S.G. Rajeev (Rajeev, 1999) developed a non-perturbative renormalization method of point interactions which can also be applied to some simple field theories by hoping that these ideas will work in more realistic situations and the cases where standard perturbative approaches do not work, such as in QCD. The basic idea in his work (Rajeev, 1999) is based on finding a way for a finite expression of the resolvent in terms of a new operator, called principal operator $\Phi(E)$ (it is going to be a matrix or a function depending on the number of centers) as a proper limit of the regularized resolvent of the regularized Hamiltonian given formally at the beginning after the renormalization procedure. (At the end of this procedure the model is free of divergences without any explicit expression of Hamiltonian despite the well-defined resolvent expression.) Nevertheless, it is sufficient to know the resolvent because it contains all the information about the spectrum. One advantage of this point of view is that there are no subtleties in the definition of the domain of Hamiltonian as in the self-adjoint extension method. Secondly, the renormalization is performed without actually solving the dynamics of the problem as opposed to the standard perturbative treatment given in quantum field theory. Once we have a finite expression of the principal matrix, the spectral information can be obtained exactly or approximately. The complete information about the system is hidden in the resolvent formula and the interaction is described by an explicit expression for $\Phi(E)$. The eigenvalues of the bound state energies are given by the solutions to $\Phi(E)A = 0$ and the scattering amplitude is determined by the inverse of $\Phi(E)$. No matter how complicated

the equation is, some approximation methods (variational principles, perturbation theory) can be applied to the principal matrix. Actually, this formulation also admits an extension of the model to Riemannian manifolds and even in this case, it has been proved that there exists a densely-defined self-adjoint operator, say H , after the renormalization procedure even if we do not know what the exact formal expression is (Dogan & Erman & Turgut, 2012).

In this thesis, we follow the Rajeev's approach and study the point interactions from a non-perturbative renormalization point of view without worrying about the issue of the domains of the operator to find the self-adjoint extension of the free Hamiltonian. Instead of constructing the self-adjoint extension, we are going to give an explicit expression of the resolvent (which corresponds to densely-defined self-adjoint Hamiltonian) after taking the suitable limit of the regularized resolvent associated to the given formal regularized Hamiltonian by renormalizing the coupling constant.

We now give the content and the organization of this thesis as follows.

In Chapter 2, we first give the heuristic definition of the Dirac delta functions. Secondly, the theory of the distributions and the Fourier transform of the distributions are briefly introduced. Lastly, the Dirac Calculus, which is very useful in our calculations, is given.

In Chapter 3, we summarize some basics notions in quantum mechanics that we need in this thesis. Then we formally discuss one-dimensional time-independent Schrödinger equation with point interaction for bound states and scattering states by using Fourier transformation. The bound state solution for finitely many point δ -interactions are also investigated. Two-center case is discussed in detail. Then, two-dimensional point interactions are formally investigated by introducing the renormalization idea. We also discuss finitely many point interactions in two dimensions and study the bound state spectrum. When the delta centers are located at the vertices of a equilateral triangle and square, the bound state problem is also analyzed and an explicit expression for the principal matrix is given.

In Chapter 4, we briefly introduce the notion of resolvent with the basic properties and the related theorems. We find the resolvent of one-dimensional time-independent Schrödinger equation with point interaction and find the resolvent kernel. So, we immediately have the bound state energy and by using the Riesz integral representation, we find the corresponding wave function. We apply this procedure to our system with point interaction and finitely many point interactions for two-dimensional case (here we do renormalization again). We find a lower bound for the ground state energy for finitely many Dirac delta centers in two dimensions and show that the ground state wave function corresponding to this system is positive and non-degenerate. We also prove that there exist at most N bound states for this system.

In Chapter 5, we review the heat kernel in one dimension and two dimensions and then we give the heat kernel eigenfunction expansion. In terms of this expansion, we find

the heat kernel of the harmonic oscillator in one dimension. We solve one-dimensional time-independent Schrödinger equation with point interaction and harmonic oscillator and examine the spectrum case by case. We also discuss the two-dimensional version of this problem and find the resolvent. A very short analysis of the bound state of the system is discussed.

Proofs of some theorems and formulas used in the thesis are explicitly given in Appendices.

CHAPTER 2

DIRAC DELTA DISTRIBUTIONS

We shall first give a heuristic motivation to define Dirac delta functions and then shortly introduce the theory of distributions.

2.1. Heuristic Way of Defining Dirac Delta Functions

Suppose that $f(x)$ is a function defined on the real axis. We ask the following question: Can we construct a kind of filter, say δ , such that it selects the value of the function at any given point x_0 (see Figure 2.1)? (Balakrishnan, 2003)

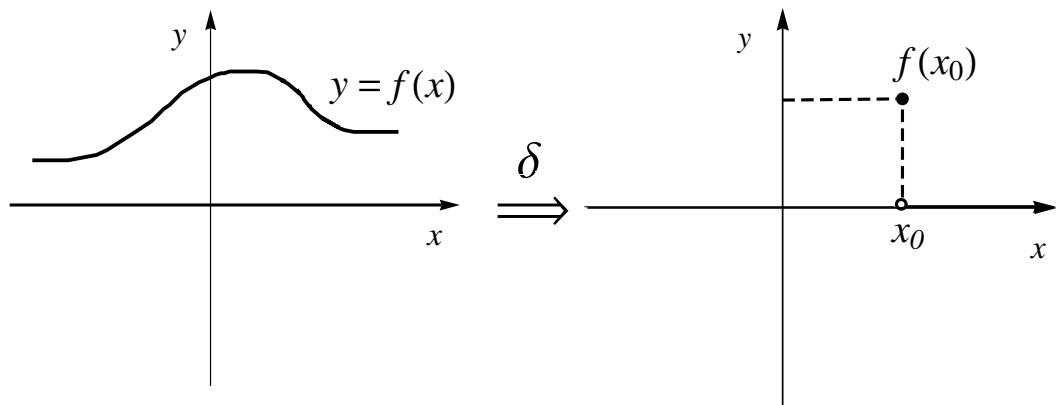


Figure 2.1. δ filter

In order to answer this question, it is a good idea to start with the discrete analog of the question. Suppose that we have a sequence $\{f_j\}_{j=1}^{\infty}$ rather than a function $f(x)$. Then, the above question becomes: Can we construct a kind of filter, say δ , such that it selects a

particular member f_i from the given sequence? If we define

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases} \quad (2.1)$$

then, it follows that

$$\sum_{j=1}^{\infty} \delta_{ij} f_j = f_i. \quad (2.2)$$

Here the filter δ_{ij} is called the Kronecker delta symbol. It has the following properties:

- The normalization property:

$$\sum_{j=1}^{\infty} \delta_{ij} = 1, \quad (2.3)$$

for each value of i .

- The symmetry property:

$$\delta_{ij} = \delta_{ji}. \quad (2.4)$$

Now, we replace the discrete indices i, j by continuous variables x_0, x and the summation over j by an integral over x . The point x_0 in the continuous problem is the analog of the index i in the discrete problem. So, we are looking for a “function” $\delta_{x_0}(x)$ such that

$$\int_{\mathbb{R}} \delta_{x_0}(x) f(x) dx = f(x_0), \quad (2.5)$$

for a given continuous function $f(x)$. The continuous analogs of the normalization and symmetry properties of Kronecker delta symbol must be

- $\int_{\mathbb{R}} \delta_{x_0}(x) dx = 1.$ (2.6)

and

$$\bullet \delta_{x_0}(x) = \delta_x(x_0) . \quad (2.7)$$

The above symbol $\delta_{x_0}(x)$ is known as the Dirac delta function introduced by Dirac (Dirac, 1958), Kirchoff and Heaviside. (An another notation for Dirac delta function $\delta_{x_0}(x)$ is also widely used: $\delta_{x_0}(x) = \delta(x - x_0)$.) The form of Eq. (2.5) looks like the kernel of an integral operator and we can intuitively think that $\delta_{x_0}(x)$ must almost vanish except at x_0 to satisfy (2.5). But this is not so obvious if $\delta_{x_0}(x)$ is considered to be an ordinary function. The next natural question is that how does the Dirac delta function defined above look like? Consider a rectangular window function

$$W_{x_0}^\epsilon(x) = \begin{cases} \frac{1}{2\epsilon} & \text{if } x_0 - \epsilon < x < x_0 + \epsilon , \\ 0 & \text{otherwise} , \end{cases} \quad (2.8)$$

which is shown in the red color in Figure 2.2. The integral of $f(x)$ weighted with this window function $W_{x_0}^\epsilon(x)$, is simply

$$\int_{\mathbb{R}} W_{x_0}^\epsilon(x) f(x) dx = \frac{1}{2\epsilon} \int_{x_0 - \epsilon}^{x_0 + \epsilon} f(x) dx . \quad (2.9)$$

Of course, this does not select $f(x_0)$ alone. But, it is going to do so as $\epsilon \rightarrow 0$ by using the mean value theorem, namely

$$\lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} (2\epsilon f(\xi)) = f(x_0) , \quad (2.10)$$

where $x_0 - \epsilon < \xi < x_0 + \epsilon$. In this limit, the width of the window goes to zero and its height becomes arbitrarily large, so as to catch all of the ordinate in the graph of $f(x)$. Then, $\delta_{x_0}(x)$ is given by

$$\delta_{x_0}(x) = \begin{cases} \lim_{\epsilon \rightarrow 0} \left(\frac{1}{2\epsilon} \right) & \text{for } x_0 - \epsilon < x < x_0 + \epsilon , \\ 0 & \text{otherwise} . \end{cases} \quad (2.11)$$

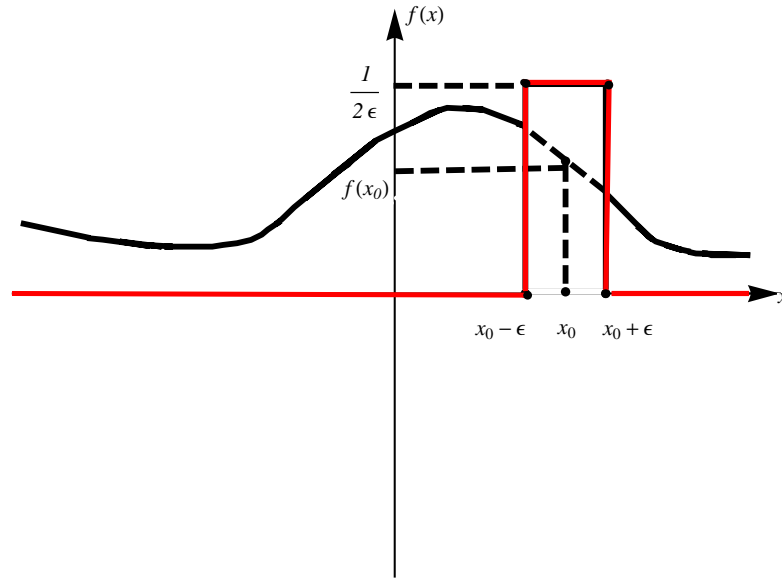


Figure 2.2. Window function

This is not a rigorous definition. If it is taken literally, then $\delta_{x_0}(x)$ must be zero for all $x \neq x_0$ while it must be infinite at $x = x_0$. The Dirac delta function is always to be understood as something that only makes sense when it appears in an integral. Hence, the Dirac delta function can be understood in the following way:

$$\int_{\mathbb{R}} \delta_{x_0}(x) f(x) dx = \lim_{\epsilon \rightarrow 0} \int_{\mathbb{R}} W_{x_0}^\epsilon(x) f(x) dx = f(x_0), \quad (2.12)$$

or

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}} W_{x_0}^n(x) f(x) dx = f(x_0), \quad (2.13)$$

for a continuous function $f(x)$ and the sequence satisfies

$$\int_{\mathbb{R}} W_{x_0}^n(x) dx = 1, \quad (2.14)$$

and each number of the sequence has a peak at x_0 . Also, they are symmetric about the point x_0 .

The definition of Dirac delta function, given in terms of the sequence of functions, can be easily generalized for any dimension D :

$$\int_{\mathbb{R}^D} \delta_{\mathbf{r}_0}^{(D)}(\mathbf{r}) f(\mathbf{r}) d^D r = \lim_{n \rightarrow \infty} \int_{\mathbb{R}^D} W_{\mathbf{r}_0}^n(\mathbf{r}) f(\mathbf{r}) d^D r = f(\mathbf{r}_0), \quad (2.15)$$

where $d^D r = dx^1 dx^2 \dots dx^D$. In physics literature, the following notation is used for the Dirac delta functions

$$\delta_{\mathbf{r}_0}^{(D)}(\mathbf{r}) = \delta^{(D)}(\mathbf{r} - \mathbf{r}_0). \quad (2.16)$$

2.2. Distributions and Some Useful Properties

L. Schwartz (Schwartz, 1966) and I. Gelfand (Gelfand & Shilov, 1964) showed that the above heuristic approach for defining the Dirac delta functions could be justified in a rigorous way and the theory they constructed are called the theory of distributions or generalized functions. The idea is basically as follows. For simplicity, let us choose $x_0 = 0$. We are going to construct a mathematical filter “ δ ” acting on a continuous function f which gives its value at $x = 0$. That means (Appel, 2007)

$$\delta(f) = f(0) \quad \text{or} \quad \langle \delta, f \rangle = f(0). \quad (2.17)$$

The above rule happens to be linear as a function of f , so it is natural that the filter δ is a mapping from a certain vector space of functions to complex numbers.

$$\begin{aligned} \delta : \text{space of functions} &\longrightarrow \mathbb{C} \\ \text{function} &\longmapsto \text{number}. \end{aligned} \quad (2.18)$$

This object δ is called a linear functional on space of functions. To be more precise, one has to specify the space of functions on which this functional is defined. The notation $\langle \delta, f \rangle$ should not be confused with the inner product.

Definition 2.1 *The support of a function f is the closure of the set where it is non-zero*

(Gustafson & Sigal, 2011):

$$\text{supp}(f) := \overline{\{\mathbf{x} \in \mathbb{R}^D : f(\mathbf{x}) \neq 0\}} . \quad (2.19)$$

Definition 2.2 (Appel, 2007)

Let $D \geq 1$. The test space, denoted by $\mathcal{D}(\mathbb{R}^D)$, is the vector space of functions φ from \mathbb{R}^D into \mathbb{C} , which are class of C^∞ and have bounded support. A test function is any function $\varphi \in \mathcal{D}(\mathbb{R}^D)$.

Example 2.1 One of the examples of a test function is given by (Debnath & Mikusiński, 2005)

$$\varphi(x) = \begin{cases} e^{(x^2-1)^{-1}} & \text{if } |x| < 1 , \\ 0 & \text{otherwise .} \end{cases} \quad (2.20)$$

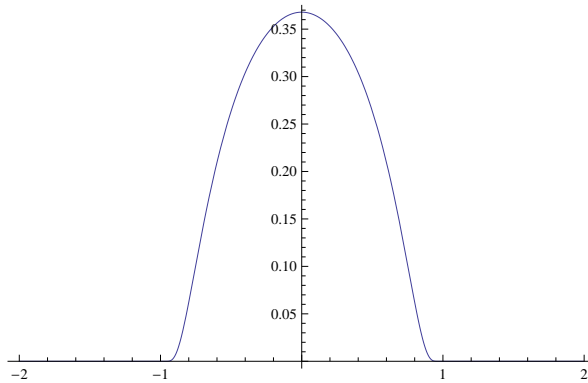


Figure 2.3. An example for a test function

Remark 2.1 One useful property of the above test functions is that when we perform integration by parts, the boundary terms vanish. The reason why we have restrictions in defining \mathcal{D} is due to the fact that the dual of \mathcal{D} gets “bigger” in contrast to the case in finite dimensions. The restriction C^∞ regularity is necessary but the condition of bounded supportness can be relaxed, as we will see later on.

Definition 2.3 (Debnath & Mikusiński, 2005)

A linear functional T on the space $\mathcal{D}(\mathbb{R}^D)$ is a rule by which we assign to every test function

φ a real number denoted $\langle T, \varphi \rangle$, such that

$$\langle T, c_1\varphi_1 + c_2\varphi_2 \rangle = c_1\langle T, \varphi_1 \rangle + c_2\langle T, \varphi_2 \rangle , \quad (2.21)$$

for arbitrary test functions φ_1 and φ_2 .

Definition 2.4 (Appel, 2007)

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

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

Definition 2.5 (Kanwal, 2004)

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

Definition 2.6 (Appel, 2007)

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

Any locally integrable function defines a distribution with the help of the following theorem.

Theorem 2.1 (Appel, 2007)

For any locally integrable function f , there is an associated distribution, also denoted by f , defined by

$$\langle f, \varphi \rangle := \int f(x)\varphi(x) dx , \quad (2.22)$$

for all $\varphi \in \mathcal{D}(\mathbb{R}^D)$. Such a distribution is called a regular distribution associated to the locally integrable function f .

All the other distributions are called singular distributions. However, we may symbolically use the formula (2.22) also for singular distributions, which are commonly used in physics literature. As an example for singular distributions, the Dirac delta distribution is the most well-known:

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.,

$$\langle \delta, \varphi \rangle := \varphi(0) , \quad (2.23)$$

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

For $\mathbf{r}_0 \in \mathbb{R}^D$, we define similarly the Dirac delta distribution centered at \mathbf{r}_0 , denoted $\delta_{\mathbf{r}_0}^{(D)}$, by its action on any test function:

$$\langle \delta_{\mathbf{r}_0}^{(D)}, \varphi \rangle := \varphi(\mathbf{r}_0) , \quad (2.24)$$

for all $\varphi \in \mathcal{D}(\mathbb{R}^D)$. In physics literature, it is usually denoted by $\delta^{(D)}(\mathbf{r} - \mathbf{r}_0)$.

Definition 2.8 (Appel, 2007)

The m – th derivative of a distribution is defined by

$$\langle T^{(m)}, \varphi \rangle := (-1)^{(m)} \langle T, \varphi^{(m)} \rangle , \quad (2.25)$$

for any $\varphi \in \mathcal{D}$ and any $m \in \mathbb{N}$.

Definition 2.9 (Appel, 2007)

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

$$\langle \psi T, \varphi \rangle := \langle T, \psi \varphi \rangle , \quad (2.26)$$

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

Theorem 2.2 (Appel, 2007)

Let ψ be a function of C^∞ class. Then,

$$\psi(x)\delta(x) = \psi(0)\delta(x) , \quad (2.27)$$

and in particular;

$$x\delta(x) = 0 , \quad (2.28)$$

which is also true for any dimension D .

Definition 2.10 (Appel, 2007)

Let S and T be two distributions. The direct product, or tensor product, of the distributions S and T is the distribution $S(x)T(y)$ defined on the space of test functions on $\mathbb{R}^P \times \mathbb{R}^D$ by

$$\langle S(\mathbf{x})T(\mathbf{y}), \varphi(\mathbf{x}, \mathbf{y}) \rangle := \langle S(\mathbf{x}), \langle T(\mathbf{y}), \varphi(\mathbf{x}, \mathbf{y}) \rangle \rangle . \quad (2.29)$$

It is denoted by $S \otimes T$ or $S(\mathbf{x})T(\mathbf{y})$. Note that tensor product is not commutative.

Example 2.2 (Appel, 2007)

The Dirac delta distribution in D dimensions can be defined as a tensor product of D Dirac delta distributions in one dimension:

$$\delta^{(D)}(\mathbf{r}) = \delta^{(D)}(x_1, x_2, \dots, x_D) := \delta(x_1)\delta(x_2) \dots \delta(x_D) . \quad (2.30)$$

There are different classes of Dirac delta distributions, e.g., point-like, surface and curvilinear. The point-like Dirac delta distribution acting on a test function has been defined by Eq. (2.24). As a physical example for point-like Dirac delta distributions, we consider:

Example 2.3 (Appel, 2007)

The electric field at any point \mathbf{r} in $\mathbb{R}^3 \setminus \{\mathbf{r}_0\}$ of a point-like particle with electric charge q , placed at a point \mathbf{r}_0 in \mathbb{R}^3 is given by $\mathbf{E}(\mathbf{r}) = \frac{q}{4\pi\epsilon_0} \frac{\mathbf{r}-\mathbf{r}_0}{\|\mathbf{r}-\mathbf{r}_0\|^3}$, where ϵ_0 is the electric permittivity constant (Griffiths, 1999). If we have a continuous charge distribution, we usually introduce a function $\rho : \mathbb{R}^3 \rightarrow \mathbb{R}$, which associates, to each point in \mathbb{R}^3 , density of electric charge at this point. Then, the total charge contained in the infinitesimal volume element $dx dy dz$ around \mathbf{r}_0 is given by $\rho(\mathbf{r}_0) dx dy dz$. Then, the electric field produced by the continuous charge density ρ is given by

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \rho(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{\|\mathbf{r} - \mathbf{r}'\|^3} d^3r' , \quad (2.31)$$

and the total charge contained in a volume $V \subset \mathbb{R}^3$ is $q = \int_V \rho(\mathbf{r}) d^3r$. The point-like charge in electrostatics must then be represented by a distribution:

$$\rho(\mathbf{r}) = q\delta^{(3)}(\mathbf{r} - \mathbf{r}_0) . \quad (2.32)$$

Note that the dimension of three-dimensional point-like Dirac delta distribution has the dimension of the inverse of a value: $[\delta^{(3)}] = \frac{1}{L^3}$.

In order to describe a surface carrying charges, we may also use a different kind of Dirac delta distributions:

Definition 2.11 (Appel, 2007)

Let S be a smooth surface in \mathbb{R}^3 . The (normalized) Dirac delta surface distribution on S is given by its action on any $\varphi \in \mathcal{D}(\mathbb{R}^3)$:

$$\langle \delta_S, \varphi \rangle := \int_S \varphi d^2S , \quad (2.33)$$

where d^2S is the integration element over the surface S .

Example 2.4 (Spherical shell Dirac delta distribution:) (Appel, 2007)

In \mathbb{R}^3 , the Dirac delta surface distribution $\delta_{\mathbb{S}^2}$ is denoted by $\delta(\|\mathbf{x}\| - R)$, for $R > 0$, where \mathbb{S}^2 is the two-sphere of radius R , i.e., $\mathbb{S}^2 = \{\mathbf{x} \in \mathbb{R}^3 ; \|\mathbf{x}\| = R\}$. From Definition 2.11, we have

$$\begin{aligned} \langle \delta_{\mathbb{S}^2}, \varphi \rangle &= \int_{\mathbb{S}^2} \varphi(R, \theta, \phi) d^2S \\ &= \int_V \varphi(r, \theta, \phi) \delta(r - R) \underbrace{r^2 \sin \theta dr d\theta d\phi}_{dV} = \langle \delta_R, \varphi \rangle . \end{aligned} \quad (2.34)$$

where we have parameterized the sphere by the spherical coordinates (Arfken & Weber, 2005), i.e., $d^2S = R^2 \sin \theta dR d\theta d\phi$ and use the fact that $\int_V \delta(r - R)f(r) dr = f(R)$.

Similarly, one can also define Dirac delta distributions on a smooth curve by analogy with Definition 2.11. However, we will only deal with the point-like Dirac delta distributions in this thesis.

One can also define the Fourier transform of the distributions.

Definition 2.12 (Appel, 2007)

The Fourier transform of a distribution T which is defined by its action on a test function φ is

given by

$$\langle \mathcal{F}[T], \varphi \rangle := \langle T, \mathcal{F}[\varphi] \rangle . \quad (2.35)$$

One can use the notation \widehat{T} and $\widehat{\varphi}$ instead of $\mathcal{F}[T]$ and $\mathcal{F}[\varphi]$:

$$\langle \widehat{T}, \varphi \rangle := \langle T, \widehat{\varphi} \rangle . \quad (2.36)$$

Remark 2.2 (Appel, 2007)

If φ has compact support and is non-zero, its Fourier transform $\widehat{\varphi}$ cannot have compact support; then the quantity $\langle T, \widehat{\varphi} \rangle$ is not always defined. Therefore, we cannot say that all distributions have an associated Fourier transform. For this reason, the idea of the tempered distributions is introduced.

Definition 2.13 (Appel, 2007)

The Schwartz space is a space of functions which are infinitely differentiable and rapidly decaying (i.e. decaying faster than any polynomial as $x \rightarrow \infty$) along with all derivatives and is denoted by \mathcal{S} . The space of linear continuous functionals on \mathcal{S} is denoted by \mathcal{S}' . A tempered distribution is an element of \mathcal{S}' .

We now introduce the Fourier transform of tempered distributions. Let T be a tempered distribution and $\varphi \in \mathcal{S}$, then the Fourier transform $\mathcal{F}[\varphi]$ is also in the space \mathcal{S} . Therefore, the quantity $\langle T, \mathcal{F}[\varphi] \rangle$ is defined and hence, it is possible to define the Fourier transform of T .

Theorem 2.3 (Appel, 2007)

$$\mathcal{F}[\delta] = 1 \quad \text{and} \quad \mathcal{F}[1] = \delta.$$

Let us give very briefly the rigorous definition and some basic properties of the Dirac calculus or Dirac's bra-ket notation which is commonly used in physics literature.

2.3. Dirac Calculus

We want to show how to define the formal Dirac calculus by using the idea of a Gelfand triplet or rigged Hilbert space. The motivation in defining rigged Hilbert spaces is based on the fact that the standard Dirac's kets such as $|x\rangle$, $|p\rangle$ and their bras do not belong to Hilbert

spaces. They live in a more general spaces. (For the discussion of rigged Hilbert spaces, see 1.7 on (Bohm, 2001).)

2.3.1. Eigendistributions

The chain of inclusions is given by (Zeidler, 2006)

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R}) , \quad (2.37)$$

which is called a Gelfand triplet with respect to the Hilbert space $L^2(\mathbb{R})$.

The momentum operator in quantum mechanics is defined by

$$(P\varphi)(x) := -i\hbar \frac{d}{dx} \varphi(x) , \quad (2.38)$$

where $P : \mathcal{S}(\mathbb{R}) \rightarrow \mathcal{S}(\mathbb{R})$ and the coordinate operator is

$$(X\varphi)(x) := x\varphi(x) , \quad (2.39)$$

where $X : \mathcal{S}(\mathbb{R}) \rightarrow \mathcal{S}(\mathbb{R})$ for all $x \in \mathbb{R}$ and all functions $\varphi(x) \in \mathcal{S}(\mathbb{R})$. But, these operators do not have eigenfunctions which lie in the Hilbert space $L^2(\mathbb{R})$. In order to see this, let us consider the following example:

Example 2.5 (Zeidler, 2006)

The solution to the eigenvalue problem $-i\hbar \frac{d}{dx} \varphi(x) = p\varphi(x)$ is $\varphi_p(x) := \frac{e^{\frac{ipx}{\hbar}}}{2\pi\hbar}$ since

$$P\varphi_p = -i\hbar \frac{d}{dx} \left(\frac{e^{\frac{ipx}{\hbar}}}{2\pi\hbar} \right) = p\varphi_p , \quad (2.40)$$

for all $p \in \mathbb{R}$. But $\varphi_p \notin L^2(\mathbb{R})$.

Although the eigenfunctions do not belong to $L^2(\mathbb{R})$, we will show that there exists a complete system of eigendistributions.

The momentum operator (Zeidler, 2006): Define $F_p(\varphi) := \int_{\mathbb{R}} \varphi_p^*(x) \varphi(x) dx$ for all test functions $\varphi \in \mathcal{S}(\mathbb{R})$. Afterwards, $F_p \in \mathcal{S}'(\mathbb{R})$. The family $\{F_p\}_{p \in \mathbb{R}}$ of tempered distributions F_p defines a complete system of eigendistributions of the momentum operator P . Explicitly, that means

- **Eigenvalue Relation:** $F_p(P\varphi) = pF_p(\varphi)$ for all $p \in \mathbb{R}$ and $\varphi \in \mathcal{S}(\mathbb{R})$. In the Dirac's notation, the above relation reads $P |F_p\rangle = p |F_p\rangle$ for all $p \in \mathbb{R}$. Physicists simply write $|p\rangle$ instead of $|F_p\rangle$, i.e., $P |p\rangle = p |p\rangle$.
- **Completeness Relation:** If $F_p(\varphi) = 0$ for all $p \in \mathbb{R}$ and fixed $\varphi \in \mathcal{S}(\mathbb{R})$, then $\varphi = 0$.

Proof For the first relation, we have

$$F_p(P\varphi) = \int_{\mathbb{R}} \varphi_p^*(x) [P\varphi(x)] dx = -\frac{i}{2\pi} \int_{\mathbb{R}} e^{-\frac{ipx}{\hbar}} \varphi'(x) dx . \quad (2.41)$$

Since $\varphi \in \mathcal{S}(\mathbb{R})$, integration by parts yields us

$$F_p(P\varphi) = p \int_{\mathbb{R}} \frac{e^{-\frac{ipx}{\hbar}}}{2\pi\hbar} \varphi(x) dx = pF_p(\varphi) . \quad (2.42)$$

For the second relation, let

$$F_p(\varphi) = 0 = \int_{\mathbb{R}} \frac{e^{-\frac{ipx}{\hbar}}}{2\pi\hbar} \varphi(x) dx , \quad (2.43)$$

for all $p \in \mathbb{R}$. Then, $\widehat{\varphi}(p) = 0 \Rightarrow \varphi = 0$. □

The coordinate operator (Zeidler, 2006): Similarly, we have the family $\{\delta_x\}_{x \in \mathbb{R}}$ of tempered distributions δ_x defines a complete system of eigendistributions of the coordinate operator X . That means

- **Eigenvalue Relation:** $\delta_x(X\varphi) = x\delta_x(\varphi)$ for all $x \in \mathbb{R}$ and $\varphi \in \mathcal{S}(\mathbb{R})$. In the Dirac's notation, the above relation reads $X |\delta_x\rangle = x |\delta_x\rangle$ for all $x \in \mathbb{R}$. Physicists simply write $|x\rangle$ instead of $|\delta_x\rangle$, i.e., $X |x\rangle = x |x\rangle$.
- **Completeness Relation:** If $\delta_x(\varphi) = 0$ for all $x \in \mathbb{R}$ and fixed $\varphi \in \mathcal{S}(\mathbb{R})$, then $\varphi = 0$.

Proof For the first relation,

$$\delta_x(X\varphi) = \delta_x[x\varphi(x)] = x\varphi(x) . \quad (2.44)$$

For the second relation, if

$$\delta_x(\varphi) = 0 = \varphi(x) , \quad (2.45)$$

for all $x \in \mathbb{R}$, then $\varphi = 0$. □

The energy operator (Zeidler, 2006): Define the Hamiltonian (the energy operator) for the free particle on the real line

$$H := \frac{P^2}{2m} , \quad (2.46)$$

where $H : \mathcal{S}(\mathbb{R}) \rightarrow \mathcal{S}(\mathbb{R})$. The family $\{F_p\}_{p \in \mathbb{R}}$ defines a complete system of eigendistributions. Explicitly;

- **Eigenvalue Relation:** $F_p(H\varphi) = E(p)F_p(\varphi)$ for all $p \in \mathbb{R}$ and $\varphi \in \mathcal{S}(\mathbb{R})$ where the eigenvalue $E(p) := \frac{p^2}{2m}$ is the energy of a free particle of momentum p . In the Dirac's notation, simply we have $H |p\rangle = E(p) |p\rangle$ for all $p \in \mathbb{R}$.
- **Completeness Relation:** If $F_p(\varphi) = 0$ for all $p \in \mathbb{R}$ and fixed $\varphi \in \mathcal{S}(\mathbb{R})$, then $\varphi = 0$.

Proof For the first relation,

$$F_p(H\varphi) = \int_{\mathbb{R}} \varphi_p^*(x)[H\varphi(x)] dx = -\frac{\hbar}{4m\pi} \int_{\mathbb{R}} e^{-\frac{ipx}{\hbar}} \varphi''(x) dx . \quad (2.47)$$

After doing integration by parts with using the property of $\varphi \in \mathcal{S}(\mathbb{R})$, we obtain

$$F_p(H\varphi) = \frac{p^2}{2m} \int_{\mathbb{R}} \frac{e^{-\frac{ipx}{\hbar}}}{2\pi\hbar} \varphi(x) dx = E(p)F_p(\varphi) . \quad (2.48)$$

For the second relation, let $F_p(\varphi) = 0$ for all $p \in \mathbb{R}$ and fixed $\varphi \in \mathcal{S}(\mathbb{R})$, then $\varphi = 0$ which we have showed it in completeness relation for the momentum operator. □

Above definitions can be generalized to the higher dimensions.

2.4. Formal Dirac Calculus

In quantum mechanics, we formally use the above Dirac's bra-ket notation in a more compact way and they satisfy the following formal relations: (Zeidler, 2006)

- $\langle \mathbf{x} | \mathbf{y} \rangle = \delta^{(D)}(\mathbf{x} - \mathbf{y})$.
- $\langle \mathbf{x} | \mathbf{p} \rangle = e^{\frac{i\mathbf{p} \cdot \mathbf{x}}{\hbar}}$.
- $\int_{\mathbb{R}^D} |\mathbf{x}\rangle \langle \mathbf{x}| d^D x = I$.
- $\int_{\mathbb{R}^D} |\mathbf{p}\rangle \langle \mathbf{p}| \frac{d^D p}{(2\pi\hbar)^D} = I$.
- $P |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle$.
- $X |\mathbf{x}\rangle = \mathbf{x} |\mathbf{x}\rangle$.

These formulae are going to be very practical in our calculations that we will use throughout the thesis.

CHAPTER 3

HEURISTIC APPROACH TO THE POINT INTERACTIONS: A SIMPLE TOY MODEL OF RENORMALIZATION

3.1. Some Basic Notions in Quantum Mechanics

We are first going to give the physical background and the basic notions of quantum mechanics that we need in this thesis.

According to the postulate of quantum mechanics, the state of a particle is described by a complex-valued function $\Psi(\mathbf{r}, t)$, where $\mathbf{r} = (x_1, x_2, \dots, x_D) \in \mathbb{R}^D$ and $t \in \mathbb{R}$ (Gustafson & Sigal, 2011). The function $\Psi(\mathbf{r}, t)$ is called the wave function or state vector. In probabilistic interpretation of quantum mechanics, the quantity $|\Psi(\mathbf{r}, t)|^2$ represents the probability distribution for the position of the particle. The probability that a particle is in the region $\Omega \subset \mathbb{R}^D$ at time t is given by $\int_{\Omega} |\Psi(\mathbf{r}, t)|^2 d^D r$. Hence,

$$\int_{\mathbb{R}^D} |\Psi(\mathbf{r}, t)|^2 d^D r = 1, \quad (3.1)$$

is required (total probability should be one). The time evolution of the wave function is given by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}, t) + V(\mathbf{r}, t) \Psi(\mathbf{r}, t), \quad (3.2)$$

where \hbar is the reduced Planck's constant $\hbar = \frac{h}{2\pi}$, one of the fundamental constants in nature, and $\Delta = \sum_{j=1}^D \partial_j^2$ is the Laplace operator, m is the mass of the particle and $V(\mathbf{r}, t)$ is the potential energy of the system. In physics literature, the Laplace operator Δ is denoted by ∇^2 .

If V does not depend on t explicitly, i.e., $V(\mathbf{r}, t) = V(\mathbf{r})$, we can do the separation of

variables $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})\varphi(t)$ and obtain a differential equation for $\psi(\mathbf{r})$:

$$(H\psi)(\mathbf{r}) = \langle \mathbf{r} | H\psi \rangle = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) , \quad (3.3)$$

where $H = -\frac{\hbar^2}{2m}\Delta + V$ is the Schrödinger operator or the Hamilton operator and the equation is called the time-independent Schrödinger equation and the separation constant E is known as the total energy. This equation can be also interpreted as an eigenvalue problem. The space of all possible states of a particle at a given time is called the state space and it is assumed to be the following Hilbert space:

$$L^2(\mathbb{R}^D) : \left\{ \Psi : \mathbb{R}^D \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^D} |\Psi(\mathbf{r})|^2 d^D r < \infty \right\} . \quad (3.4)$$

Here, the inner product is defined by

$$\langle \Psi, \phi \rangle = \langle \Psi | \phi \rangle = \int_{\mathbb{R}^D} \Psi^*(\mathbf{r})\phi(\mathbf{r}) d^D r , \quad (3.5)$$

where $*$ denotes the complex conjugation. We are going to use either $\langle \Psi, \phi \rangle$ or $\langle \Psi | \phi \rangle$ (Dirac's bra-ket notation) as notations for the inner product interchangeably according to the context throughout the thesis. If the state is space localized for all times, then such a state is called the bound state. Later on we are going to study the discrete and continuous spectrum of the Hamiltonian from the resolvent which is going to be discussed in Chapter 4 and actually the classification of the spectrum into discrete and continuous parts (strictly speaking, absolutely continuous parts (Reed & Simon, 1978)) corresponds to a classification of the dynamics into bound states and scattering states, respectively (Gustafson & Sigal, 2011).

3.2. Formal Analysis of Point Interaction in One Dimension

We start with a standard quantum mechanical textbook problem, where a particle of mass m interacts with a point interaction centered at the origin in one dimension. The time-independent Schrödinger equation of this system is formally given by (Griffiths, 1995)

$$\langle x | H\psi \rangle = (H\psi)(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \lambda\delta(x) \right] \psi(x) = E\psi(x) , \quad (3.6)$$

where $\lambda > 0$ is the strength of the point interaction (or sometimes called coupling constant). (It corresponds to an attractive point interaction.)

We are interested in finding the solution of the eigenvalue problem (3.6) for bound states.

Theorem 3.1 *The bound state energy and corresponding bound state wave function of the system (3.6) in one dimension are*

$$E = -\frac{m\lambda^2}{2\hbar^2}, \quad (3.7)$$

and

$$\psi(x) = \frac{\sqrt{m\lambda}}{\hbar} e^{-\frac{m\lambda}{\hbar^2}|x|}, \quad (3.8)$$

respectively.

Proof One formal way of finding the solution is to go to the Fourier space. The Fourier transform of $\psi(x)$ is

$$\mathcal{F}[\psi(x)] = \widehat{\psi}(p) = \int_{\mathbb{R}} e^{-\frac{ipx}{\hbar}} \psi(x) dx, \quad (3.9)$$

and the inverse Fourier transform is given by

$$\psi(x) = \int_{\mathbb{R}} e^{\frac{ipx}{\hbar}} \widehat{\psi}(p) [dp], \quad (3.10)$$

where we have used the notation $[dp] = \frac{dp}{2\pi\hbar}$ in order to keep track of the factor $2\pi\hbar$ in our calculations. In higher dimensions: $[d^D p] = \frac{d^D p}{(2\pi\hbar)^D}$. We expect that the bound state energy is negative because we have $\int_{\mathbb{R}} V(x) dx = -\lambda < 0$ (Schechter, 1981). So that we parameterize the energy $E = -\nu^2$ such that $\nu \in \mathbb{R}^+$. By applying formal Fourier transformation to the Schrödinger equation and using the convolution theorem, we get

$$\left(\frac{p^2}{2m} + \nu^2\right) \widehat{\psi}(p) = \lambda\psi(0), \quad (3.11)$$

which can be written as a singular integral equation:

$$\widehat{\psi}(p) = \int_{\mathbb{R}} \left[\frac{\lambda}{\nu^2} - \frac{q^2(2\pi\hbar)\delta(q-p)}{2m\nu^2} \right] \widehat{\psi}(q) [dq], \quad (3.12)$$

where the expression inside of the bracket can be interpreted as the integral kernel.

In Eq. (3.11), if we define $\lambda\psi(0) = C$ and apply the consistency condition (solve $\widehat{\psi}(p)$ from (3.11) in terms of C and then substitute it into Eq. (3.10) for $x = 0$), we obtain

$$C = \lambda \int_{\mathbb{R}} \frac{C}{\frac{p^2}{2m} + \nu^2} [dp]. \quad (3.13)$$

Since $C \neq 0$ (if C was zero, then we would have free Hamiltonian problem that is $C = \lambda\psi(0) = 0$, then $\lambda\delta(x)\psi(x) = \lambda\delta(x)\psi(0) = 0$), we can simplify C 's in the above equation and evaluating the integral by changing of the variable $p = \sqrt{2m\nu} \tan \theta$ gives the bound state energy as in (3.7). By the inverse formal Fourier transform and using the residue theorem (Greene & Krantz, 2006) and then from the normalization condition given in (3.1), we find the corresponding bound state wave function given in (3.8). \square

Lemma 3.1 *The average value of the Hamiltonian is*

$$\langle \psi | H | \psi \rangle = -\frac{m\lambda^2}{2\hbar^2}. \quad (3.14)$$

Proof The average value of the free Hamiltonian is

$$\begin{aligned} \langle \psi, H_0 \psi \rangle = \langle \psi | H_0 | \psi \rangle &= -\frac{\hbar^2}{2m} \int_{\mathbb{R}} \psi^*(x) \left[\frac{d^2}{dx^2} \psi(x) \right] dx \\ &= -\frac{\lambda}{2} \int_{\mathbb{R}} e^{-\frac{m\lambda}{\hbar^2}|x|} \left[\frac{d^2}{dx^2} e^{-\frac{m\lambda}{\hbar^2}|x|} \right] dx = \frac{m\lambda^2}{2\hbar^2}, \end{aligned} \quad (3.15)$$

where we have used $\frac{d}{dx}|x| = \text{sgn}(x)$ and $\frac{d}{dx}\text{sgn}(x) = 2\delta(x)$. (The derivative here should be understood in the distributional sense.) This tells us that the wave function for the bound state is contained in the domain of the free Hamiltonian H_0 , that is, $\psi \in \mathcal{D}(H_0)$. Also, if we compute the average value of our potential energy, we have

$$\langle \psi | V | \psi \rangle = -\frac{m\lambda^2}{\hbar^2} \int_{\mathbb{R}} e^{-\frac{m\lambda}{\hbar^2}|x|} \delta(x) e^{-\frac{m\lambda}{\hbar^2}|x|} dx = -\frac{m\lambda^2}{\hbar^2}. \quad (3.16)$$

Since the average value of the sum is equal to sum of the average value (Schechter, 1981), we have (3.14) which is consistent with Eq. (3.7). \square

The above formal analysis in finding the bound states of our system could be performed also in the coordinate representation, which can be found in any elementary quantum mechanics textbook (Griffiths, 1995), which we also summarize in Appendix A.

Remark 3.1 *Actually, the Hamiltonian $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \lambda\delta(x)$ is just a formal expression since a $\delta(x)$ does not correspond to an operator in $L^2(\mathbb{R})$. This can be seen as follows: Given any function $\psi(x) \in L^2(\mathbb{R})$, the function $\delta(x)\psi(x)$ is not square-integrable, hence not in $L^2(\mathbb{R})$. Nevertheless, it is possible to define point interactions rigorously in several ways and find a self-adjoint operator in $L^2(\mathbb{R})$ such that it has the same result with the above formal analysis.*

In order to construct such an operator, we first start with a symmetric Laplace operator which does not act on the location of Dirac delta potential. Then we construct all the self-adjoint extensions of the initial symmetric operator. After that we select one of those extension operators which gives the same results introduced formally. The construction of self-adjoint extensions can be achieved in two ways. First one is based on Von Neumann approach and the second one is known as Krein's approach. In two and three dimensions, these rigorous constructions should be performed by renormalizing the coupling constant.

3.2.1. Point Interaction as a Sequence of Regular Potentials with Finite Support

Actually, there is no point interaction (Dirac delta potential) in nature. It is an idealization as many other potentials used in quantum mechanics (such as square well potential, infinite square well potential, step potential, harmonic oscillator, etc. (Eisberg & Resnick, 1985)). However, point interactions can be used in many areas of physics under the appropriate circumstances. For example, when the de Broglie wavelength of the particle $\lambda = \frac{\hbar}{p}$ is much larger than the range of the potential, of a given system, it is a very good approximation to the real physical systems. The scattering of slow neutrons by heavy nuclei could be such a system.

As we have stated in Chapter 2, Dirac delta functions can be defined by the sequence of functions. Instead of solving the Schrödinger equation with a point interaction $-\lambda\delta(x)$ directly, we can pick the sequence of Dirac delta potential and solve it first and then take the limit of these solutions at the end. This is an indirect approach to the problem which sounds more physically since there is no point interaction in nature.

Let us pick a simplest possible sequence of Dirac delta function such that its exact solution is known. One such a potential is the finite square well potential (Griffiths, 1995):

$$V_n(x) = \begin{cases} 0 & \text{if } x \notin \left(-\frac{1}{n}, \frac{1}{n}\right), \\ -\frac{\lambda n}{2} & \text{if } x \in \left(-\frac{1}{n}, \frac{1}{n}\right), \end{cases} \quad (3.17)$$

where $\lambda > 0$. For bound states, let us again write $E = -\nu^2$.

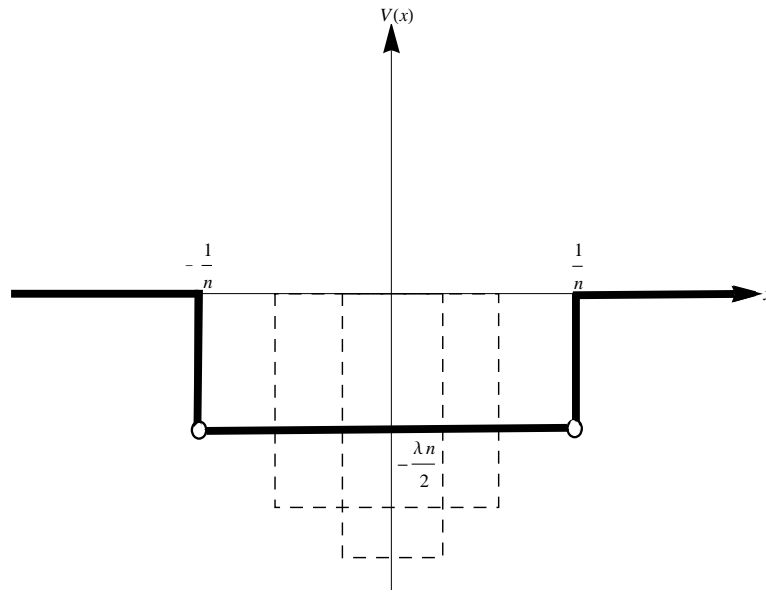


Figure 3.1. Finite square well potential

Note that the area under $V_n(x)$ is constant for all n . Then, the general solution for bound states can be easily found as

$$\psi(x) = \begin{cases} Ae^{-kx} & \text{if } x > \frac{1}{n}, \\ B \cos(lx) + C \sin(lx) & \text{if } -\frac{1}{n} < x < \frac{1}{n}, \\ De^{kx} & \text{if } x < -\frac{1}{n}, \end{cases} \quad (3.18)$$

where $k = \frac{\nu\sqrt{2m}}{\hbar}$ is real and positive, $l = \sqrt{\frac{2m}{\hbar^2} \left(\frac{\lambda n}{2} - \nu^2\right)}$ is also real and positive due to the fact that $E > V_{min} = -\frac{\lambda n}{2}$ for normalizable solution (otherwise we cannot have bound states).

The coefficients A, B, C, D are arbitrary constants to be determined. Since the potential is symmetric, we expect that there are either even or odd-parity solutions. Let us consider the even-parity solutions, that is,

$$\psi_e(x) = \begin{cases} Ae^{-kx} & \text{if } x > \frac{1}{n}, \\ B \cos(lx) & \text{if } -\frac{1}{n} < x < \frac{1}{n}, \\ Ae^{kx} & \text{if } x < -\frac{1}{n}. \end{cases} \quad (3.19)$$

From the boundary conditions (the continuity of $\psi_e(x)$ and $\frac{d\psi_e(x)}{dx}$ at $x = -\frac{1}{n}$ and $x = \frac{1}{n}$), we obtain

$$l \tan\left(\frac{l}{n}\right) = k. \quad (3.20)$$

A solution to the above transcendental equation expressed as a function of ν gives the allowed bound state energies. In order to solve the above equation, we first make the change of variables for simplification. Let $z \equiv \frac{l}{n}$ and $z_0 \equiv \sqrt{\frac{m\lambda}{n\hbar^2}}$. Then, the above equation becomes

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}. \quad (3.21)$$

This transcendental equation has no exact analytical solution. Therefore, we analyze this equation graphically and asymptotically as $n \rightarrow \infty$.

If $\frac{1}{n}$ goes to zero, z_0 is expected to be small by keeping λ fixed. When n is large, the intersection occurs at small values of z and the right-hand side of (3.21) is dominated so that we treat the left-hand side as a correction. Hence, as a first approximation (Olver, 1974) we obtain

$$\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} = \tan z \simeq z, \quad (3.22)$$

or

$$z_0^2 - z^2 \simeq z^4 \ll 1, \quad (3.23)$$

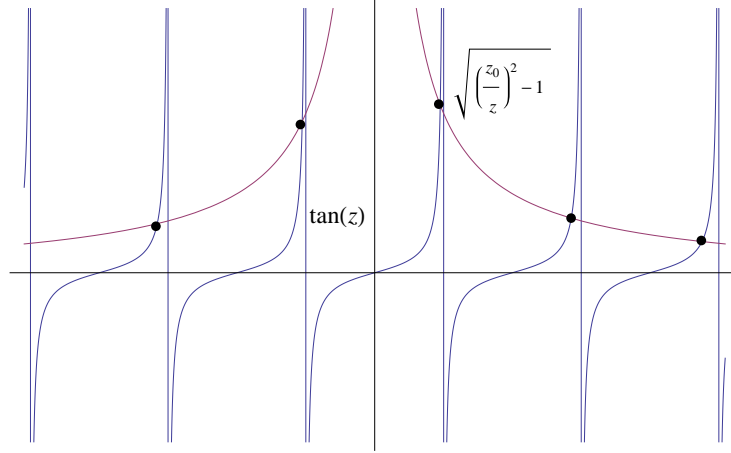


Figure 3.2. Graph of $\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ and $\tan z$

then, $z \simeq z_0$. The expression

$$z_0^2 - z^2 = \frac{m\lambda}{n\hbar^2} - \frac{2m}{n^2\hbar^2} \left(\frac{\lambda n}{2} - \nu^2 \right) \simeq \frac{2m\nu^2}{n^2\hbar^2}, \quad (3.24)$$

as $n \rightarrow \infty$. Also, due to Eq. (3.23) and by using the fact that $z \simeq z_0$, we find

$$E = -\nu^2 \simeq -\frac{m\lambda^2}{2\hbar^2}, \quad (3.25)$$

which is the same result obtained directly from the point interaction in one dimension. Here, the limiting procedure is performed in such a way that the area of the potential is fixed as its width is getting smaller and smaller. We actually demonstrate that limiting and direct solution procedures are commutative, that is,

One can also show that the limit of the scattering solutions of the finite well approaches the scattering solutions of the Dirac delta potential.

Corollary 3.1 *Point interactions are considered as a zero range limit of the finite well potentials.*

Remark 3.2 *Actually, the choice for $V_n(x)$ can be more general and it has been shown that if $V_n(x)$ belongs to Rollnick class, the above analysis is still true under certain circumstances (Albeverio & Gesztesy & Høegh-Krohn & Holden & Exner, 1988).*

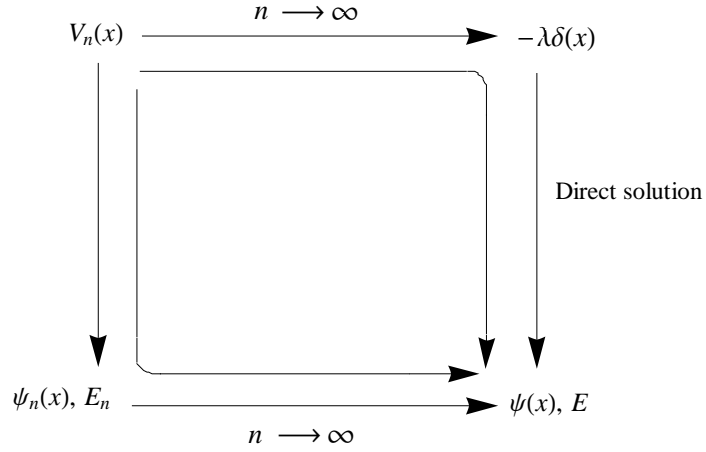


Figure 3.3. Commutativity diagram of the solutions

3.2.2. Scattering from Point Interaction

Now, we are going to analyze the scattering problem of the point interaction. Let $E = \frac{\hbar^2 k^2}{2m} > 0$ where $\frac{\hbar^2 k^2}{2m}$ is the free particle's energy and $k = \frac{p}{\hbar}$ is the wave vector (Merzbacher, 1961). Then, the time-independent Schrödinger equation in one dimension can be written as

$$\left(\frac{d^2}{dx^2} + k^2 \right) \psi(x) = \frac{2m}{\hbar^2} V(x) \psi(x) = \varrho(x), \quad (3.26)$$

where we have defined the right-hand side as $\varrho(x)$.

Theorem 3.2 *The transmission and reflection coefficients of the system (3.26) are*

$$T(k) = \frac{1}{1 + \left(\frac{m^2 \lambda^2}{\hbar^4 k^2} \right)}, \quad (3.27)$$

and

$$R(k) = \frac{1}{1 + \left(\frac{\hbar^4 k^2}{m^2 \lambda^2} \right)}, \quad (3.28)$$

respectively.

Proof By treating the right-hand side of (3.26) as a source term, the particular solution $\psi(x)$ can be given in terms of Green's function $G(x, x')$ (Byron & Fuller, 1992):

$$\psi(x) = \int_{\mathbb{R}} G(x, x') \rho(x') dx' = \frac{2m}{\hbar^2} \int_{\mathbb{R}} G(x, x') V(x') \psi(x') dx' , \quad (3.29)$$

and it satisfies

$$\left(\frac{d^2}{dx^2} + k^2 \right) G(x, x') = \delta(x, x') = \delta(x - x') . \quad (3.30)$$

Since the solution of the homogeneous equation $\left(\frac{d^2}{dx^2} + k^2 \right) \psi(x) = 0$ is $\psi(x) = Ae^{ikx}$, where A is a constant, we can add a particular solution (3.29) to the homogeneous solution: (solution is not unique)

$$\psi(x) = Ne^{ikx} + \frac{2m}{\hbar^2} \int_{\mathbb{R}} G(x - x') V(x') \psi(x') dx' , \quad (3.31)$$

where $G(x - x') = G(x, x')$ due to the translation symmetry of the differential operator. Let us take the formal Fourier transform of both sides of Eq. (3.30):

$$\int_{\mathbb{R}} e^{-\frac{ipy}{\hbar}} \left(\frac{d^2}{dy^2} + k^2 \right) G(y) dy = 1 , \quad (3.32)$$

where we denoted $G(x - x') = G(y)$. From the Green's formula (Appel, 2007) (or just integration by parts):

$$\int_{\mathbb{R}} e^{-\frac{ipy}{\hbar}} \left(\frac{d^2}{dy^2} + k^2 \right) G(y) dy = \int_{\mathbb{R}} G(y) \left(\frac{d^2}{dy^2} + k^2 \right) e^{-\frac{ipy}{\hbar}} dy , \quad (3.33)$$

where $G(y)$ is chosen such that the boundary terms vanish. Hence,

$$\int_{\mathbb{R}} G(y) \left(\frac{d^2}{dy^2} + k^2 \right) e^{-\frac{ipy}{\hbar}} dy = \left(k^2 - \frac{p^2}{\hbar^2} \right) \widehat{G}(p) , \quad (3.34)$$

where $\widehat{G}(p)$ is the formal Fourier transformed Green's function and from Eq. (3.32), we obtain

$$\widehat{G}(p) = \frac{1}{k^2 - \frac{p^2}{\hbar^2}}. \quad (3.35)$$

The formal inverse Fourier transform is then

$$G(y) = \int_{\mathbb{R}} \frac{e^{\frac{ipy}{\hbar}}}{k^2 - \frac{p^2}{\hbar^2}} [dp]. \quad (3.36)$$

Since the poles appear on the real axis, we should specify the contour associated with the proper boundary conditions for the scattering problem, where we have only outgoing wave solutions. In order to compute the contour integral, we are going to use Feynman's trick (Merzbacher, 1961) which is related with casual Green's functions in quantum field theory. The simple poles will be shifted up to $\pm \frac{i\epsilon}{2\hbar k}$ where $\epsilon > 0$.

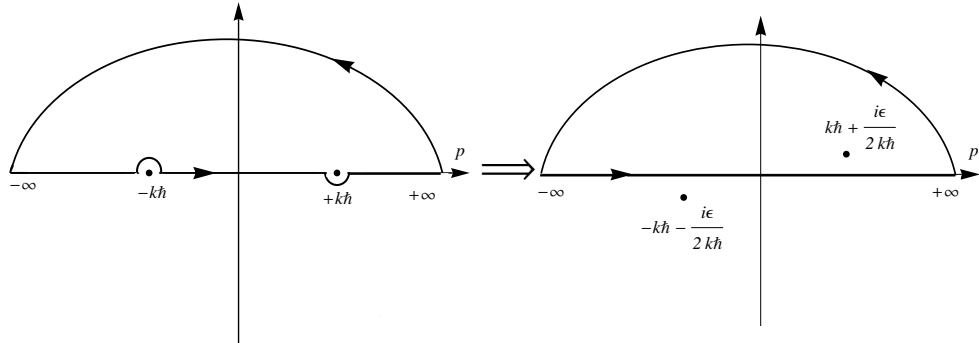


Figure 3.4. Feynman's trick

Therefore,

$$G_{\epsilon}^{(+)}(x - x') = -\frac{\hbar}{2\pi} \int_{\mathbb{R}} \frac{e^{\frac{ip(x-x')}{\hbar}}}{p^2 - (\hbar^2 k^2 + i\epsilon)} dp, \quad (3.37)$$

Because of

$$\sqrt{1 + \frac{i\epsilon}{\hbar^2 k^2}} = 1 + \frac{i\epsilon}{2\hbar^2 k^2}, \quad (3.38)$$

by Taylor expansion near $\epsilon = 0$, simple poles are at $p = \pm (\hbar k + \frac{i\epsilon}{2\hbar k})$. After using the residue theorem and then taking the limit $\epsilon \rightarrow 0$, we obtain

$$\lim_{\epsilon \rightarrow 0} G_\epsilon^{(+)}(x - x') = G^{(+)}(x - x') = -\frac{i}{2k} e^{ik|x-x'|}. \quad (3.39)$$

Substituting this into Eq. (3.31), we obtain

$$\psi^{(+)}(x) = N e^{ikx} - \frac{im}{\hbar^2 k} \int_{\mathbb{R}} e^{ik|x-x'|} V(x') \psi^{(+)}(x') dx', \quad (3.40)$$

which is called the Lippmann-Schwinger equation in the coordinate representation in one dimension (Merzbacher, 1961). By inserting the point interaction $V(x) = -\lambda\delta(x)$ into the above equation, we have

$$\psi^{(+)}(x) = N e^{ikx} + \frac{im\lambda}{\hbar^2 k} e^{ik|x|} \psi^{(+)}(0), \quad (3.41)$$

The consistency check yields

$$\psi^{(+)}(0) = \frac{N}{1 - \frac{im\lambda}{\hbar^2 k}}. \quad (3.42)$$

Then,

$$\psi^{(+)}(x) = \begin{cases} N e^{ikx} + \frac{im\lambda N}{\hbar^2 k - im\lambda} e^{-ikx} & \text{if } x < 0, \\ [N + \frac{im\lambda N}{\hbar^2 k - im\lambda}] e^{ikx} & \text{if } x > 0. \end{cases} \quad (3.43)$$

From the above equation, we obtain transmission and reflection coefficients given in (3.27) and (3.28) by using their definitions:

$$T(k) = \left| \frac{\text{Amplitude of the transmitted wave}}{\text{Amplitude of the incoming wave}} \right|^2, \quad (3.44)$$

and

$$R(k) = \left| \frac{\text{Amplitude of the reflected wave}}{\text{Amplitude of the incoming wave}} \right|^2. \quad (3.45)$$

Moreover, note that this coefficients are independent of the sign of the strength of point interaction. \square

Remark 3.3 For fixed value of k , $R \rightarrow 1$, $T \rightarrow 0$ as $\lambda \rightarrow \infty$ and $R \rightarrow 0$, $T \rightarrow 1$ as $\lambda \rightarrow 0$.

Remark 3.4 For fixed value of λ , $R \rightarrow 1$, $T \rightarrow 0$ as $k \rightarrow 0$ and $R \rightarrow 0$, $T \rightarrow 1$ as $k \rightarrow \infty$.

These results are physically expected.

3.3. Formal Analysis of Finitely Many Point Interactions in One Dimension

The time-independent Schrödinger equation in one dimension with N point interactions (formally) is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \sum_{i=1}^N \lambda_i \delta(x - a_i) \psi(x) = -\nu^2 \psi(x), \quad (3.46)$$

where a_i is the location of the i -th point interaction for $i = 1, \dots, N$. We assume that $a_i \neq a_j$ for $i \neq j$ and let $d_{min} = \min_{i,j} |a_i - a_j| > 0$. By applying the formal Fourier transform to Eq. (3.46), we have

$$\left(\frac{p^2}{2m} + \nu^2 \right) \widehat{\psi}(p) = \sum_{i=1}^N \lambda_i \psi(a_i) e^{-\frac{ipa_i}{\hbar}}, \quad (3.47)$$

or, it can be rewritten as the following singular integral equation:

$$\widehat{\psi}(p) = \int_{\mathbb{R}} \left[\sum_{i=1}^N \frac{\lambda_i e^{\frac{i(q-p)a_i}{\hbar}}}{\nu^2} - \frac{q^2(2\pi\hbar)\delta(q-p)}{2m\nu^2} \right] \widehat{\psi}(q) [dq], \quad (3.48)$$

where the expression inside of the bracket is the integral kernel.

Let $\lambda_i \psi(a_i) = A_i$. After the consistency check, we have

$$\left[\frac{1}{\lambda_i} - \int_{\mathbb{R}} \frac{1}{\frac{p^2}{2m} + \nu^2} [dp] \right] A_i - \int_{\mathbb{R}} \sum_{\substack{j=1 \\ j \neq i}}^N \left[\frac{e^{\frac{ip|a_i - a_j|}{\hbar}}}{\frac{p^2}{2m} + \nu^2} [dp] \right] A_j = 0. \quad (3.49)$$

These equations can be written as homogeneous system of linear equations in a matrix form:

$$\sum_{j=1}^N \Phi_{ij}(\nu) A_j = 0 \quad \text{or} \quad \Phi A = 0, \quad (3.50)$$

where

$$\Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda_i} - \int_{\mathbb{R}} \frac{1}{\frac{p^2}{2m} + \nu^2} [dp] & \text{if } i = j, \\ - \int_{\mathbb{R}} \frac{e^{\frac{ip|a_i - a_j|}{\hbar}}}{\frac{p^2}{2m} + \nu^2} [dp] & \text{if } i \neq j. \end{cases} \quad (3.51)$$

After solving integrals by using the residue theorem, we find

$$\Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda_i} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & \text{if } i = j, \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m}\nu|a_i - a_j|}{\hbar}}}{\hbar\nu} & \text{if } i \neq j. \end{cases} \quad (3.52)$$

which is called the principal matrix. This terminology is first introduced by S. G. Rajeev when he discuss many-body version of these potentials (Rajeev, 1999). From (3.50), for non-trivial solutions, we must have $\det \Phi_{ij}(\nu) = 0$, from which we can find the bound state energies as

a function of λ_i 's. In general, $\det \Phi$ is a complicated function of ν , so it is difficult to find the solution of $\det \Phi(\nu) = 0$ exactly. In other words, the linear differential equation problem $H\psi = E\psi$ turns out to be a non-linear transcendental algebraic problem $\det \Phi(E) = 0$.

3.3.1. Two-center Case: A Toy Model for Chemical Bonds

Theorem 3.3 For $N = 2$, we have at most two bound states. The critical distance to have two bound states is

$$d > \frac{\hbar^2}{2m} \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2} \right) = d_{critical} , \quad (3.53)$$

where $d = |a_1 - a_2|$.

Proof For $N = 2$, Eq. (3.52) becomes

$$\Phi(\nu) = \begin{pmatrix} \frac{1}{\lambda_1} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m\nu}|a_1-a_2|}{\hbar}}}{\hbar\nu} \\ -\sqrt{\frac{m}{2}} \frac{e^{-\frac{\sqrt{2m\nu}|a_1-a_2|}{\hbar}}}{\hbar\nu} & \frac{1}{\lambda_2} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \end{pmatrix} . \quad (3.54)$$

We need to solve $\det \Phi(\nu) = 0$ to find bound state energies. Hence,

$$\left(\frac{1}{\lambda_1} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \right) \left(\frac{1}{\lambda_2} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} \right) = \frac{m}{2\hbar^2\nu^2} e^{-\frac{2\sqrt{2m\nu}|a_1-a_2|}{\hbar}} . \quad (3.55)$$

By multiplying both sides with $\lambda_1\lambda_2\nu^2$ and putting in order, we obtain

$$\left(\nu - \sqrt{\frac{m}{2}} \frac{\lambda_1}{\hbar} \right) \left(\nu - \sqrt{\frac{m}{2}} \frac{\lambda_2}{\hbar} \right) = \frac{m\lambda_1\lambda_2}{2\hbar^2} e^{-\frac{2\sqrt{2m\nu}|a_1-a_2|}{\hbar}} . \quad (3.56)$$

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

$$(x - c_1)(x - c_2) = c_1c_2e^{-\beta x} , \quad (3.57)$$

which is a transcendental equation and difficult to solve. We get help from the graphs of the

functions to solve this equation. Without loss of generality, let us assume that $c_1 < c_2$. We have one bound state which can be easily seen from the Figure 3.5. In this figure, there is only one root corresponding to the bound state energy (the root $x = 0$ does not correspond to the bound state energy). For particular values of c_1 and c_2 , we may have two roots which can be seen in Figure 3.6. We have two bound states if the following condition is satisfied:

$$(x - c_1)(x - c_2) > c_1 c_2 e^{-\beta x} \text{ near } x = 0 . \quad (3.58)$$

Since $e^{-\beta x} = 1 - \beta x$ near $x = 0$, the above equation becomes

$$c_1 + c_2 < \beta c_1 c_2 , \quad (3.59)$$

and by substituting the original variables, we obtain (3.53). This equation tells us that if the distance between the point interactions' centers is larger than this critical distance, then we have two bound states. Note that two-center case of the problem is a toy model for chemical bonds (Cohen Tannoudji & Diu & Laloe, 1996).

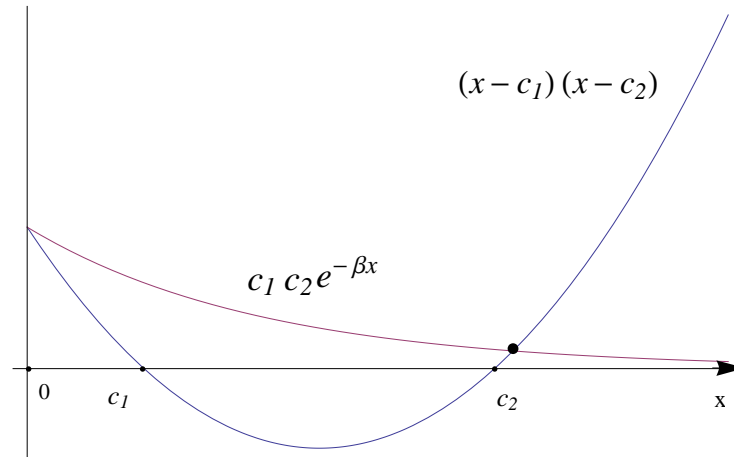


Figure 3.5. Graph of $(x - c_1)(x - c_2)$ and $c_1 c_2 e^{-\beta x}$ for $c_1 = 5$, $c_2 = 20$ and $\beta = 0.1$

□

Theorem 3.4 *The bound state energies of the particle in the presence of two point interac-*

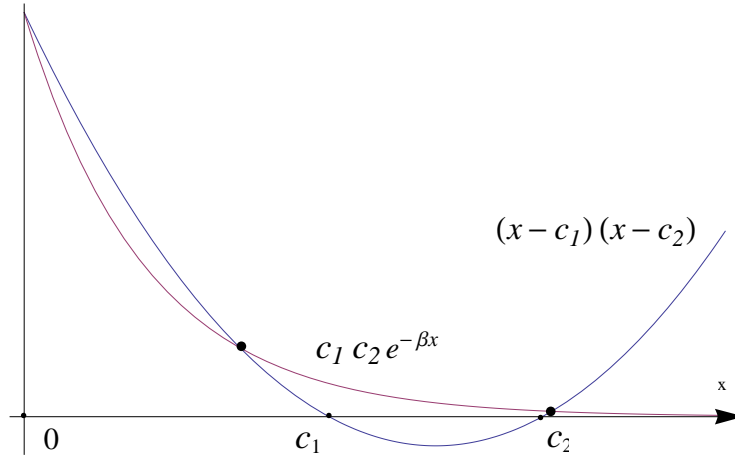


Figure 3.6. Graph of $(x - c_1)(x - c_2)$ and $c_1 c_2 e^{-\beta x}$ for $c_1 = 1$, $c_2 = 1.7$ and $\beta = 2.5$

tions ($N = 2$) for $c_1 = c_2 = c$ are

$$E_{\pm} = - \left\{ \sqrt{\frac{m}{2}} \frac{\lambda}{\hbar} + \frac{\hbar}{\sqrt{2m}|a_1 - a_2|} W \left[\pm \frac{m\lambda|a_1 - a_2|}{\hbar^2} e^{-\frac{m\lambda|a_1 - a_2|}{\hbar^2}} \right] \right\}^2, \quad (3.60)$$

where $W[z]$ is the Lambert W function.

Proof For $c_1 = c_2 = c$ ($\lambda_1 = \lambda_2 = \lambda$), Eq. (3.57) becomes

$$(x - c)e^{\frac{\beta x}{2}} = \pm c. \quad (3.61)$$

Let us rewrite this equation in the following form

$$\frac{\beta}{2}(x - c)e^{\frac{\beta(x-c)}{2}} = \pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}}. \quad (3.62)$$

Solutions of this equation can be explicitly expressed in terms of Lambert W function. It has many applications such as enumeration of trees in combinatorics, in the solution of iterated exponentiation, a jet fuel problem and an enzyme kinetics problem and also in Wien's displacement law, capacitor fields and conformal mapping (Corless & Gonnet & Hare & Jeffrey & Knuth, 1996) (Valluri & Jeffrey & Corless, 1988). The definition of the function is given

by the solution of the following transcendental equation

$$y e^y = z \Rightarrow y \equiv W[z] . \quad (3.63)$$

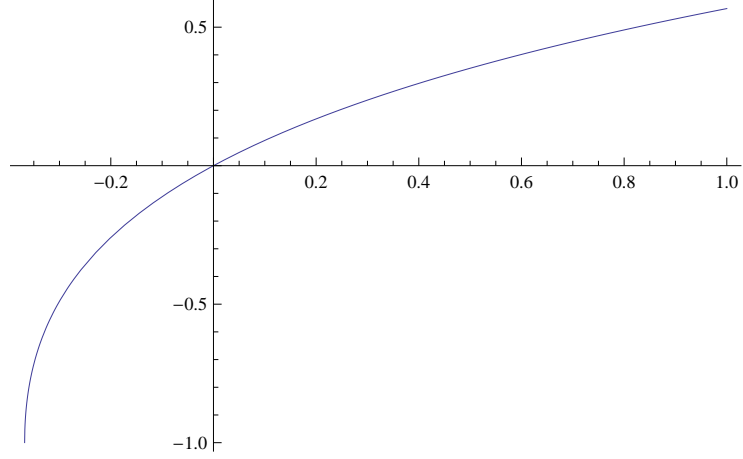


Figure 3.7. Graph of Lambert W function

So, the solution to Eq. (3.62) turns out to be

$$\frac{\beta}{2}(x_{\pm} - c) = W \left[\pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}} \right] , \quad (3.64)$$

and then

$$x_{\pm} = c + \frac{2}{\beta} W \left[\pm \frac{\beta c}{2} e^{-\frac{\beta c}{2}} \right] . \quad (3.65)$$

By substituting back to our original variables, we obtain

$$\nu = \sqrt{\frac{m \lambda}{2 \hbar}} + \frac{\hbar}{\sqrt{2m}|a_1 - a_2|} W \left[\pm \frac{m\lambda|a_1 - a_2|}{\hbar^2} e^{-\frac{m\lambda|a_1 - a_2|}{\hbar^2}} \right] . \quad (3.66)$$

Since $E = -\nu^2$, one can immediately find (3.60). □

Theorem 3.5 For $N = 2$ and $\lambda_1 = \lambda_2 = \lambda$ and also $a_1 = -a$ and $a_2 = a$, we have at most

two bound states. The critical distance to have two bound states is

$$d > \frac{\hbar^2}{m\lambda} = d_{critical} . \quad (3.67)$$

Proof If we choose same strengths of the point interactions: $\lambda_1 = \lambda_2 = \lambda$ and the location of the centers are assumed to be symmetric: $a_1 = -a$ and $a_2 = a$ in (3.56), then we obtain

$$\pm \left(\sqrt{\frac{2}{m} \frac{\hbar\nu}{\lambda}} - 1 \right) = e^{-\frac{2\sqrt{2m}a\nu}{\hbar}} . \quad (3.68)$$

By choosing $\nu \equiv \frac{\kappa\hbar}{\sqrt{2m}}$ for convenience, we have

$$e^{-2a\kappa_+} = \frac{\hbar^2\kappa_+}{m\lambda} - 1 , \quad (3.69)$$

and

$$e^{-2a\kappa_-} = 1 - \frac{\hbar^2\kappa_-}{m\lambda} , \quad (3.70)$$

which correspond to the even and odd-parity solutions, respectively (Griffiths, 1995). One can easily see that the former has definitely one (and only one) root but the latter may or may not have a root. In order (3.70) have a root, the condition $a > \frac{\hbar^2}{2m\lambda}$ should be satisfied because of the slopes near $\kappa_- = 0$. Since the distance between the point interactions is $d = 2a$, we have two roots when (3.67) is satisfied. We can also check that this result is consistent with (3.53) by writing $\lambda_1 = \lambda_2 = \lambda$ in that equation. \square

If $d > d_{critical}$, we can calculate the difference between odd and even-parity energy levels ΔE as $d = 2a \rightarrow \infty$. When a is large, the right-hand side of Eq. (3.69) dominates. Hence, we treat the left-hand side of this equation as a correction. In the first approximation ($a \rightarrow \infty$), the left-hand side of Eq. (3.69) becomes zero and we obtain $\kappa_+ = \frac{m\lambda}{\hbar^2}$. By substituting this solution into the left-hand side of Eq. (3.69) as a second approximation by successive approximations (Olver, 1974), we find

$$\kappa_+ = \frac{m\lambda}{\hbar^2} \left(1 + e^{-\frac{2m\lambda a}{\hbar^2}} \right) . \quad (3.71)$$

Similarly, one can easily find that

$$\kappa_- = \frac{m\lambda}{\hbar^2} \left(1 - e^{-\frac{2m\lambda a}{\hbar^2}} \right). \quad (3.72)$$

Since $E_{\pm} = -\nu_{\pm}^2 = -\frac{\kappa_{\pm}^2 \hbar^2}{2m}$, the difference between the energy levels is

$$\Delta E = E_- - E_+ \sim \frac{2m\lambda^2}{\hbar^2} e^{-\frac{2m\lambda a}{\hbar^2}}, \quad (3.73)$$

which goes to zero exponentially as $a \rightarrow \infty$. In other words, the energy levels become degenerate.

3.3.2. The Case When Centers Coincide

Let us consider the case when N point interactions coincide at the origin and take $\lambda_1 = \dots = \lambda_N = \lambda$ for simplicity. Then, the principal matrix given in (3.52) becomes

$$\Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda} - \sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & \text{if } i = j, \\ -\sqrt{\frac{m}{2}} \frac{1}{\hbar\nu} & \text{if } i \neq j. \end{cases} \quad (3.74)$$

To find bound state energies from the $\det \Phi_{ij}(\nu) = 0$, we are going to use the below formula (Meyer, 2001):

$$\det \begin{pmatrix} \alpha & \gamma & \dots & \gamma \\ \gamma & \alpha & \dots & \gamma \\ \gamma & \gamma & \ddots & \gamma \\ \gamma & \gamma & \dots & \alpha \end{pmatrix}_{(N \times N)} = (\alpha - \gamma)^N \left(1 + \frac{N\gamma}{\alpha - \gamma} \right). \quad (3.75)$$

Hence,

$$\det \Phi_{ij}(\nu) = \left(\frac{1}{\lambda}\right)^N \left[1 + \frac{N \left(-\sqrt{\frac{m}{2}} \frac{1}{\hbar\nu}\right)}{\frac{1}{\lambda}}\right] = 0. \quad (3.76)$$

Then, we have $1 - \sqrt{\frac{m}{2}} \frac{N\lambda}{\hbar\nu} = 0$ which means that

$$\nu = \sqrt{\frac{m}{2}} \frac{N\lambda}{\hbar}. \quad (3.77)$$

Therefore, the bound state energy is

$$E = -\nu^2 = -\frac{mN^2\lambda^2}{2\hbar^2}. \quad (3.78)$$

Remark 3.5 *The result is evident because $\lambda_1\delta(x) + \dots + \lambda_N\delta(x) = N\lambda\delta(x)$ and replacing $\lambda \rightarrow N\lambda$ for one Dirac delta potential in Eq. (3.7) gives the same result.*

Let us examine this problem for different values of λ_j . The matrix in Eq. (3.75) can be generalized by

$$\Phi_{ij}(\nu) = \begin{pmatrix} \alpha_1 & \gamma & \dots & \gamma \\ \gamma & \alpha_2 & \dots & \gamma \\ \gamma & \gamma & \ddots & \gamma \\ \gamma & \gamma & \dots & \alpha_N \end{pmatrix}_{(N \times N)}. \quad (3.79)$$

This matrix can be written as

$$\Phi_{ij}(\nu) = (\alpha_i - \gamma)\delta_{ij} + \gamma e_i e_j^T. \quad (3.80)$$

Here, $e_i = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}_{(N \times 1)}$ where 1 is located at the i -th row. We are going to use the formula given by (Meyer, 2001):

$$\det(A + cd^T) = \det A(1 + d^T A^{-1}c), \quad (3.81)$$

where A is nonsingular and c, d are $N \times 1$ columns. Therefore,

$$\det \Phi_{ij}(\nu) = \det[(\alpha_i - \gamma)\mathbb{I}] \left[1 + \sum_{i,j=1}^N e_j^T [(\alpha_i - \gamma)\delta_{ij}]^{-1} \gamma e_i \right], \quad (3.82)$$

then

$$\begin{aligned} \det \Phi_{ij}(\nu) &= \prod_{i=1}^N (\alpha_i - \gamma) \left[1 + \gamma \sum_{j=1}^N e_j^T \frac{1}{(\alpha_j - \gamma)} e_j \right] \\ &= \prod_{i=1}^N (\alpha_i - \gamma) \left[1 + \gamma \sum_{j=1}^N \frac{1}{(\alpha_j - \gamma)} \right]. \end{aligned} \quad (3.83)$$

We want to find the bound state energy, so $\det \Phi_{ij}(\nu) = 0$:

$$1 + \gamma \sum_{j=1}^N \frac{1}{(\alpha_j - \gamma)} = 0. \quad (3.84)$$

By inserting the original variables, $\gamma = -\sqrt{\frac{m}{2}} \frac{1}{\hbar \nu}$ and $\alpha_j = \frac{1}{\lambda_j} - \sqrt{\frac{m}{2}} \frac{1}{\hbar \nu}$, we obtain

$$\nu = \sqrt{\frac{m}{2}} \frac{1}{\hbar} \sum_{j=1}^N \lambda_j, \quad (3.85)$$

then

$$E = -\nu^2 = -\frac{m}{2\hbar^2} \left(\sum_{j=1}^N \lambda_j \right)^2 . \quad (3.86)$$

Remark 3.6 *It is also an evident answer since $\lambda_1\delta(x) + \dots + \lambda_N\delta(x) = (\lambda_1 + \dots + \lambda_N)\delta(x)$ and replacing $\lambda \rightarrow \lambda_1 + \dots + \lambda_N$ for one Dirac delta potential in Eq. (3.7) gives the same result. But, interesting point is that to derive such simple results we need to use quite sophisticated formulas from linear algebra.*

3.4. Formal Analysis of Point Interaction in Two Dimensions

The time-independent Schrödinger equation in two dimensions with a point interaction (formally), centered at the origin, is

$$-\frac{\hbar^2}{2m} \Delta \psi(x, y) - \lambda \delta^{(2)}(x, y) \psi(x, y) = -\nu^2 \psi(x, y) , \quad (3.87)$$

where $\delta^{(2)}(x, y) = \delta(x)\delta(y)$ defined in Eq. (2.30) and Δ is the Laplace operator defined on $L^2(\mathbb{R}^2)$. By applying the formal Fourier transform to the Schrödinger equation, we obtain

$$\left(\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \nu^2 \right) \widehat{\psi}(p_x, p_y) = \lambda \psi(0, 0) , \quad (3.88)$$

or, equivalently, it can be written as a singular integral equation:

$$\widehat{\psi}(\mathbf{p}) = \int_{\mathbb{R}^2} \left[\frac{\lambda}{\nu^2} - \frac{(\mathbf{q}^2)(2\pi\hbar)^2 \delta^{(2)}(\mathbf{q} - \mathbf{p})}{2m\nu^2} \right] \widehat{\psi}(\mathbf{q}) [d^2q] , \quad (3.89)$$

where the expression inside of the bracket is the integral kernel where \mathbf{p} denotes (p_x, p_y) and \mathbf{q} denotes (q_x, q_y) .

Let us define $\lambda\psi(0,0) = C$ in Eq. (3.88), where C is a constant and after the consistency condition, to find

$$\frac{1}{\lambda} = \int_{\mathbb{R}^2} \frac{1}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^2p]. \quad (3.90)$$

But, this integral is divergent, as can be easily checked in polar coordinates, namely

$$\begin{aligned} \frac{1}{\lambda} &= \frac{m}{\pi\hbar^2} \int_0^\infty \frac{p}{p^2 + 2m\nu^2} dp = \frac{m}{\pi\hbar^2} \lim_{\Lambda \rightarrow \infty} \int_0^\Lambda \frac{p}{p^2 + 2m\nu^2} dp \\ &= \frac{m}{2\pi\hbar^2} \lim_{\Lambda \rightarrow \infty} \ln \left| \frac{\Lambda^2 + 2m\nu^2}{2m\nu^2} \right|, \end{aligned} \quad (3.91)$$

where $|\mathbf{p}| = p$. This happens due to the large values of momenta and it is known as ultraviolet divergence (UV). Actually, this divergence occurs due to the scaling symmetry of the problem (Jackiw, 1995): Suppose that the ground state energy is $E = -\nu^2$. Let us rescale \mathbf{x} with η , i.e., $\mathbf{x} \rightarrow \eta\mathbf{x}$ ($\mathbf{x} = \eta\mathbf{x}'$) where $\eta \in \mathbb{R}^+$. Then the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{1}{\eta^2} \Delta' \tilde{\psi}(\mathbf{x}') - \frac{\lambda}{\eta^2} \delta^{(2)}(\mathbf{x}') \tilde{\psi}(\mathbf{x}') = -\nu^2 \tilde{\psi}(\mathbf{x}'), \quad (3.92)$$

where $\mathbf{x} = (x, y)$, Δ' denotes the Laplacian with respect to the \mathbf{x}' variables and $\psi(\eta\mathbf{x}') = \tilde{\psi}(\mathbf{x}')$. Also, we have used the fact that $\Delta \rightarrow \frac{1}{\eta^2} \Delta$ and the normalization of $\delta^{(2)}(\mathbf{x})$ from Eq. (2.6) gives that $\delta^{(2)}(\eta\mathbf{x}') \rightarrow \frac{1}{\eta^2} \delta^{(2)}(\mathbf{x}')$. Hence,

$$-\frac{\hbar^2}{2m} \Delta \tilde{\psi}(\mathbf{x}) - \lambda \delta^{(2)}(\mathbf{x}) \tilde{\psi}(\mathbf{x}) = -\eta^2 \nu^2 \tilde{\psi}(\mathbf{x}), \quad (3.93)$$

where we have relabeled the variables $\mathbf{x}' \leftrightarrow \mathbf{x}$. This means that we can always find a ground state energy lower than $-\nu^2$, energy is unbounded from below which has no sense physically. In the following section, we are going to show how to make sense of these infinities.

Although one-dimensional problem works very well in physical applications, what could go wrong in its two-dimensional version? In order to cure this problem, we need to consult a well-known procedure, called renormalization, firstly introduced in quantum field theory.

Actually, this problem still appears in the higher-dimensional cases, as well. One reason is: A typical Hamiltonian contains the kinetic and the potential energy operators. Al-

though the formal expression is Hermitian (symmetric), it may not be self-adjoint in general (that is $D(H) \neq D(H^\dagger)$) (Reed & Simon, 1975) and when the short-distance behavior of the potential function is same or more singular than that of the kinetic energy part, this problem appears and the eigenvalue problem $H\psi = E\psi$ leads to nonphysical results and the dynamics are not well-defined (Jackiw, 1995).

3.5. Renormalization of Point Interaction

Let us explain the basic idea of the renormalization method, which is commonly used in quantum field theory (Zee, 2010). Then, we apply this method to our problem and show how we can remove the divergences in the problem.

Let O_1, O_2, O_3, \dots be measurable quantities for a given physical system (they are functions of parameters in the system, e.g., coupling constant, mass, charge, etc...) (Mead & Godines, 1991). We first modify the theory by changing the large momentum behavior of the potential involved. The theory is assumed to be correct up to a definite momentum scale, say Λ (called cut-off) since we expect that every theory should have a domain of validity. Next, we make all the divergent integrals finite by restricting the upper limit of the integrals via the cut-off parameter. Then, these quantities O_1, O_2, O_3, \dots become functions of Λ and finite:

$$\begin{aligned} O_1 &= f_1(\lambda, \Lambda) \\ O_2 &= f_2(\lambda, \Lambda) \\ &\vdots \end{aligned} \tag{3.94}$$

However, they are divergent as $\Lambda \rightarrow \infty$. This part of the procedure is called regularization (for different regularization schemes, see Appendix B). In general, measurable quantities O_1, O_2, \dots are difficult to calculate exactly so they are computed perturbatively. Then, we solve the first equation for λ as a function of O_1 and Λ and insert the experimentally measured value, say $\langle O_1 \rangle$, to get

$$\lambda(\Lambda) = f_1^{-1}(\langle O_1 \rangle, \Lambda) . \tag{3.95}$$

After that, we substitute this value of $\lambda(\Lambda)$ into the expressions for all other observables:

$$\begin{aligned} O_2 &= f_2(f_1^{-1}(\langle O_1 \rangle, \Lambda), \Lambda) \\ O_3 &= f_3(f_1^{-1}(\langle O_1 \rangle, \Lambda), \Lambda), \text{ etc. ,} \end{aligned} \quad (3.96)$$

and we take the limit $\Lambda \rightarrow \infty$ at the end. If all measurable quantities O_2, O_3, \dots are found to be finite at the end of the procedure, then the procedure is completed and one can check O_2, O_3, \dots with experiments for the predictability of the theory. If O_2, O_3, \dots are still divergent, we must go back to the beginning of the procedure and repeat it for the other parameters in the model. If we are able to find finite results for all measurable quantities at the end of these procedures, the theory is said to be renormalizable.

Let us return now to our problem and apply this formal procedure. Let O_1 be the bound state energy of our system and O_2 be the scattering cross section of the particle from the Dirac delta-center located at $\mathbf{x} = \mathbf{0}$. Now we are going to regularize the system by introducing the characteristic function:

$$\Theta_\Lambda(\mathbf{p}) = \begin{cases} 0 & \text{if } |\mathbf{p}| > \Lambda, \\ 1 & \text{if } |\mathbf{p}| \leq \Lambda. \end{cases} \quad (3.97)$$

Firstly, let us insert the characteristic function into (3.90) and solve the integral for $E = -nu^2$, then

$$O_1 = E = -\frac{\left(\frac{\Lambda^2}{2m}\right)}{\left(e^{\frac{2\pi\hbar^2}{m\lambda}} - 1\right)}. \quad (3.98)$$

Since right-hand side is not real-analytic function in terms of λ (the right hand side of (3.98) cannot be written as a geometric sum), this shows that the bound state energies cannot be analyzed perturbatively. Next, we solve the above equation for λ and insert the experimentally measured bound state energy, say $E = -\nu^2 = -\mu^2$. Therefore,

$$\frac{1}{\lambda(\Lambda)} = \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \mu^2} [d^2p], \quad (3.99)$$

where $\lambda(\Lambda)$ is called the bare coupling constant. Note that as $\Lambda \rightarrow \infty$, $\lambda(\Lambda) \rightarrow 0$. This

is called the asymptotic freedom in quantum field theory. One should then check that the scattering cross section of this problem is finite by choosing (3.99). For this reason, let us rewrite the time-independent Schrödinger equation in two dimensions in the following form (Merzbacher, 1961)

$$(\Delta + k^2) \psi(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r}) \psi(\mathbf{r}) , \quad (3.100)$$

where $E = \frac{\hbar^2 k^2}{2m}$ is the energy of the incoming particle and $\mathbf{r} = (x, y)$. This equation is an inhomogeneous differential equation, so the Green's function method would be useful. After similar calculations as we did in one-dimensional scattering problem, the Green's function in two dimensions associated with $-\frac{\hbar^2}{2m} \Delta + V$ can be easily found as

$$G(\mathbf{r}) = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}}}{k^2 - \frac{p^2}{\hbar^2}} [d^2 p] . \quad (3.101)$$

By using the polar coordinates, the above integral turns out to be

$$G(\mathbf{r}) = -\frac{1}{4\pi^2} \int_0^{2\pi} \int_0^\infty \frac{e^{\frac{ipr \cos \theta}{\hbar}}}{p^2 - \hbar^2 k^2} p \, dp \, d\theta . \quad (3.102)$$

Since the integral representation of the Bessel function of the first kind is (Lebedev, 1965):

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix \cos \theta} \, d\theta , \quad (3.103)$$

the integral over θ can be evaluated, so that

$$G(\mathbf{r}) = -\frac{1}{2\pi} \int_0^\infty \frac{J_0\left(\frac{pr}{\hbar}\right)}{p^2 - \hbar^2 k^2} p \, dp . \quad (3.104)$$

By using an another integral representation of $J_0(x)$ (Lebedev, 1965):

$$J_0(x) = \frac{2}{\pi} \int_1^\infty \frac{\sin(xt)}{\sqrt{t^2 - 1}} \, dt , \quad (3.105)$$

we obtain

$$G(\mathbf{r}) = -\frac{1}{\pi^2} \int_1^\infty \left[\int_0^\infty \frac{\sin(\frac{prt}{\hbar})}{p^2 - \hbar^2 k^2} p \, dp \right] \frac{1}{\sqrt{t^2 - 1}} \, dt . \quad (3.106)$$

It is clear that

$$\begin{aligned} I(\mathbf{r}) &= \int_0^\infty \frac{\sin(\frac{prt}{\hbar})}{p^2 - \hbar^2 k^2} p \, dp = \frac{1}{2i} \int_0^\infty \frac{e^{\frac{iprt}{\hbar}} - e^{-\frac{iprt}{\hbar}}}{p^2 - \hbar^2 k^2} p \, dp \\ &= \frac{1}{2i} \int_{\mathbb{R}} \frac{e^{\frac{iprt}{\hbar}}}{p^2 - \hbar^2 k^2} p \, dp . \end{aligned} \quad (3.107)$$

After Feynman's trick, the above integral becomes

$$I_\epsilon^{(+)}(\mathbf{r}) = \frac{1}{2i} \int_{\mathbb{R}} \frac{e^{\frac{iprt}{\hbar}}}{p^2 - (\hbar^2 k^2 + i\epsilon)} p \, dp . \quad (3.108)$$

From Eq. (3.38), the simple poles are at $p = \pm (\hbar k + \frac{i\epsilon}{2\hbar k})$. After using the residue theorem and then taking the limit $\epsilon \rightarrow 0$, we obtain

$$\lim_{\epsilon \rightarrow 0} I_\epsilon^{(+)}(\mathbf{r}) = I^{(+)}(\mathbf{r}) = \frac{\pi}{2} e^{ikrt} . \quad (3.109)$$

Therefore, Eq. (3.106) becomes

$$G^{(+)}(\mathbf{r}) = -\frac{1}{2\pi} \int_1^\infty \frac{e^{ikrt}}{\sqrt{t^2 - 1}} \, dt . \quad (3.110)$$

By using the integral representation of the Hankel function of the first kind of order zero (Lebedev, 1965):

$$H_0^{(1)}(z) = \frac{2}{\pi i} \int_1^\infty \frac{e^{izt}}{\sqrt{t^2 - 1}} \, dt , \quad (3.111)$$

the Green's function in two dimensions becomes

$$G^{(+)}(\mathbf{r} - \mathbf{r}') = -\frac{i}{4}H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|) . \quad (3.112)$$

Since the general solution to the scattering problem is given by

$$\psi^{(+)}(\mathbf{r}) = Ne^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2} \int_{\mathbb{R}^2} G^{(+)}(\mathbf{r} - \mathbf{r}')V(\mathbf{r}')\psi^{(+)}(\mathbf{r}') d^2r' , \quad (3.113)$$

called the Lippmann-Schwinger equation in the coordinate representation in two dimensions (Merzbacher, 1961), we obtain

$$\psi^{(+)}(\mathbf{r}) = Ne^{i\mathbf{k}\cdot\mathbf{r}} - \frac{im}{2\hbar^2} \int_{\mathbb{R}^2} H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|)V(\mathbf{r}')\psi^{(+)}(\mathbf{r}') d^2r' . \quad (3.114)$$

If we substitute $V(\mathbf{r}) = -\lambda(\Lambda)\delta^{(2)}(\mathbf{r})$ into the above equation, we get

$$\psi^{(+)}(\mathbf{r}) = Ne^{i\mathbf{k}\cdot\mathbf{r}} + \frac{im\lambda(\Lambda)}{2\hbar^2}H_0^{(1)}(kr)\psi^{(+)}(\mathbf{0}) . \quad (3.115)$$

As $r \rightarrow \infty$, the asymptotic expansion of the Hankel function of the first kind of order zero is given by (Lebedev, 1965):

$$\frac{im\lambda(\Lambda)}{2\hbar^2}H_0^{(1)}(kr) \sim \frac{im\lambda(\Lambda)}{2\hbar^2} \sqrt{\frac{2}{\pi kr}} e^{i(kr - \frac{\pi}{4})} = \frac{m\lambda(\Lambda)}{\hbar^2\sqrt{2\pi kr}} e^{i(kr + \frac{\pi}{4})} . \quad (3.116)$$

Therefore, asymptotically Eq. (3.115) becomes

$$\psi^{(+)}(\mathbf{r}) \sim Ne^{i\mathbf{k}\cdot\mathbf{r}} + \frac{m\lambda(\Lambda)}{\hbar^2\sqrt{2\pi kr}}\psi^{(+)}(\mathbf{0})e^{i(kr + \frac{\pi}{4})} . \quad (3.117)$$

The asymptotic behavior of the wave function in two dimensions for the scattering problem is expected to be

$$\psi^{(+)}(\mathbf{r}) \sim Ne^{i\mathbf{k}\cdot\mathbf{r}} + \frac{f_{\mathbf{k}}(\mathbf{r})}{\sqrt{r}}e^{i(kr + \frac{\pi}{4})} , \quad (3.118)$$

where $f_{\mathbf{k}}(\mathbf{r})$ is the scattering amplitude. If we compare equations (3.117) and (3.118), we get

$$f_{\mathbf{k}}^{\Lambda}(\mathbf{r}) = \frac{m\lambda(\Lambda)\psi^{(+)}(\mathbf{0})}{\hbar^2\sqrt{2\pi k}}. \quad (3.119)$$

In order to evaluate this expression, we must find $\lambda(\Lambda)\psi^{(+)}(\mathbf{0})$. For this reason, we take the formal Fourier transform of $\psi(\mathbf{r}) = Ne^{i\mathbf{k}\cdot\mathbf{r}}$, where $N = (2\pi\hbar)^2$ is the normalization constant, and Eq. (3.100) with the potential $V(\mathbf{r}) = -\lambda(\Lambda)\delta(\mathbf{r})$, then after Feynman's trick, the distributional solution of (3.100) is

$$\widehat{\psi}^{(+)}(\mathbf{p}) = (2\pi\hbar)^2\delta^{(2)}\left(\frac{\mathbf{p}}{\hbar} - \mathbf{k}\right) + \frac{2m\lambda(\Lambda)\psi^{(+)}(\mathbf{0})}{p^2 - (\hbar^2k^2 + i\epsilon)}. \quad (3.120)$$

By substituting this solution into the formal inverse Fourier transform given by

$$\psi^{(+)}(\mathbf{0}) = \int_{\mathbb{R}^2} \widehat{\psi}^{(+)}(\mathbf{p}) [d^2p], \quad (3.121)$$

we obtain

$$\psi^{(+)}(\mathbf{0}) = 1 + 2m\lambda(\Lambda)\psi^{(+)}(\mathbf{0}) \int_{\mathbb{R}^2} \frac{\Theta_{\Lambda}(\mathbf{p})}{p^2 - (\hbar^2k^2 + i\epsilon)} [d^2p]. \quad (3.122)$$

Let us define $I_{\epsilon}^{\Lambda}(\mathbf{k}) = 2m \int_{\mathbb{R}^2} \frac{\Theta_{\Lambda}(\mathbf{p})}{p^2 - (\hbar^2k^2 + i\epsilon)} [d^2p]$. Therefore,

$$\begin{aligned} \lambda(\Lambda)\psi^{(+)}(\mathbf{0}) &= \left[\frac{1}{\lambda(\Lambda)} - I_{\epsilon}^{\Lambda}(\mathbf{k}) \right]^{-1} \\ &= \left[2m \int_{\mathbb{R}^2} \left(\frac{\Theta_{\Lambda}(\mathbf{p})}{p^2 + 2m\mu^2} - \frac{\Theta_{\Lambda}(\mathbf{p})}{p^2 - (\hbar^2k^2 + i\epsilon)} \right) [d^2p] \right]^{-1}, \end{aligned} \quad (3.123)$$

where $\frac{1}{\lambda(\Lambda)}$ was chosen as in (3.99). After calculating this and taking the limit $\Lambda \rightarrow \infty$, we find

$$\lim_{\Lambda \rightarrow \infty} \lambda(\Lambda)\psi^{(+)}(\mathbf{0}) = \left[\frac{m}{2\pi\hbar^2} \ln \left(-\frac{\hbar^2k^2 + i\epsilon}{2m\mu^2} \right) \right]^{-1}. \quad (3.124)$$

By taking the limit $\epsilon \rightarrow 0^+$ yields

$$\lim_{\epsilon \rightarrow 0^+} \left[\lim_{\Lambda \rightarrow \infty} \lambda(\Lambda) \psi^{(+)}(\mathbf{0}) \right] = \frac{\pi \hbar^2}{m} \left[\ln \left(\frac{\hbar k}{\sqrt{2m\mu}} \right) - \frac{i\pi}{2} \right]^{-1}, \quad (3.125)$$

where we have chosen the principal branch of the logarithm while taking the limit. By inserting this value into Eq. (3.119), we get

$$f_{\mathbf{k}}(\mathbf{r}) = \sqrt{\frac{\pi}{2k}} \left[\ln \left(\frac{\hbar k}{\sqrt{2m\mu}} \right) - \frac{i\pi}{2} \right]^{-1}. \quad (3.126)$$

Notice that the scattering amplitude does not depend on θ , that is the scattering is isotropic, which is physically expected. Since the scattering differential cross section is given by $\frac{d\sigma}{d\theta} = |f(\theta)|^2$, the total cross section can be easily found as

$$O_2 = \sigma = \frac{4\pi^2 \hbar}{\sqrt{2mE}} \left[\frac{1}{\ln^2 \left(\frac{E}{\mu^2} \right) + \pi^2} \right], \quad (3.127)$$

which is the second measurable quantity and it is finite and completes the renormalization procedure. Since the parameter μ appears due to the renormalization procedure, it is an example of dimensional transmutation. Note that total cross section decreases as the bound state energy $-\mu^2$ increases. The generalization for multiple Dirac delta centers can be done by the above formulation. The result for two centers is given in (Altunkaynak, 2002) if the wave number of incoming particle is perpendicular to the distance between the centers.

Let us calculate the bound state wave function now. In order to do this, we should first write the regularized wave function $\psi_\Lambda(\mathbf{x})$ and let us assume that $\lim_{\Lambda \rightarrow \infty} 2\pi\lambda(\Lambda)\psi_\Lambda(\mathbf{0}) = C$, where C is some constant. Since the regularized momentum space wave function

$$\hat{\psi}_\Lambda(\mathbf{p}) = \frac{\lambda(\Lambda)\psi_\Lambda(\mathbf{0})}{\frac{\mathbf{p}^2}{2m} + \mu^2}, \quad (3.128)$$

where we have used Eq. (3.89), we obtain the bound state wave function for point interaction

in \mathbb{R}^2 after taking the limit $\Lambda \rightarrow \infty$

$$\psi(\mathbf{x}) = \frac{\sqrt{2m\mu}}{\hbar\sqrt{\pi}} K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} |\mathbf{x}| \right), \quad (3.129)$$

where we find C from the normalization condition. Here, we have used the integral representation of the modified Bessel function of the third kind (Lebedev, 1965)

$$K_0(ab) = \int_0^\infty \frac{x}{x^2 + a^2} J_0(bx) dx, \quad (3.130)$$

and the integral representation of the Bessel function of the first kind given in Eq. (3.103).

Remark 3.7 *We will give a more rigorous proof of the above result in Chapter 4.*

Remark 3.8 *The asymptotic expansion of K_0 for small values of x is given by (Lebedev, 1965)*

$$K_0(x) \sim -\ln\left(\frac{x}{2}\right) + \gamma, \quad (3.131)$$

where γ is the Euler's constant. Hence, the bound state wave function (3.129) blows up near the origin.

Lemma 3.2 *The bound state wave function (3.129) is an element of $L^2(\mathbb{R}^2)$ but $\Delta\psi(\mathbf{x}) \notin L^2(\mathbb{R}^2)$.*

Proof In polar coordinates, we have

$$\int_{\mathbb{R}^2} |\psi(\mathbf{x})|^2 d^2x = \frac{4m\mu^2}{\hbar^2} \int_0^\infty r \left[K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} r \right) \right]^2 dr. \quad (3.132)$$

If we change the variables $\frac{\sqrt{2m\mu}}{\hbar} r = y$, we obtain

$$\int_{\mathbb{R}^2} |\psi(\mathbf{x})|^2 d^2x = 2 \int_0^\infty y [K_0(y)]^2 dy = 1, \quad (3.133)$$

where we have used $\int_0^\infty y[K_0(y)]^2 dy = \frac{1}{2}$ (Gradshteyn & Ryzhik, 2000). This means that the wave function is normalized and an element of $L^2(\mathbb{R}^2)$. However, consider

$$\begin{aligned} \int_{\mathbb{R}^2} |\Delta\psi(\mathbf{x})|^2 d^2x &= \frac{2m\mu^2}{\hbar^2\pi} \int_{\mathbb{R}^2} \left| \Delta K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} |\mathbf{x}| \right) \right|^2 d^2x \\ &= \frac{4m\mu^2}{\hbar^2} \int_0^\infty \left[\frac{d^2}{dr^2} K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} r \right) \right]^2 r dr . \end{aligned} \quad (3.134)$$

Here, we have used polar coordinates. From recurrence relations of the Bessel functions (Lebedev, 1965), we have

$$\frac{d^2 K_0(ar)}{dr^2} = a^2 K_0(ar) + \frac{a}{r} K_1(ar) . \quad (3.135)$$

Therefore,

$$\begin{aligned} \int_0^\infty \left[\frac{d^2}{dr^2} K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} r \right) \right]^2 r dr &= \int_0^\infty \left[\frac{2m\mu^2}{\hbar^2} K_0 \left(\frac{\sqrt{2m\mu}}{\hbar} r \right) \right. \\ &\quad \left. + \frac{\sqrt{2m\mu}}{\hbar r} K_1 \left(\frac{\sqrt{2m\mu}}{\hbar} r \right) \right]^2 r dr . \end{aligned} \quad (3.136)$$

From the asymptotic expansion of K_0 given by (3.131), we have

$$\int_0^\infty K_0(ar) K_1(ar) dr \sim a \int_0^\infty \left[-\ln \left(\frac{ar}{2} \right) + \gamma \right] \frac{1}{r} dr , \quad (3.137)$$

where $a = \frac{\sqrt{2m\mu}}{\hbar}$ and we have used $K_1(ar) = -a \frac{dK_0(ar)}{dr}$ (Lebedev, 1965). But, one can easily see that this integral is divergent near $r = 0$ because of the second term. \square

3.6. Formal Analysis of Finitely Many Point Interactions in Two Dimensions

The time-independent Schrödinger equation in two dimensions with N point interactions (formally) is

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x}) - \sum_{i=1}^N \lambda_i \delta^{(2)}(\mathbf{x} - \mathbf{a}_i)\psi(\mathbf{x}) = -\nu^2\psi(\mathbf{x}), \quad (3.138)$$

where \mathbf{a}_i is the location of the i -th point interaction for $i = 1, \dots, N$. Suppose that $\mathbf{a}_i \neq \mathbf{a}_j$ for $i \neq j$ and let $d_{min} = \min_{i,j} |\mathbf{a}_i - \mathbf{a}_j| > 0$. By applying the formal Fourier transform, we obtain

$$\left(\frac{\mathbf{p}^2}{2m} + \nu^2\right) \widehat{\psi}(\mathbf{p}) = \sum_{i=1}^N \lambda_i \psi(\mathbf{a}_i) e^{-\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}}, \quad (3.139)$$

or, it can be written as a singular integral equation:

$$\widehat{\psi}(\mathbf{p}) = \int_{\mathbb{R}^2} \left[\sum_{i=1}^N \frac{\lambda_i e^{\frac{i(\mathbf{q}-\mathbf{p})\cdot\mathbf{a}_i}{\hbar}}}{\nu^2} - \frac{\mathbf{q}^2 (2\pi\hbar)^2 \delta^{(2)}(\mathbf{q} - \mathbf{p})}{2m\nu^2} \right] \widehat{\psi}(\mathbf{q}) [d^2q], \quad (3.140)$$

where the expression inside of the bracket is the integral kernel.

Let us denote $\lambda_i \psi(\mathbf{a}_i) = A_i$ in Eq. (3.139). The consistency after the regularization implies

$$\left[\frac{1}{\lambda_i} - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^2p] \right] A_i - \int_{\mathbb{R}^2} \sum_{\substack{j=1 \\ j \neq i}}^N \left[\frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^2p] \right] A_j = 0. \quad (3.141)$$

This equation can be written as a matrix equation:

$$\sum_{j=1}^N \Phi_{ij}^\Lambda(\nu) A_j = 0, \quad (3.142)$$

where

$$\Phi_{ij}^{\Lambda}(\nu) = \begin{cases} \frac{1}{\lambda_i(\Lambda)} - \int_{\mathbb{R}^2} \frac{\Theta_{\Lambda}(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^2p] & \text{if } i = j, \\ - \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{p} \cdot (\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \Theta_{\Lambda}(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^2p] & \text{if } i \neq j, \end{cases} \quad (3.143)$$

is called the regularized principal matrix. In this problem, we may have several measurable quantities, namely

O_1 : The bound state energy of the particle to the i -th point interaction in the absence of the other centers.

O_2 : The bound state energy of the particle to the i -th and j -th point interactions in the absence of the other centers.

⋮

O_N : The bound state energy of the particle to the N point interactions.

O_{N+1} : Scattering cross section of the particle from the N point interactions.

For $N = 1$ sector, $\det \Phi_{ij}^{\Lambda}(\nu) = 0$ reduces to

$$\frac{1}{\lambda_i(\Lambda)} = \int_{\mathbb{R}^2} \frac{\Theta_{\Lambda}(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \mu_i^2} [d^2p], \quad (3.144)$$

where $-\mu_i^2$ is the experimentally measured bound state energy of the particle to the i -th point interaction. We then substitute this value of $\lambda_i(\Lambda)$ to check whether the other measurable quantities are finite or not. For this purpose, we take the limit $\Lambda \rightarrow \infty$ after inserting this value into Eq. (3.143), then we find the renormalized principal matrix:

$$\Phi_{ij}(\nu) = \begin{cases} \frac{m}{\pi \hbar^2} \ln \left(\frac{\nu}{\mu_i} \right) & \text{if } i = j, \\ - \frac{m}{\pi \hbar^2} K_0 \left(\frac{\nu \sqrt{2m} |\mathbf{a}_i - \mathbf{a}_j|}{\hbar} \right) & \text{if } i \neq j, \end{cases} \quad (3.145)$$

where we have used the integral representation of the Bessel function of the first kind J_0 and the modified Bessel function of the third kind K_0 which were given in Eq. (3.103) and Eq. (3.130), respectively.

This matrix can also be written as

$$\Phi_{ij}(\nu) = \delta_{ij} \frac{m}{\pi \hbar^2} \ln \left(\frac{\nu}{\mu_i} \right) + (1 - \delta_{ij}) \left(-\frac{m}{\pi \hbar^2} \right) K_0 \left(\frac{\nu \sqrt{2m} |\mathbf{a}_i - \mathbf{a}_j|}{\hbar} \right), \quad (3.146)$$

where δ_{ij} is the Kronecker's delta given in (2.1).

Remark 3.9 *In contrast to the one-dimensional case for N point interactions, the centers of the point interactions here are not allowed to coincide because of the divergence in the off-diagonal term of the renormalized principal matrix (3.145). There is a nonphysical singularity.*

3.6.1. Two-center Case

Theorem 3.6 *For two-center case, there are at most two bound states. If $d > d_{critical} = \frac{\sqrt{2}\hbar e^\gamma}{\sqrt{m\mu_1\mu_2}}$, there are exactly two bound states.*

Proof For $N = 2$ in Eq. (3.145), we have a 2×2 renormalized principal matrix:

$$\Phi(\nu) = \frac{m}{\pi \hbar^2} \begin{pmatrix} \ln \left(\frac{\nu}{\mu_1} \right) & -K_0 \left(\frac{\nu \sqrt{2m} |\mathbf{a}_1 - \mathbf{a}_2|}{\hbar} \right) \\ -K_0 \left(\frac{\nu \sqrt{2m} |\mathbf{a}_1 - \mathbf{a}_2|}{\hbar} \right) & \ln \left(\frac{\nu}{\mu_2} \right) \end{pmatrix}. \quad (3.147)$$

We need to solve $\det \Phi(\nu) = 0$ for the purpose of finding the bound state energies. Then,

$$\ln \left(\frac{\nu}{\mu_1} \right) \ln \left(\frac{\nu}{\mu_2} \right) = K_0^2 \left(\frac{\nu}{\mu_d} \right), \quad (3.148)$$

where $\mu_d = \frac{\hbar}{d\sqrt{2m}}$ and $d = |\mathbf{a}_1 - \mathbf{a}_2|$. Let us write this equation in terms of the dimensionless variables:

$$\ln(\alpha_1 x) \ln(\alpha_2 x) = K_0^2(x), \quad (3.149)$$

where $x = \frac{\nu}{\mu_d}$, $\alpha_1 = \frac{\mu_d}{\mu_1}$ and $\alpha_2 = \frac{\mu_d}{\mu_2}$. Since this equation is a transcendental equation, it is difficult to find the exact solution so we are going to study the equation graphically and

asymptotically. Let us choose $\alpha_1 > \alpha_2$ without loss of generality. Firstly, let us show that we have at least one bound state energy.

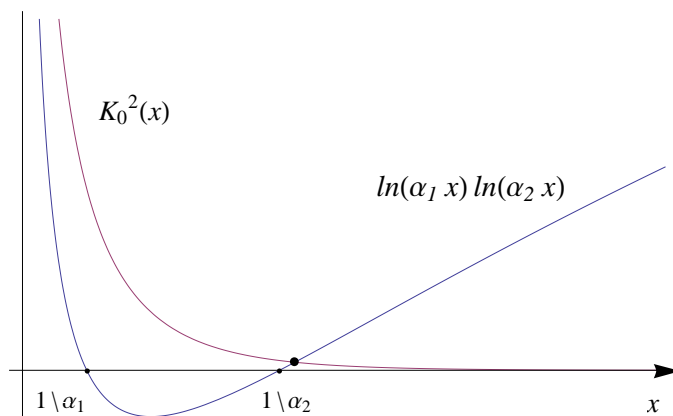


Figure 3.8. Graph of $\ln(\alpha_1 x) \ln(\alpha_2 x)$ and $K_0^2(x)$ for $\alpha_1 = 2$ and $\alpha_2 = 0.5$

On the interval $(0, \frac{1}{\alpha_1})$, $\ln(\alpha_1 x) \ln(\alpha_2 x)$ is monotonically decreasing and positive function. When $x > \frac{1}{\alpha_2}$, the function is monotonically increasing and positive. It is easy to see that $\ln(\alpha_1 x) \ln(\alpha_2 x)$ has a local minimum at $x = \frac{1}{\sqrt{\alpha_1 \alpha_2}}$, $\frac{1}{\alpha_1} < \frac{1}{\sqrt{\alpha_1 \alpha_2}} < \frac{1}{\alpha_2}$ (see Figure 3.8). Also, $K_0^2(x)$ is a monotonically decreasing function for $x > 0$. So, they should intersect each other at only one point for $x > \frac{1}{\alpha_2}$. Then, we have at least one root.

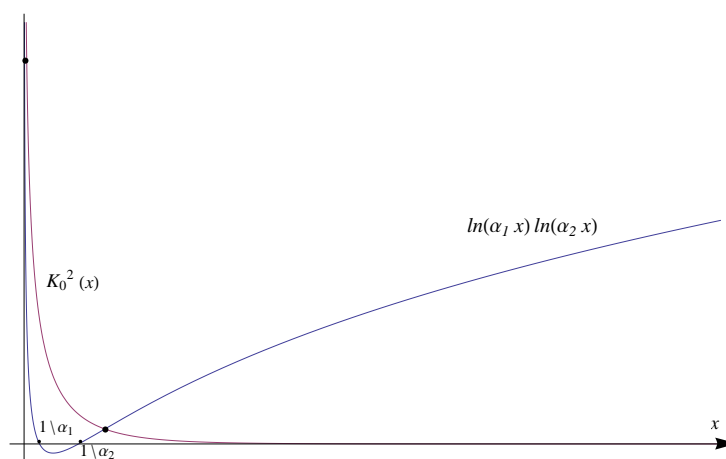


Figure 3.9. Graph of $\ln(\alpha_1 x) \ln(\alpha_2 x)$ and $K_0^2(x)$ for $\alpha_1 = 9$ and $\alpha_2 = 2.5$

If α_1 and α_2 are properly chosen, one can see that there may exist two bound state energies (see Figure 3.9). The necessary condition to have two roots is that

$$\ln(\alpha_1 x) \ln(\alpha_2 x) \gtrsim \left[-\ln\left(\frac{x}{2}\right) + \gamma \right]^2, \quad (3.150)$$

where we have used the asymptotic expansion of $K_0(x)$ near $x = 0$, which is given in Eq. (3.131). The above equation can be rewritten as

$$\ln(\alpha_1 x) \left[\ln(\alpha_1 x) + \ln\left(\frac{\alpha_2}{\alpha_1}\right) \right] \gtrsim \left[-\ln\left(\frac{\alpha_1 x}{\alpha_1}\right) + \ln 2 + \ln e^\gamma \right]^2. \quad (3.151)$$

Hence,

$$\ln(\alpha_1 x) \left[2 \ln(2\alpha_1 e^\gamma) + \ln\left(\frac{\alpha_2}{\alpha_1}\right) \right] \gtrsim \ln^2(2\alpha_1 e^\gamma) > 0. \quad (3.152)$$

We are interested in the region $x < \frac{1}{\alpha_1}$, so $\ln(\alpha_1 x) < 0$. Therefore,

$$\ln\left(\frac{\alpha_2}{\alpha_1}\right) + 2 \ln(2\alpha_1 e^\gamma) < 0. \quad (3.153)$$

After solving this, we obtain

$$d > \frac{\sqrt{2}\hbar e^\gamma}{\sqrt{m\mu_1\mu_2}} = d_{critical}, \quad (3.154)$$

which is the condition for the existence of two bound states.

One also easily check that for $d > \frac{\sqrt{2}\hbar e^\gamma}{\sqrt{m\mu_1\mu_2}}$,

$$\left| \frac{d}{dx} [\ln(\alpha_1 x) \ln(\alpha_2 x)] \right| > \left| \frac{d}{dx} K_0^2(x) \right|, \quad (3.155)$$

near $x = 0$. (This condition guarantees that the function $\ln(\alpha_1 x) \ln(\alpha_2 x)$ should blow up faster than $K_0^2(x)$ near $x = 0$.)

We can say that if the distance between the centers of point interactions is greater than some critical distance, then we have two bound state energies. Otherwise, we have one bound state energy. \square

We are going to show also that for N point interactions, we have at most N bound states. But, this is going to be shown in the next chapter using the resolvent formulation of the problem.

In particular, let us take $\mu = \mu_1 = \mu_2$ in Eq. (3.148). Then,

$$\ln \left(\frac{\nu}{\mu} \right) = \pm K_0 \left(\frac{d\sqrt{2m}}{\hbar} \nu \right). \quad (3.156)$$

We are going to find the difference between odd and even-parity energy levels ΔE as $d \rightarrow \infty$ as we did for N point interactions in one dimension. The asymptotic expansion of $K_0(x)$ as $x \rightarrow \infty$ is given by (Lebedev, 1965)

$$K_0(x) \sim \sqrt{\frac{\pi}{2x}} e^{-x}. \quad (3.157)$$

Therefore, for the positive root ν_+ , Eq. (3.156) becomes

$$\ln \left(\frac{\nu_+}{\mu} \right) \sim \sqrt{\frac{\pi \hbar}{2d\sqrt{2m}\nu_+}} e^{-\frac{2d\sqrt{2m}\nu_+}{\hbar}}. \quad (3.158)$$

As $d \rightarrow \infty$, the left-hand side of the above equation dominates so that we treat the right-hand side of this equation as a correction and it goes to zero as $d \rightarrow \infty$. So that we obtain $\nu_+ \sim \mu$ for the first order by the successive approximation (Olver, 1974). After substituting this value of ν_+ into the right-hand side of Eq. (3.158) for the second order approximation, we have

$$\nu_+ \sim \mu \exp \left[\sqrt{\frac{\pi \hbar}{2d\mu\sqrt{2m}}} e^{-\frac{2d\mu\sqrt{2m}}{\hbar}} \right] = \mu e^\tau, \quad (3.159)$$

where $\tau \equiv \sqrt{\frac{\pi \hbar}{2d\mu\sqrt{2m}}} e^{-\frac{2d\mu\sqrt{2m}}{\hbar}}$ for simplicity. One can similarly obtain that

$$\nu_- \sim \mu e^{-\tau}. \quad (3.160)$$

Then,

$$\Delta E = -\nu_-^2 + \nu_+^2 \sim 2\mu^2 \sinh(2\tau) . \quad (3.161)$$

Since $\tau \rightarrow 0$ exponentially as $d \rightarrow \infty$, $\Delta E \rightarrow 0$ and that means the energy levels become degenerate.

Finally, we must notice that the linear eigenvalue problem given at the beginning, $H\psi = E\psi$, is converted to a non-linear eigenvalue algebraic problem $\det \Phi(\nu) = 0$ after the renormalization procedure.

Remark 3.10 (Point Interactions in \mathbb{R}^3)

The above analysis can be also easily extended to three dimensions and the procedure is basically the same. Then, the regularized principle matrix is found as

$$\Phi_{ij}^\Lambda(\nu) = \begin{cases} \frac{1}{\lambda_i(\Lambda)} - \int_{\mathbb{R}^3} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^3p] & \text{if } i = j , \\ - \int_{\mathbb{R}^3} \frac{e^{\frac{i\mathbf{p} \cdot (\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \nu^2} [d^3p] & \text{if } i \neq j . \end{cases} \quad (3.162)$$

After choosing $\frac{1}{\lambda_i(\Lambda)} = \int_{\mathbb{R}^3} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \mu_i^2} [d^3p]$, one can apply the same procedure as we did for two-dimensional case and obtain

$$\lim_{\Lambda \rightarrow \infty} \Phi_{ij}^\Lambda(\nu) = \Phi_{ij}(\nu) = \begin{cases} \frac{\sqrt{m}}{2\sqrt{2\pi}\hbar^3} (\nu - \mu_i) & \text{if } i = j , \\ - \frac{m}{2\pi\hbar^2} \frac{e^{-\frac{\nu|\mathbf{a}_i - \mathbf{a}_j|\sqrt{2m}}{\hbar}}}{|\mathbf{a}_i - \mathbf{a}_j|} & \text{if } i \neq j , \end{cases} \quad (3.163)$$

which is the renormalized principal matrix in three dimensions. Note that Remark 3.9 is also consistent with this problem, namely, we have a divergence problem due to the off-diagonal term if the centers coincide.

Remark 3.11 (*Two-center Case in \mathbb{R}^3*)

From (3.163), the transcendental equation for this system can be found as

$$(\nu - \mu_1)(\nu - \mu_2) = \frac{2m\hbar^2}{d^2} e^{-\frac{2d\sqrt{2m}\nu}{\hbar}}. \quad (3.164)$$

By denoting $\nu = x$, $\mu_1 = c_1$, $\mu_2 = c_2$, $\frac{2m\hbar^2}{d^2} = A$ and $\frac{2d\sqrt{2m}}{\hbar} = \beta$, the above equation becomes

$$(x - c_1)(x - c_2) = Ae^{-\beta x}. \quad (3.165)$$

This above equation has the same form with (3.57). After the similar calculations as we did in two dimensions, we find a

$$d > \sqrt{\frac{2m}{\mu_1\mu_2}} \hbar = d_{critical}, \quad (3.166)$$

condition for the distance between the centers of point interactions in order to have two bound states in three dimensions. If this condition is not satisfied, then we have only one bound state. But, we are mainly going to discuss the problem in two dimensions.

We can also determine the flows of the eigenvalues of the renormalized principal matrix for two, three and four-center cases.

3.6.2. Flows of the Eigenvalues in Two-center Case in Two Dimensions

Let $\mu_1 = \mu_2 = \mu$ in (3.147). Then, the eigenvalues of the renormalized principal matrix can be easily found as

$$w_1(\nu) = \frac{1}{\pi} \left[\ln \left(\frac{\nu}{\mu} \right) + K_0(\sqrt{2}\nu d) \right], \quad (3.167)$$

and

$$w_2(\nu) = \frac{1}{\pi} \left[\ln \left(\frac{\nu}{\mu} \right) - K_0(\sqrt{2}\nu d) \right]. \quad (3.168)$$

(We have chosen $m = \hbar = 1$ for simplicity and numerical calculations.) So, $w_1(\nu) \neq w_2(\nu)$ (no degeneracy). The flows of the eigenvalues for different values of $d = [1, 100]$ can be seen in Figure 3.10.

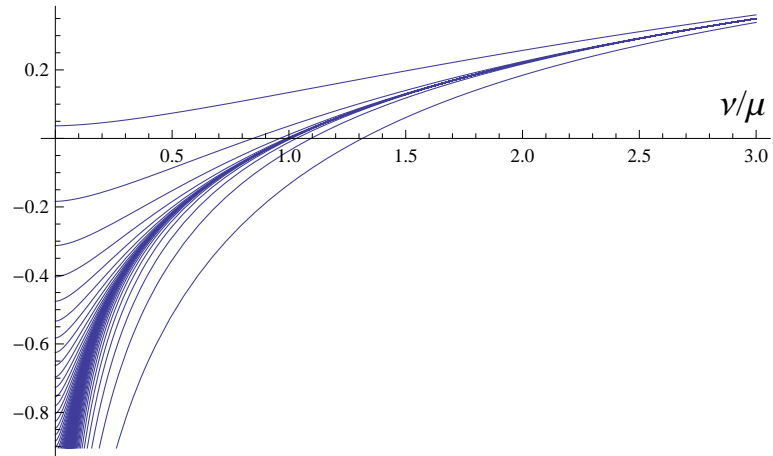


Figure 3.10. Flows of the eigenvalues w_1, w_2 for $d = [1, 100]$ in two-center case

In particular, for $\sqrt{2}\mu d = 1$, it can be seen from Figure 3.11 that there exists only one bound state energy which is the ground state energy as well. For $\sqrt{2}\mu d = 5$, we have two bound state energies (see Figure 3.12).

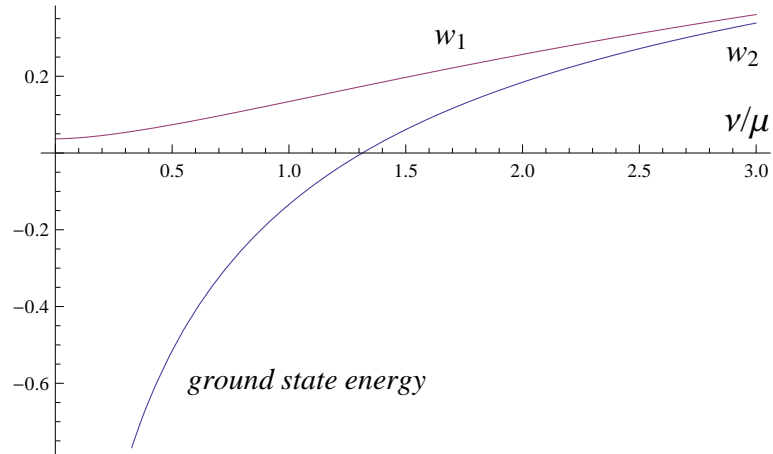


Figure 3.11. Flows of the eigenvalues w_1, w_2 for $\sqrt{2}\mu d = 1$

Remark 3.12 We see that the above curve in Figure 3.11 does not intersect the horizontal axis, which means that there cannot be a bound state solution associated with w_1 . The reason lies in the fact that the renormalized principal matrix is not analytic at $\nu = 0$.

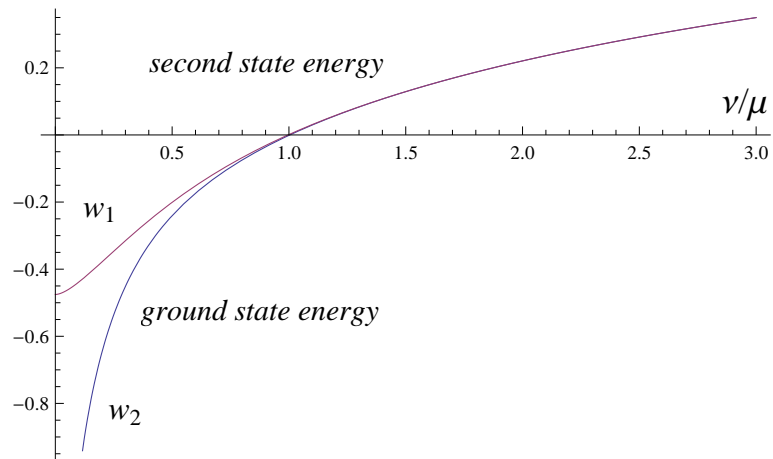


Figure 3.12. Flows of the eigenvalues w_1, w_2 for $\sqrt{2}\mu d = 5$

3.6.3. Flows of the Eigenvalues in Three-center Case in Two Dimensions

Let us consider three point interactions centered at the vertices of an equilateral triangle with $\mu_1 = \mu_2 = \mu_3 = \mu$ in two dimensions. Let d be one of the sides of the equilateral triangle.

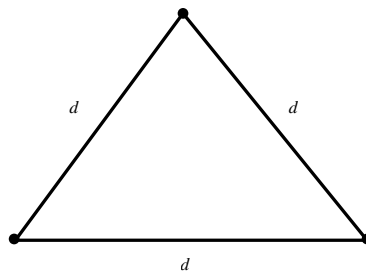


Figure 3.13. Equilateral triangle with three point interactions

Then, from Eq. (3.145), we have the following explicit form of the renormalized principle matrix

$$\Phi(\nu) = \frac{1}{\pi} \begin{pmatrix} \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d) & -K_0(\sqrt{2}\nu d) \\ -K_0(\sqrt{2}\nu d) & \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d) \\ -K_0(\sqrt{2}\nu d) & -K_0(\sqrt{2}\nu d) & \ln\left(\frac{\nu}{\mu}\right) \end{pmatrix}, \quad (3.169)$$

where we have chosen units such that $m = \hbar = 1$. The eigenvalues of the above matrix can be calculated as

$$w_1(\nu) = \frac{1}{\pi} \left[\ln\left(\frac{\nu}{\mu}\right) + K_0(\sqrt{2}\nu d) \right] = w_2(\nu) \text{ (2-fold degeneracy)}, \quad (3.170)$$

and

$$w_3(\nu) = \frac{1}{\pi} \left[\ln\left(\frac{\nu}{\mu}\right) - 2K_0(\sqrt{2}\nu d) \right]. \quad (3.171)$$

The flows of the eigenvalues for different values of $d = [1, 500]$ are shown in Figure 3.14.

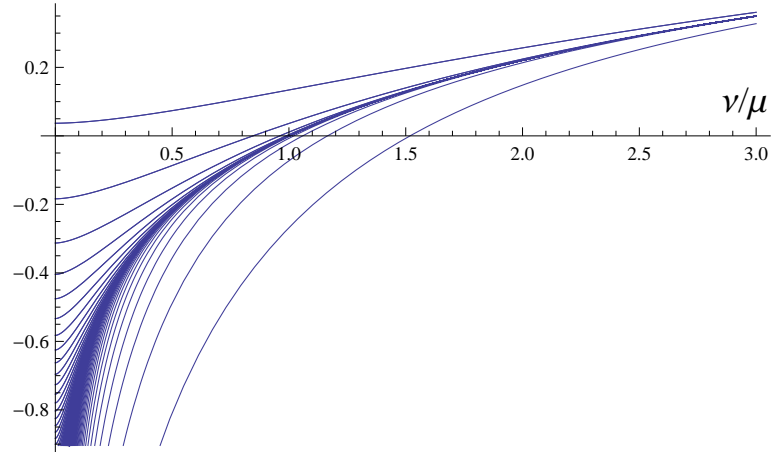


Figure 3.14. Flows of the eigenvalues w_1, w_2, w_3 for $d = [1, 500]$ in three-center case

In particular, for $\sqrt{2}\mu d = 1$, we have only the ground state energy (see Figure 3.15) and for $\sqrt{2}\mu d = 5$, we have two bound state energies with one of them has a 2-fold degeneracy (see Figure 3.16).

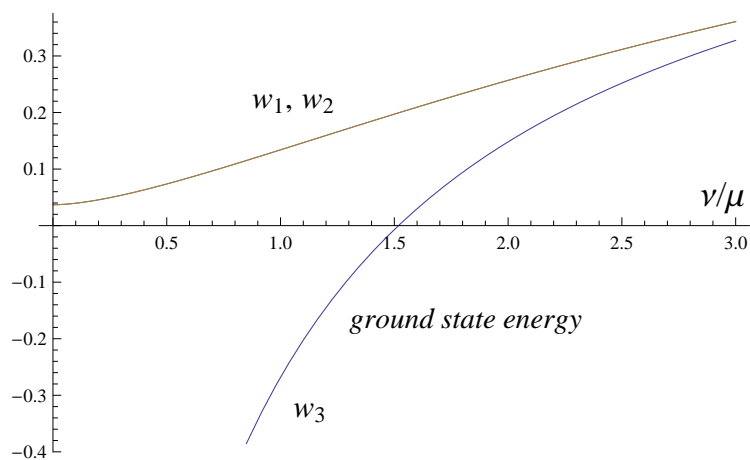


Figure 3.15. Flows of the eigenvalues w_1, w_2, w_3 for $\sqrt{2}\mu d = 1$

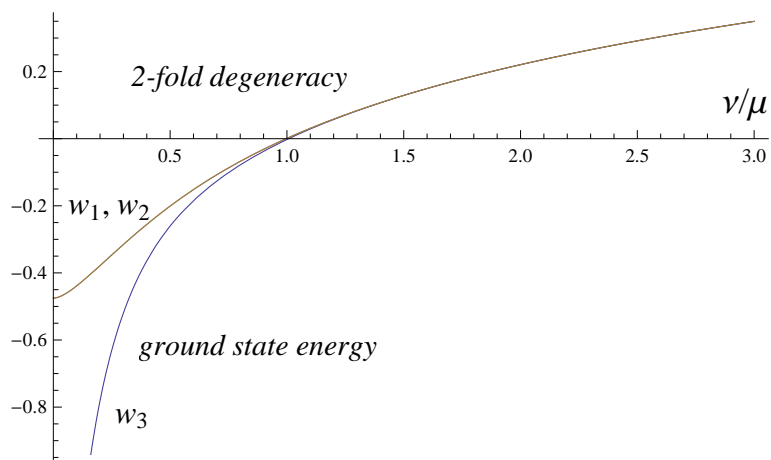


Figure 3.16. Flows of the eigenvalues w_1, w_2, w_3 for $\sqrt{2}\mu d = 5$

3.6.4. Flows of the Eigenvalues in Four-center Case in Two Dimensions

Let us now examine four point interactions centered at the vertices of a square with $\mu_1 = \mu_2 = \mu_3 = \mu_4 = \mu$ and $m = \hbar = 1$ in two dimensions. Let d be one of the sides of the square.

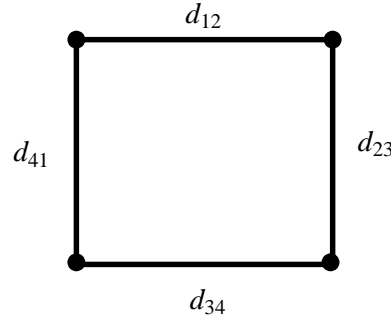


Figure 3.17. Square with four point interactions

Then the renormalized matrix (3.145) becomes

$$\Phi(\nu) = \frac{1}{\pi} \begin{pmatrix} \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d_{12}) & -K_0(\sqrt{2}\nu d_{13}) & -K_0(\sqrt{2}\nu d_{14}) \\ -K_0(\sqrt{2}\nu d_{21}) & \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d_{23}) & -K_0(\sqrt{2}\nu d_{24}) \\ -K_0(\sqrt{2}\nu d_{31}) & -K_0(\sqrt{2}\nu d_{32}) & \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d_{34}) \\ -K_0(\sqrt{2}\nu d_{41}) & -K_0(\sqrt{2}\nu d_{42}) & -K_0(\sqrt{2}\nu d_{43}) & \ln\left(\frac{\nu}{\mu}\right) \end{pmatrix} \quad (3.172)$$

where we denoted $d_{ij} = |\mathbf{a}_i - \mathbf{a}_j|$. Since $d_{12} = d_{21} = d_{23} = d_{32} = d_{34} = d_{43} = d_{41} = d_{14} = d$ and $d_{13} = d_{31} = d_{24} = d_{42} = d\sqrt{2}$, the above matrix becomes

$$\Phi(\nu) = \frac{1}{\pi} \begin{pmatrix} \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d) & -K_0(2\nu d) & -K_0(\sqrt{2}\nu d) \\ -K_0(\sqrt{2}\nu d) & \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d) & -K_0(2\nu d) \\ -K_0(2\nu d) & -K_0(\sqrt{2}\nu d) & \ln\left(\frac{\nu}{\mu}\right) & -K_0(\sqrt{2}\nu d) \\ -K_0(\sqrt{2}\nu d) & -K_0(2\nu d) & -K_0(\sqrt{2}\nu d) & \ln\left(\frac{\nu}{\mu}\right) \end{pmatrix}, \quad (3.173)$$

which is a circulant matrix (Aldrovandi, 2001). In general, $N \times N$ circulant matrices have

this form

$$\begin{pmatrix} c_0 & c_{N-1} & \dots & c_2 & c_1 \\ c_1 & c_0 & c_{N-1} & \dots & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{N-2} & \dots & \ddots & \ddots & c_{N-1} \\ c_{N-1} & c_{N-2} & \dots & c_1 & c_0 \end{pmatrix}, \quad (3.174)$$

and the eigenvalues of this matrix are given by (Aldrovandi, 2001)

$$w_j = c_0 + c_{N-1}U_j + c_{N-2}U_j^2 + \dots + c_1U_j^{N-1}, \quad (3.175)$$

where $j = 0, 1, \dots, N - 1$ and $U_j = e^{\frac{2\pi ij}{N}}$. Therefore, the eigenvalues of the matrix (3.173) are

$$w_1(\nu) = \frac{1}{\pi} \left[\ln \left(\frac{\nu}{\mu} \right) - 2K_0(\sqrt{2}\nu d) - K_0(2\nu d) \right], \quad (3.176)$$

and

$$w_2(\nu) = \frac{1}{\pi} \left[\ln \left(\frac{\nu}{\mu} \right) + K_0(2\nu d) \right] = w_3(\nu) \text{ (2-fold degeneracy)}, \quad (3.177)$$

and

$$w_4(\nu) = \frac{1}{\pi} \left[\ln \left(\frac{\nu}{\mu} \right) + 2K_0(\sqrt{2}\nu d) - K_0(2\nu d) \right]. \quad (3.178)$$

For different values of $d = [1, 500]$, the flows of the eigenvalues can be seen from Figure 3.18. Also, we have three bound state energies with one of them has 2-fold degeneracy for $\sqrt{2}\mu d = 1$ and four bound state energies with one of them has 2-fold degeneracy for $\sqrt{2}\mu d = 5$ which are shown in Figure 3.19 and 3.20, respectively.

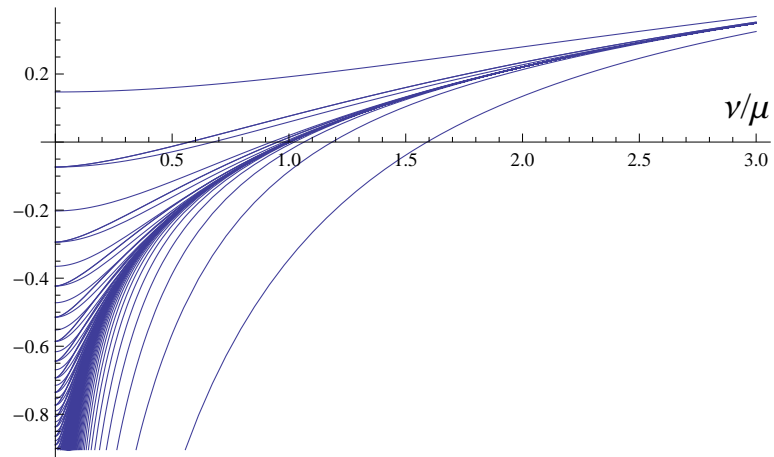


Figure 3.18. Flows of the eigenvalues w_1, w_2, w_3, w_4 for $d = [1, 500]$ in four-center case

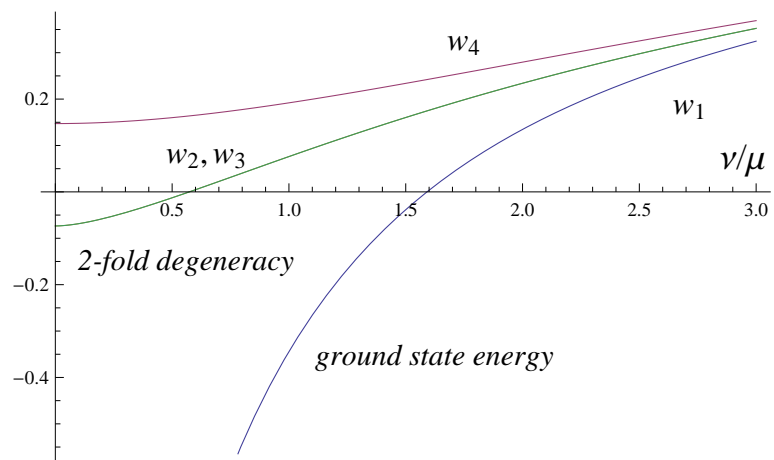


Figure 3.19. Flows of the eigenvalues w_1, w_2, w_3, w_4 for $\sqrt{2}\mu d = 1$

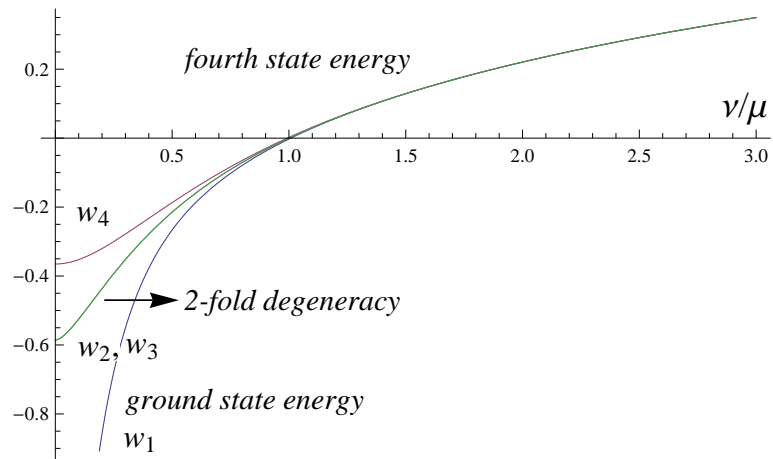


Figure 3.20. Flows of the eigenvalues w_1, w_2, w_3, w_4 for $\sqrt{2}\mu d = 5$

These ideas can be generalized for the point interactions located at the vertices of the regular polygons because they all have a form of a circulant matrix and their eigenvalues can be found via the formula given in (3.175). After that one can similarly plot the flows of the eigenvalues.

CHAPTER 4

RESOLVENT FORMULA FOR POINT INTERACTIONS

Since the resolvent includes all the information about the spectrum of the operators and it allows us to discuss the renormalization procedure in a more rigorous way, we will use this approach from now on.

4.1. Resolvent

Definition 4.1 (Hislop & Sigal, 1996) (Reed & Simon, 1980)

Let H be a linear operator on a Banach space X with domain $\mathcal{D}(H) \subset X$.

- The spectrum of H , $\sigma(H)$, is the set of all points $\lambda \in \mathbb{C}$ for which $H - \lambda\mathbb{I}$ is not invertible.
- The resolvent set of H , $\rho(H)$, is the set of all points $\lambda \in \mathbb{C}$ for which $H - \lambda\mathbb{I}$ is invertible.
- If $\lambda \in \rho(H)$, then the inverse of $H - \lambda$ is called the resolvent of H at λ and is written as $R_H(\lambda) := (H - \lambda\mathbb{I})^{-1}$.

When the operator is defined in the context, it can be simply written as $R(\lambda)$.

Definition 4.2 (Reed & Simon, 1980)

Let X be a Banach space and let D be a region in the complex plane, i.e., a connected open subset of \mathbb{C} . A function, $T(z)$ defined on D and taking values in the set of all linear operators on X to Y , namely $B(X, Y)$ is said to be analytic at $z_0 \in D$ if $\lim_{h \rightarrow 0} \frac{T(z_0+h) - T(z_0)}{h}$ exists in $B(X, Y)$.

Theorem 4.1 (Hislop & Sigal, 1996)

The resolvent set $\rho(H)$ is an open subset of \mathbb{C} (and hence $\sigma(H)$ is closed) and $R_H(\lambda)$ is an analytic (holomorphic) operator-valued function of λ on $\rho(H)$.

Definition 4.3 (Hislop & Sigal, 1996)

- If $\lambda \in \sigma(H)$ is such that $\text{Ker}(H - \lambda\mathbb{I}) \neq \{0\}$, then λ is an eigenvalue of H and any $u \in \text{Ker}(H - \lambda\mathbb{I})$, $u \neq 0$, is an eigenvector of H for λ and satisfies $Hu = \lambda u$. Moreover,

$\dim(\text{Ker}(H - \lambda\mathbb{I}))$ is called the (geometric) multiplicity of λ and $\text{Ker}(H - \lambda\mathbb{I})$ is the (geometric) eigenspace of H at λ . (Note that the kernel $\text{Ker}(H - \lambda\mathbb{I})$ is a linear subspace of X .)

- The discrete (point) spectrum of H , $\sigma_d(H)$, is the set of all eigenvalues of H with finite (algebraic) multiplicity and which are isolated points of $\sigma(H)$.
- The essential spectrum of H is defined as the complement of $\sigma_d(H)$ in $\sigma(H)$: $\sigma_{\text{ess}}(H) \equiv \sigma(H) \setminus \sigma_d(H)$.

Remark 4.1 Space-time behavior of the wave function are related to the classification of spectrum according to the resolvent. For instance, bound state energies are associated with point spectrum and scattering states are associated with absolutely continuous spectrum (for the definition of absolutely continuous spectrum, see (Reed & Simon, 1978)).

Theorem 4.2 (Hislop & Sigal, 1996)

Let X be a complex Banach space, $H \in B(X, X)$ and $\lambda, \mu \in \rho(H)$ where $B(X, X)$ is the space of bounded linear operators. Then, the resolvent $R(\lambda)$ of H satisfies the resolvent equation or so called the first resolvent identity:

$$R(\lambda) - R(\mu) = (\lambda - \mu)R(\lambda)R(\mu) , \quad (4.1)$$

and

$$R(\lambda)R(\mu) = R(\mu)R(\lambda) . \quad (4.2)$$

In addition, resolvent also satisfies the second resolvent identity:

$$\begin{aligned} R_H(\lambda) - R_A(\lambda) &= R_H(\lambda)(H - A)R_A(\lambda) \\ &= R_H(\lambda)(A - H)R_A(\lambda) , \end{aligned} \quad (4.3)$$

where $A \in B(X, X)$.

Definition 4.4 (Riesz Integral Representation) (Hislop & Sigal, 1996)

Let H be a closed operator on X and z_0 be an isolated point of $\sigma(H)$. Then, for an admissible

contour Γ_{z_0}

$$\mathbb{P}_{z_0} := -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} R_H(z) dz, \quad (4.4)$$

is called the Riesz integral representation for H and z_0 , where admissible contour is a simple closed contour Γ_{z_0} around z_0 , whose closure of the region bounded by the contour containing z_0 intersects $\sigma(H)$ only at z_0 (see Figure 4.1).

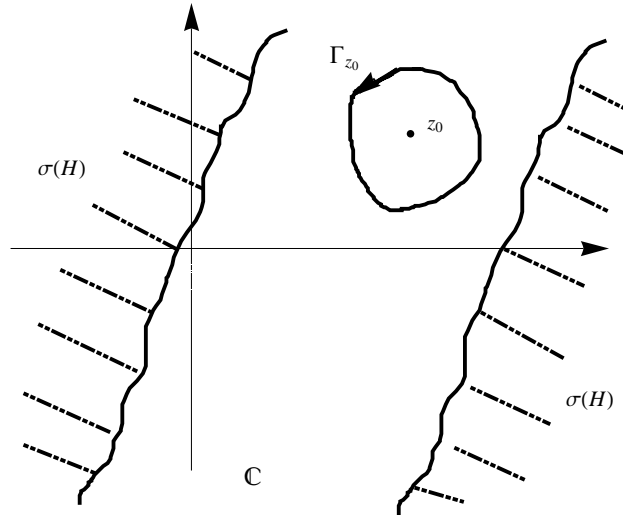


Figure 4.1. Admissible contour Γ_{z_0} for H and z_0

Proposition 4.1 (Hislop & Sigal, 1996)

Let \mathbb{P}_{z_0} be the Riesz integral for H and z_0 :

1. \mathbb{P}_{z_0} is a projection.
2. $\text{Ran}(\mathbb{P}_{z_0}) \supset \text{Ker}(H - z_0\mathbb{I})$.
3. If X is a Hilbert space and H is self-adjoint, therefore \mathbb{P}_{z_0} is the orthogonal projection onto $\text{Ker}(H - z_0\mathbb{I})$.

Here, Ran denotes the range of the operator.

(For the proof, one can consult on Appendix C.1.)

We now apply the resolvent formalism to our problem.

4.2. Resolvent of Free Hamiltonian with Point Interaction in One Dimension

Lemma 4.1 *The resolvent of point interaction Hamiltonian $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \lambda \delta(x)$ in one dimension is given by*

$$R(p, q; E) = \frac{(2\pi\hbar)\delta(p-q)}{\frac{q^2}{2m} - E} + \frac{1}{\frac{p^2}{2m} - E} \frac{1}{\Phi(E)} \frac{1}{\frac{q^2}{2m} - E}, \quad (4.5)$$

where $\Phi(E) = \lambda^{-1} - \int_{\mathbb{R}} \frac{1}{\frac{p^2}{2m} - E} [dp]$. Also, $R_0(p, q; E) = \frac{(2\pi\hbar)\delta(p-q)}{\frac{q^2}{2m} - E}$ is the free resolvent kernel in the momentum representation.

Proof The time-independent Schrödinger equation in one dimension with a point interaction centered at the origin was given in Eq. (3.6). In order to find the resolvent of the formal Hamiltonian, we must solve $(H - E)|\psi\rangle = |\rho\rangle$. (Since solving $|\psi\rangle$ is equivalent to finding the resolvent, $|\psi\rangle = (H - E)^{-1}|\rho\rangle = R(E)|\rho\rangle$.) In the coordinate representation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \lambda\delta(x)\psi(x) - E\psi(x) = \rho(x), \quad (4.6)$$

where ρ is a sufficiently regular function such that all the expressions below make sense and $E \in \mathbb{C}$. By applying the formal Fourier transform to the above equation, we can easily find

$$\widehat{\psi}(p) = \frac{C}{\frac{p^2}{2m} - E} + \frac{\widehat{\rho}(p)}{\frac{p^2}{2m} - E}, \quad (4.7)$$

where $C = \lambda\psi(0)$. Then, the consistency condition implies

$$C = \frac{\int_{\mathbb{R}} \frac{\widehat{\rho}(p)}{\frac{p^2}{2m} - E} [dp]}{\left[\lambda^{-1} - \int_{\mathbb{R}} \frac{1}{\frac{p^2}{2m} - E} [dp] \right]}. \quad (4.8)$$

Let us substitute Eq. (4.8) into Eq. (4.7) and get

$$\widehat{\psi}(p) = \int_{\mathbb{R}} \left[\frac{(2\pi\hbar)\delta(p-q)}{\frac{q^2}{2m} - E} + \frac{1}{\frac{p^2}{2m} - E} \frac{1}{\Phi(E)} \frac{1}{\frac{q^2}{2m} - E} \right] \widehat{\rho}(q) [dq], \quad (4.9)$$

where $\Phi(E) = \lambda^{-1} - \int_{\mathbb{R}} \frac{1}{\frac{p^2}{2m} - E} [dp]$ is called the principal function (Rajeev, 1999). By comparing (4.9) with its integral form

$$\widehat{\psi}(p) = \int_{\mathbb{R}} R(p, q; E) \widehat{\rho}(q) [dq] , \quad (4.10)$$

the resolvent kernel is found to be (4.5). □

Theorem 4.3 *The bound state energy and corresponding wave function of the point interaction in one dimension are (3.7) and (3.8), respectively.*

Proof After evaluating the integral in $\Phi(E)$, we have

$$\Phi(E) = \frac{1}{\lambda} - \frac{\sqrt{m}}{\hbar} \frac{1}{\sqrt{-2E}} . \quad (4.11)$$

The poles of the resolvent kernel gives the point spectrum (bound state energies) and we expect that poles in the negative real E axis should only come from zeros of the principal function $\Phi(E)$ due to the fact that the free resolvent kernel $R_0(p, q; E)$ has no pole in the negative real axis. Hence, $\Phi(E) = 0$ gives us (3.7). In order to find the bound state wave function, we are going to use Definition 4.4. This representation can be written in this form:

$$\frac{1}{2\pi i} \oint_{\Gamma} R(E) dE = -|\psi\rangle \langle\psi| , \quad (4.12)$$

where Γ is the contour which includes the isolated pole $E = -\frac{m\lambda^2}{2\hbar^2}$ of $R(E)$ and $|\psi\rangle \langle\psi|$ (in the Dirac's bra-ket notation or it can be written as $(\cdot, \psi)\psi$) is the projection operator onto the eigenspaces of the bound state energy $E = -\frac{m\lambda^2}{2\hbar^2}$. In the momentum representation, the above formula becomes

$$\frac{1}{2\pi i} \oint_{\Gamma} R(p, q; E) dE = -\widehat{\psi}(p) \widehat{\psi}(q) . \quad (4.13)$$

Since the free resolvent kernel is analytic inside Γ (see Figure 4.2), we obtain

$$\widehat{\psi}(p) = \frac{\sqrt{m}\lambda^{\frac{3}{2}}}{\hbar} \frac{1}{\frac{p^2}{2m} + \frac{m\lambda^2}{2\hbar^2}} . \quad (4.14)$$

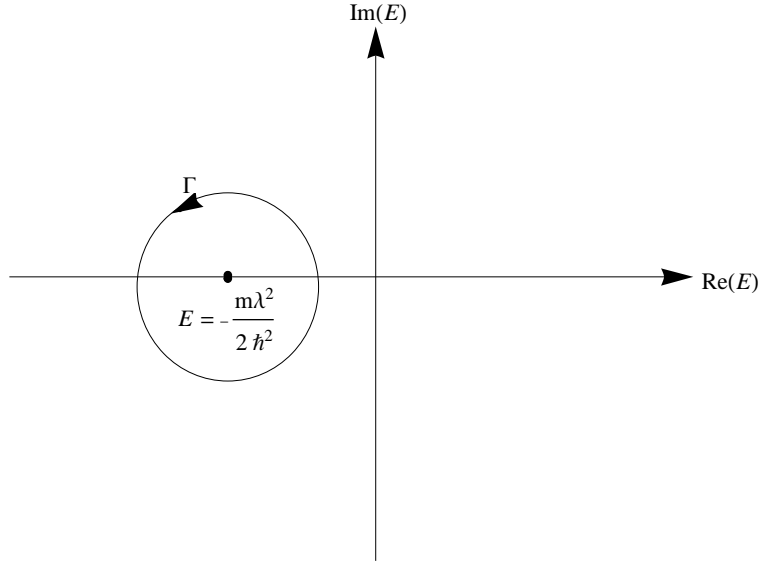


Figure 4.2. The contour enclosing the simple pole $-\frac{m\lambda^2}{2\hbar^2}$

By substituting this into the formal inverse Fourier transform and using the residue theorem, we obtain the coordinate representation of the bound state wave function (3.8). \square

Proposition 4.2 *The spectrum of the free Hamiltonian H_0 is the positive real line, i.e., $\sigma(H_0) \in [0, \infty)$.*

Proof

$$\begin{aligned}
 (R_0\hat{\psi})(p) &= \langle p | R_0(E) | \hat{\psi} \rangle = \int_{\mathbb{R}} R_0(p, q; E) \hat{\psi}(q) [dq] = \int_{\mathbb{R}} \frac{(2\pi\hbar)\delta(p-q)}{\frac{q^2}{2m} - E} \hat{\psi}(q) [dq] \\
 &= \frac{\hat{\psi}(p)}{\frac{p^2}{2m} - E}. \tag{4.15}
 \end{aligned}$$

If $E \in [0, \infty)$, then $R_0\hat{\psi}$ becomes unbounded. Therefore, $\sigma(H_0) \in [0, \infty)$. \square

Corollary 4.1

$$\frac{1}{2\pi i} \oint_{\Gamma} R_0(p, q; E) dE = 0, \tag{4.16}$$

where the contour Γ is chosen in Figure 4.2.

Proposition 4.3 *The resolvent kernel in the coordinate representation is given by*

$$R(x, y; E) = \int_{\mathbb{R}^2} e^{\frac{ipx}{\hbar}} R(p, q; E) e^{-\frac{iqy}{\hbar}} [dp][dq] . \quad (4.17)$$

Proof By using Dirac's bra-ket notation:

$$R(x, y; E) = \langle x | R(E) | y \rangle = \int_{\mathbb{R}^2} \langle x | p \rangle \langle p | R(E) | q \rangle \langle q | y \rangle [dp][dq] , \quad (4.18)$$

where we used the completeness relation $\int_{\mathbb{R}} |p\rangle \langle p| [dp] = I$. Since $\langle x | p \rangle = e^{\frac{ipx}{\hbar}}$ and $\langle q | y \rangle = e^{-\frac{iqy}{\hbar}}$, we immediately obtain the result. \square

Corollary 4.2 *The resolvent kernel in the coordinate representation for the one-dimensional Schrödinger operator with a point interaction is*

$$R(x, y; E) = \int_{\mathbb{R}} \frac{e^{\frac{ip(x-y)}{\hbar}}}{\frac{p^2}{2m} - E} [dp] + \int_{\mathbb{R}^2} \frac{e^{\frac{ipx}{\hbar}}}{\frac{p^2}{2m} - E} \Phi^{-1}(E) \frac{e^{-\frac{iqy}{\hbar}}}{\frac{q^2}{2m} - E} [dp][dq] , \quad (4.19)$$

where $\Phi(E)$ is given in Eq. (4.11). The integral representation of the free resolvent kernel in the coordinate representation is given by

$$R_0(x, y; E) = \int_{\mathbb{R}} \frac{e^{\frac{ip(x-y)}{\hbar}}}{\frac{p^2}{2m} - E} [dp] . \quad (4.20)$$

Then, Eq. (4.19) can be written in the following form:

$$R(x, y; E) = R_0(x, y; E) + R_0(x, 0; E) \Phi^{-1}(E) R_0(0, y; E) . \quad (4.21)$$

4.3. Resolvent of Free Hamiltonian with Point Interaction in Two Dimensions

Theorem 4.4 *The resolvent kernel of the Hamiltonian for point interaction in two dimensions after the renormalization procedure is given by*

$$R(\mathbf{p}, \mathbf{q}; E) = \frac{(2\pi\hbar)^2 \delta^{(2)}(\mathbf{p} - \mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} + \frac{1}{\frac{\mathbf{p}^2}{2m} - E} \Phi^{-1}(E) \frac{1}{\frac{\mathbf{q}^2}{2m} - E}, \quad (4.22)$$

where $\Phi(E) = \frac{m}{2\pi\hbar^2} \ln\left(-\frac{E}{\mu^2}\right)$.

Proof The inhomogeneous Schrödinger equation for our problem in two dimensions is

$$-\frac{\hbar^2}{2m} \Delta \psi(\mathbf{x}) - \lambda \delta^{(2)}(\mathbf{x}) \psi(\mathbf{x}) - E \psi(\mathbf{x}) = \rho(\mathbf{x}). \quad (4.23)$$

The resolvent kernel can be found in analogy with the one-dimensional case except that the expression after the formal Fourier transform must be regularized due to the divergence. The result is

$$\left(\frac{\mathbf{p}^2}{2m} - E\right) \widehat{\psi}_\Lambda(\mathbf{p}) - \lambda(\Lambda) \Theta_\Lambda(\mathbf{p}) \int_{\mathbb{R}^2} \Theta_\Lambda(\mathbf{q}) \widehat{\psi}_\Lambda(\mathbf{q}) [d^2q] = \widehat{\rho}_\Lambda(\mathbf{p}), \quad (4.24)$$

where $\Theta_\Lambda(\mathbf{p})$ is inserted to preserve the symmetry in the resolvent kernel ($R(\mathbf{x}, \mathbf{y}; E) = R^*(\mathbf{y}, \mathbf{x}; E)$) in the regularization procedure. Then, the solution $\widehat{\psi}_\Lambda(\mathbf{p})$ becomes

$$\widehat{\psi}_\Lambda(\mathbf{p}) = \frac{\widehat{\rho}_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} + \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} \lambda(\Lambda) C(\Lambda), \quad (4.25)$$

where $C(\Lambda) = \int_{\mathbb{R}^2} \Theta_\Lambda(\mathbf{q}) \widehat{\psi}_\Lambda(\mathbf{q}) [d^2q]$. The consistency condition implies that

$$C(\Lambda) = \int_{\mathbb{R}^2} \Theta_\Lambda(\mathbf{q}) \left[\frac{\widehat{\rho}_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} + \frac{\Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} \lambda(\Lambda) C(\Lambda) \right] [d^2q], \quad (4.26)$$

or

$$\lambda(\Lambda)C(\Lambda) \left[\lambda^{-1}(\Lambda) - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} [d^2p] \right] = \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{q})\widehat{\rho}_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] , \quad (4.27)$$

where we have used $\Theta_\Lambda^2(\mathbf{q}) = \Theta_\Lambda(\mathbf{q})$. By substituting this value of $\lambda(\Lambda)C(\Lambda)$ into the (4.25) with the choice of $\lambda^{-1}(\Lambda)$ given in (3.99), we have

$$\begin{aligned} \widehat{\psi}_\Lambda(\mathbf{p}) &= \frac{\widehat{\rho}_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} + \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} \frac{1}{\left[\int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} + \mu^2} [d^2p] - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} [d^2p] \right]} \\ &\quad \times \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} \widehat{\rho}_\Lambda(\mathbf{q}) [d^2q] . \end{aligned} \quad (4.28)$$

Now we take the limit $\Lambda \rightarrow \infty$ and find

$$\widehat{\psi}(\mathbf{p}) = \frac{\widehat{\rho}(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} + \frac{1}{\frac{\mathbf{p}^2}{2m} - E} \frac{1}{\Phi(E)} \int_{\mathbb{R}^2} \frac{\widehat{\rho}(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] , \quad (4.29)$$

where

$$\Phi(E) = \frac{m}{2\pi\hbar^2} \ln \left(-\frac{E}{\mu^2} \right) , \quad (4.30)$$

is called the renormalized principal function. From the above solution, we can immediately find the resolvent kernel in the momentum representation (4.22). \square

Lemma 4.2 *The bound state wave function in two dimensions is given by (3.129).*

Proof By using the Riesz integral representation:

$$\frac{1}{2\pi i} \oint_{\Gamma} R(\mathbf{p}, \mathbf{q}; E) dE = -\widehat{\psi}(\mathbf{p})\widehat{\psi}(\mathbf{q}) , \quad (4.31)$$

where Γ is the contour enclosing the pole $E = -\mu^2$ which is found from $\Phi(E) = 0$ in Eq. (4.30), the wave function in the momentum representation is

$$\widehat{\psi}(\mathbf{p}) = \sqrt{\frac{2\pi}{m}} \mu \hbar \frac{1}{\frac{\mathbf{p}^2}{2m} + \mu^2}, \quad (4.32)$$

after the evolution of the contour integral. By substituting this into the inverse formal Fourier transform, the wave function in the coordinate representation can be found exactly in (3.129). \square

Theorem 4.5 *The resolvent kernel in the coordinate representation is given by*

$$R(\mathbf{x}, \mathbf{y}; E) = R_0(\mathbf{x}, \mathbf{y}; E) + R_0(\mathbf{x}, \mathbf{0}; E) \Phi^{-1}(E) R_0(\mathbf{0}, \mathbf{y}; E). \quad (4.33)$$

Proof $R(\mathbf{x}, \mathbf{y}; E)$ is related to the resolvent kernel in the momentum representation by

$$R(\mathbf{x}, \mathbf{y}; E) = \int_{\mathbb{R}^4} e^{\frac{i\mathbf{p}\cdot\mathbf{x}}{\hbar}} R(\mathbf{p}, \mathbf{q}; E) e^{-\frac{i\mathbf{q}\cdot\mathbf{y}}{\hbar}} [d^2p][d^2q]. \quad (4.34)$$

(One can prove this also as in one-dimensional case.) Hence, after inserting $R(\mathbf{p}, \mathbf{q}; E)$ found in (4.22) into (4.34), we obtain

$$R(\mathbf{x}, \mathbf{y}; E) = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}{\hbar}}}{\frac{\mathbf{p}^2}{2m} - E} [d^2p] + \int_{\mathbb{R}^4} \frac{e^{\frac{i\mathbf{p}\cdot\mathbf{x}}{\hbar}}}{\frac{\mathbf{p}^2}{2m} - E} \Phi^{-1}(E) \frac{e^{-\frac{i\mathbf{q}\cdot\mathbf{y}}{\hbar}}}{\frac{\mathbf{q}^2}{2m} - E} [d^2p][d^2q], \quad (4.35)$$

which can also be written as (4.33) with using Eq. (4.20). \square

4.4. Resolvent of Free Hamiltonian with Finitely Many Point Interactions in Two Dimensions

Theorem 4.6 *The resolvent of finitely many point interactions in \mathbb{R}^2 after the renormalization procedure is given by*

$$R(\mathbf{p}, \mathbf{q}; E) = \frac{(2\pi\hbar)^2 \delta^{(2)}(\mathbf{q} - \mathbf{p})}{\frac{\mathbf{q}^2}{2m} - E} + \sum_{i,j=1}^N \frac{e^{-i\mathbf{p}\cdot\mathbf{a}_i}}{\frac{\mathbf{p}^2}{2m} - E} [\Phi^{-1}(E)]_{ij} \frac{e^{i\mathbf{q}\cdot\mathbf{a}_j}}{\frac{\mathbf{q}^2}{2m} - E}, \quad (4.36)$$

where $\Phi_{ij}(E)$ is (3.145) for $E = -\nu^2$.

Proof The formal Fourier transform of the inhomogeneous Schrödinger equation

$$-\frac{\hbar^2}{2m} \Delta \psi(\mathbf{x}) - \sum_{i=1}^N \lambda_i \delta^{(2)}(\mathbf{x} - \mathbf{a}_i) \psi(\mathbf{x}) - E \psi(\mathbf{x}) = \rho(\mathbf{x}) \quad (4.37)$$

is similarly obtained in the regularized form:

$$\left(\frac{\mathbf{p}^2}{2m} - E \right) \widehat{\psi}_\Lambda(\mathbf{p}) - \sum_{i=1}^N \lambda_i(\Lambda) \Theta_\Lambda(\mathbf{p}) \int_{\mathbb{R}^2} e^{-\frac{i(\mathbf{p}-\mathbf{q})\cdot\mathbf{a}_i}{\hbar}} \widehat{\psi}_\Lambda(\mathbf{q}) \Theta_\Lambda(\mathbf{q}) [d^2q] = \widehat{\rho}_\Lambda(\mathbf{p}). \quad (4.38)$$

Let us define $A_i(\Lambda) = \int_{\mathbb{R}^2} e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \widehat{\psi}_\Lambda(\mathbf{q}) \Theta_\Lambda(\mathbf{q}) [d^2q]$. Therefore, the solution $\widehat{\psi}_\Lambda(\mathbf{p})$ in the momentum representation is

$$\widehat{\psi}_\Lambda(\mathbf{p}) = \frac{\widehat{\rho}_\Lambda(\mathbf{p})}{\frac{\mathbf{p}^2}{2m} - E} + \frac{\sum_{i=1}^N \lambda_i(\Lambda) \Theta_\Lambda(\mathbf{p}) e^{-\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}} A_i(\Lambda)}{\frac{\mathbf{p}^2}{2m} - E}. \quad (4.39)$$

The consistency condition yields

$$A_i(\Lambda) = \int_{\mathbb{R}^2} e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \left[\frac{\widehat{\rho}_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} + \frac{\sum_{j=1}^N \lambda_j(\Lambda) \Theta_\Lambda(\mathbf{q}) e^{-\frac{i\mathbf{q}\cdot\mathbf{a}_j}{\hbar}} A_j(\Lambda)}{\frac{\mathbf{q}^2}{2m} - E} \right] \Theta_\Lambda(\mathbf{q}) [d^2q]. \quad (4.40)$$

If we separate the sum into two parts: $i = j$ term and $i \neq j$ terms, we obtain

$$A_i(\Lambda) = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \widehat{\rho}_\Lambda(\mathbf{q}) \Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] + \int_{\mathbb{R}^2} \frac{\lambda_i(\Lambda) \Theta_\Lambda(\mathbf{q}) A_i(\Lambda)}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] + \sum_{\substack{j=1 \\ j \neq i}}^N \frac{e^{\frac{i\mathbf{q}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \lambda_j(\Lambda) \Theta_\Lambda(\mathbf{q}) A_j(\Lambda)}{\frac{\mathbf{q}^2}{2m} - E} [d^2q]. \quad (4.41)$$

Then,

$$\lambda_i(\Lambda) A_i(\Lambda) \left[\frac{1}{\lambda_i(\Lambda)} - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] \right] - \sum_{\substack{j=1 \\ j \neq i}}^N \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \lambda_j(\Lambda) \Theta_\Lambda(\mathbf{q}) A_j(\Lambda)}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \widehat{\rho}_\Lambda(\mathbf{q}) \Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q]. \quad (4.42)$$

Let us define $\lambda_i(\Lambda) A_i(\Lambda) = B_i(\Lambda)$, then

$$\left[\frac{1}{\lambda_i} - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] \right] B_i(\Lambda) - \left[\sum_{\substack{j=1 \\ j \neq i}}^N \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] \right] B_j(\Lambda) = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \widehat{\rho}_\Lambda(\mathbf{q}) \Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q]. \quad (4.43)$$

If we define

$$\Phi_{ij}^\Lambda(E) = \begin{cases} \frac{1}{\lambda_i(\Lambda)} - \int_{\mathbb{R}^2} \frac{\Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] & \text{if } i = j, \\ - \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}} \Theta_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] & \text{if } i \neq j, \end{cases} \quad (4.44)$$

then Eq. (4.43) can be written as a matrix equation

$$\sum_{j=1}^N \Phi_{ij}^\Lambda(E) B_j(\Lambda) = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \Theta_\Lambda(\mathbf{q}) \widehat{\rho}_\Lambda(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q]. \quad (4.45)$$

By choosing $\frac{1}{\lambda_i(\Lambda)}$ as in (3.144) and taking the limit $\Lambda \rightarrow \infty$, we obtain

$$\sum_{j=1}^N \Phi_{ij}(E) B_j = \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_i}{\hbar}} \widehat{\rho}(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q], \quad (4.46)$$

or

$$B_i = \sum_{j=1}^N [\Phi^{-1}(E)]_{ij} \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_j}{\hbar}} \widehat{\rho}(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q], \quad (4.47)$$

where we have defined $\lim_{\Lambda \rightarrow \infty} B_j(\Lambda) = B_j$ and

$$\Phi_{ij}(E) = \begin{cases} \frac{m}{2\pi\hbar^2} \ln\left(-\frac{E}{\mu_i^2}\right) & \text{if } i = j, \\ -\frac{m}{\pi\hbar^2} K_0\left(\frac{\sqrt{-2mE}|\mathbf{a}_i - \mathbf{a}_j|}{\hbar}\right) & \text{if } i \neq j, \end{cases} \quad (4.48)$$

which is the renormalized principal matrix and consistent with Eq. (3.145) for $E = -\nu^2$. Hence, we find the wave function in the momentum representation after taking the limit

$$\begin{aligned} \widehat{\psi}(\mathbf{p}) &= \frac{\widehat{\rho}(\mathbf{q})}{\frac{\mathbf{p}^2}{2m} - E} + \sum_{i,j=1}^N \frac{e^{-\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}}}{\frac{\mathbf{p}^2}{2m} - E} [\Phi^{-1}(E)]_{ij} \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_j}{\hbar}} \widehat{\rho}(\mathbf{q})}{\frac{\mathbf{q}^2}{2m} - E} [d^2q] \\ &= \int_{\mathbb{R}^2} \left[\frac{(2\pi\hbar)^2 \delta^{(2)}(\mathbf{q} - \mathbf{p})}{\frac{\mathbf{q}^2}{2m} - E} + \sum_{i,j=1}^N \frac{e^{-\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}}}{\frac{\mathbf{p}^2}{2m} - E} [\Phi^{-1}(E)]_{ij} \frac{e^{\frac{i\mathbf{q}\cdot\mathbf{a}_j}{\hbar}}}{\frac{\mathbf{q}^2}{2m} - E} \right] \widehat{\rho}(\mathbf{q}) [d^2q], \end{aligned} \quad (4.49)$$

from which we deduce (4.36). □

Corollary 4.3 *The renormalized principal matrix (4.48) satisfies*

$$\Phi^\dagger(E) = \Phi(E^*). \quad (4.50)$$

(It is just a consequence of the explicit expression of the renormalized principal matrix $\Phi(E)$ given in (4.48).)

Theorem 4.7 *The resolvent kernel in the coordinate representation is given by*

$$\begin{aligned}
R(\mathbf{x}, \mathbf{y}; E) &= \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}{\hbar}}}{\frac{\mathbf{p}^2}{2m} - E} [d^2p] \\
&+ \int_{\mathbb{R}^4} \sum_{i,j=1}^N \frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{a}_i)}}}{\frac{\mathbf{p}^2}{2m} - E} [\Phi^{-1}(E)]_{ij} \frac{e^{\frac{i\mathbf{q}\cdot(\mathbf{a}_j-\mathbf{y})}{\hbar}}}{\frac{\mathbf{q}^2}{2m} - E} [d^2p][d^2q] , \quad (4.51)
\end{aligned}$$

or in terms of the free resolvent:

$$R(\mathbf{x}, \mathbf{y}; E) = R_0(\mathbf{x}, \mathbf{y}; E) + \sum_{i,j=1}^N R_0(\mathbf{x}, \mathbf{a}_i; E) [\Phi^{-1}(E)]_{ij} R_0(\mathbf{a}_j, \mathbf{y}; E) . \quad (4.52)$$

Proof The idea is the same as for one point interaction. □

4.4.1. A Lower Bound for the Ground State Energy

In this section, our goal is to find a lower bound for the ground state energy for N point interactions in two dimensions. Actually, we have to prove this because we need to complete the renormalization procedure so that the other measurable quantities must also be finite.

Theorem 4.8 (Geršgorin Theorem) *(Roger & Charles, 1992)*

All the eigenvalues w of an $N \times N$ matrix Φ are located in the union of N discs:

$$\bigcup_{i=1}^N \{z \in \mathbb{C} : |z - \Phi_{ii}| \leq R'_i(\Phi)\} \equiv G(\Phi) , \quad (4.53)$$

where

$$R'_i(\Phi) = \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}| , \quad (4.54)$$

is the deleted absolute value row sums and $1 \leq i \leq N$.

(For the proof, see Appendix C.2.)

Theorem 4.9 *The lower bound for the ground state energy for N point interactions in two dimensions is given by*

$$E_* = -\nu_*^2 = - \left\{ \mu + 2\mu_d W \left[(N-1)e^{-\frac{\mu}{2\mu_d}} \right] \right\}^2, \quad (4.55)$$

where $W[z]$ is the Lambert W function.

Proof Since $\Phi_{ij}^{-1} = \frac{c_{ij}}{\det \Phi_{ij}}$ where $c_{ij} \neq 0$ is the transposed cofactor matrix of Φ_{ij} , in order to have non-trivial solutions, we must have $\det \Phi_{ij}(\nu) = 0$, from which we can find the bound state energies. Then, the zero eigenvalues of the following eigenvalue problem

$$\Phi_{ij}(E)A_i(E) = w^k(E)A_i(E), \quad (4.56)$$

where $A_i(E)$ is the normalized eigenvector of our matrix corresponding to the eigenvalue $w^k(E)$, give the bound state energies. Let E_* be the lower bound of the ground state energy. Then, Theorem 4.8 implies that for $E < E_*$, none of the Geršgorin's discs contain the zero eigenvalue. It means that we impose

$$|\Phi_{ii}(E)| > \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}(E)|, \quad (4.57)$$

for $E < E_*$ and for all $i = 1, 2, \dots, N$. Let $E = -\nu^2 \in \mathbb{R}$ ($\nu > 0$). The question is what the critical value E_* satisfies (4.57). Recall that

$$\Phi_{ii}(\nu) = \frac{m}{\pi \hbar^2} \ln \left(\frac{\nu}{\mu_i} \right). \quad (4.58)$$

Since we physically expect that $\nu > \mu_i$ for all i , $|\Phi_{ii}|$ is a monotonically increasing function of ν . Meanwhile,

$$|\Phi_{ij}(\nu)| = \frac{m}{\pi \hbar^2} K_0 \left(\frac{\nu}{\mu_{d_{ij}}} \right), \quad (4.59)$$

where $\mu_{d_{ij}} \equiv \frac{\hbar}{\sqrt{2md_{ij}}}$, is a monotonically decreasing function of ν and so is $\sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}(\nu)|$. This means that we are looking for a critical value of ν , say ν_* , such that (4.57) is satisfied. Pictorially,

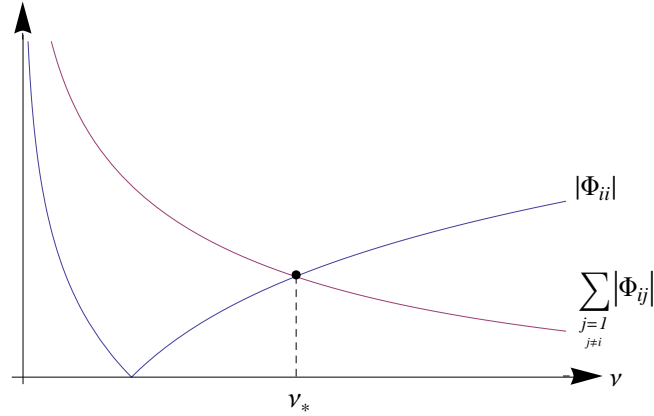


Figure 4.3. Critical value

($\nu > \nu_*$ means $E < E_*$.) Now the aim is to find the critical value ν_* or E_* . Finding ν_* is a difficult problem since it is a transcendental equation. Nevertheless, we can find the critical value analytically by simplifying the expressions in the renormalized principal matrix (3.145). Note that

$$|\Phi_{ii}(\nu)| \geq \min_i |\Phi_{ii}(\nu)|, \quad (4.60)$$

for all ν . Let $\mu = \max_i \mu_i$, then we have

$$|\Phi_{ii}(\nu)| \geq \frac{m}{\pi \hbar^2} \ln \left(\frac{\nu}{\mu} \right). \quad (4.61)$$

Since the lower bound for $\ln x$ is given by (Abramowitz & Sitegun, 1972)

$$\ln x > \frac{x-1}{x}, \quad (4.62)$$

for all $x > 0$ and $x \neq 1$, then

$$|\Phi_{ii}(\nu)| \geq \frac{m}{\pi \hbar^2} \left(1 - \frac{\mu}{\nu}\right) = |\Phi_{ii}^{lower}(\nu)|. \quad (4.63)$$

For the right-hand side, we have also

$$\begin{aligned} \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}(\nu)| &\leq (N-1) \max_j |\Phi_{ij}(\nu)| = (N-1) \max_j \left[\frac{m}{\pi \hbar^2} K_0 \left(\frac{\nu}{\mu_{d_{ij}}} \right) \right] \\ &\leq (N-1) \frac{m}{\pi \hbar^2} K_0 \left(\frac{\nu}{\mu_d} \right), \end{aligned} \quad (4.64)$$

where $d = \min_j d_{ij}$. In addition, using the upper bound of K_0 (Erman, 2010):

$$K_0(x) \leq \frac{2}{x} e^{-\frac{x}{2}}, \quad (4.65)$$

we have

$$\sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}(\nu)| \leq \frac{m}{\pi \hbar^2} (N-1) \frac{2\mu_d}{\nu} e^{-\frac{\nu}{2\mu_d}} = \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}^{upper}(\nu)|. \quad (4.66)$$

If we now impose $|\Phi_{ii}^{lower}(\nu)| > \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}^{upper}(\nu)|$ for all i , it guarantees (4.57) for all $\nu > \nu_*$.

Therefore, it is sufficient to find ν'_* from $|\Phi_{ii}^{lower}(\nu'_*)| > \sum_{\substack{j=1 \\ j \neq i}}^N |\Phi_{ij}^{upper}(\nu'_*)|$, namely

$$1 - \frac{\mu}{\nu'_*} = (N-1) \frac{2\mu_d}{\nu'_*} e^{-\frac{\nu'_*}{2\mu_d}}. \quad (4.67)$$

Let us define $\frac{\nu'_*}{\mu} = x$ and $\frac{\mu_d}{\mu} = \alpha$ for simplicity. Then,

$$(x-1)e^{\frac{x}{2\alpha}} = 2(N-1)\alpha. \quad (4.68)$$

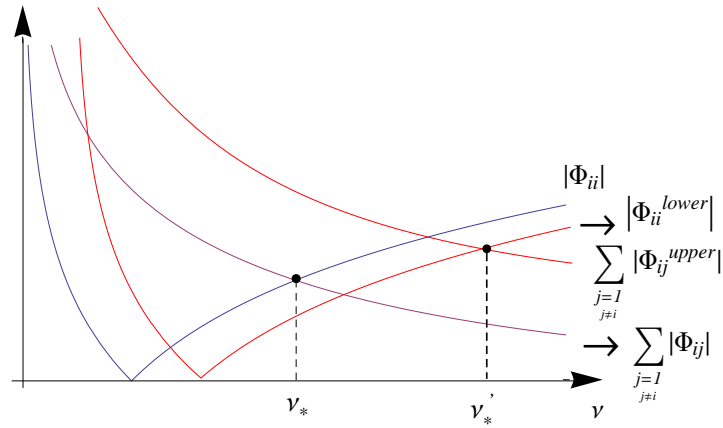


Figure 4.4. Another critical value

The solution is given by the Lambert W function which was introduced in (3.63). Therefore, we find

$$\nu'_* = \mu + 2\mu_d W \left[(N-1)e^{-\frac{\mu}{2\mu_d}} \right], \quad (4.69)$$

or

$$E'_* = - \left\{ \mu + 2\mu_d W \left[(N-1)e^{-\frac{\mu}{2\mu_d}} \right] \right\}^2. \quad (4.70)$$

Hence,

$$E \geq E'_* = - \left\{ \mu + 2\mu_d W \left[(N-1)e^{-\frac{\mu}{2\mu_d}} \right] \right\}^2. \quad (4.71)$$

□

4.4.2. Spectral Properties of Bound States

Theorem 4.10 (*Hellmann-Feynman Theorem*) (Feynman, 1939) (Hellmann, 1937)

A non-degenerate eigenvalue of a Hermitian operator (in a finite-dimensional Hilbert space) in a parameter dependent eigensystem varies with respect to the parameter according to the formula

$$\frac{\partial E(\nu)}{\partial \nu} = \left\langle \psi(\nu) \left| \frac{\partial H(\nu)}{\partial \nu} \psi(\nu) \right. \right\rangle , \quad (4.72)$$

where

$$H(\nu)\psi(\nu) = E(\nu)\psi(\nu) , \quad (4.73)$$

provided that the derivatives are well-defined and the associated normalized eigenfunction, $\psi(\nu)$, is continuous with respect to the parameter, ν .

(For the proof, see Appendix C.3. Also, the extension for the degenerate case of the theorem above can be found in Appendix D.)

Remark 4.2 *Actually, the above formula has been used in physics literature for also unbounded operators in infinite-dimensional Hilbert spaces. Then, one should be careful about the domain of the operator where the domain itself may also depend on the parameter ν . In this case, the formula (4.72) is generalized to include such cases (Esteve & Falceto & Canal, 2009). Nevertheless, we do not need this generalized version of Hellmann-Feynman theorem because we are going to apply this theorem for finite-dimensional renormalized principal matrix $\Phi(E)$.*

Definition 4.5 (Kato, 1995)

If X is an inner product space and the operator-valued function $T(x) \in B(X)$ is holomorphic in a domain D_0 of the x -plane intersecting with real axis and symmetric for real x :

$$T^\dagger(x) = T(x) , \quad (4.74)$$

the family $\{T(x)\}$ is said to be symmetric.

$T^\dagger(x^*)$ is holomorphic for $x^* \in \overline{D_0}$ ($\overline{D_0}$ is the mirror image of D_0 with respect to the real axis) and coincides with $T(x)$ for real x . Hence, $T^\dagger(x^*) = T(x)$ for $x \in D_0 \cap \overline{D_0}$ by the unique continuation property of holomorphic functions. Thus, $T^\dagger(x) = T(x^*)$ as long as both x and x^* belong to D_0 . Then we may assume without loss of generality that D_0 is symmetric with respect to the real axis.

Theorem 4.11 (*Kato, 1995*)

If the holomorphic family $T(x)$ is symmetric, the eigenvalues $w^k(x)$ and the eigenprojections $\mathbb{P}_k(x)$ are holomorphic on the real axis of x .

Corollary 4.4 *The renormalized principal matrix $\Phi(E)$ given explicitly in (4.48) is holomorphic except that it has a branch cuts along the positive real E axis. (K_0 and \log have branch cut along the positive real E axis.)*

Theorem 4.12 (*Spectral Theorem*) (*Halmos, 1974*)

If T is a normal (in particular self-adjoint) operator on a finite N -dimensional inner product space, there are always corresponding real numbers w_1, \dots, w_r where r is a strictly positive integer, not greater than the dimension of the space and orthogonal projections $\mathbb{P}_1, \dots, \mathbb{P}_r$ such that

1. w_j are pairwise distinct for $1 \leq j \leq r \leq N$.
2. \mathbb{P}_j are pairwise orthogonal and different from zero. ($\mathbb{P}_i \mathbb{P}_j = 0 = \mathbb{P}_j \mathbb{P}_i$ for all i, j where $i \neq j$.)
3. $\sum_{j=1}^r \mathbb{P}_j = 1$.
4. $\Phi = \sum_{j=1}^r w_j \mathbb{P}_j$.

Lemma 4.3 *The eigenvalues w^k of the principal matrix Φ flow according to*

$$\left(\frac{dw^k(E)}{dE} \right) \Big|_{E=-\nu^2} < 0, \quad (4.75)$$

that is, all the eigenvalues of the principal matrix strictly decreasing with respect to $E \in \mathbb{R}$ or strictly increasing with respect to ν :

$$\frac{dw^k(\nu)}{d\nu} > 0, \quad (4.76)$$

where $E = -\nu^2$.

Proof Since $w^k(E) = \langle A_i(E), \Phi_{ij}(E)A_j(E) \rangle$ from Eq. (4.56), as a consequence of the Hellmann-Feynman theorem, we obtain

$$\frac{dw^k(E)}{dE} = \left\langle A_i(E), \frac{d\Phi_{ij}(E)}{dE} A_j(E) \right\rangle = \sum_{i,j=1}^N A_i^*(E) \frac{d\Phi_{ij}(E)}{dE} A_j(E). \quad (4.77)$$

From Eq. (4.44) and (4.48), it is easy to see that

$$\frac{d\Phi_{ij}(E)}{dE} = \begin{cases} \frac{m}{2\pi\hbar^2 E} & \text{if } i = j, \\ - \int_{\mathbb{R}^2} \frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}}}{\left(\frac{\mathbf{p}^2}{2m} - E\right)^2} [d^2p] & \text{if } i \neq j, \end{cases} \quad (4.78)$$

from the definition of the matrix derivative $\frac{d\Phi(E)}{dE} = \left[\frac{d\Phi_{ij}(E)}{dE} \right]$ (Meyer, 2001). Let us substitute the above equation into Eq. (4.77) and then we have

$$\begin{aligned} \frac{dw^k(E)}{dE} &= \frac{m}{2\pi\hbar^2 E} |A_i(E)|^2 \\ &- \int_{\mathbb{R}^2} \left[\sum_{\substack{i,j=1 \\ j \neq i}}^N A_i^*(E) \frac{e^{\frac{i\mathbf{p}\cdot(\mathbf{a}_i - \mathbf{a}_j)}{\hbar}}}{\left(\frac{\mathbf{p}^2}{2m} - E\right)^2} A_j(E) \right] [d^2p]. \end{aligned} \quad (4.79)$$

By evaluating this at $E = -\nu^2$ and using the result:

$$\frac{m}{2\pi\hbar^2\nu^2} = \int_{\mathbb{R}^2} \frac{1}{\left(\frac{\mathbf{p}^2}{2m} + \nu^2\right)^2} [d^2p], \quad (4.80)$$

we obtain

$$\left. \frac{dw^k(E)}{dE} \right|_{E=-\nu^2} = - \int_{\mathbb{R}^2} \left[\frac{\left| \sum_{i=1}^N A_i^*(-\nu^2) e^{\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}} \right|^2}{\left(\frac{\mathbf{p}^2}{2m} + \nu^2\right)^2} \right] [d^2p]. \quad (4.81)$$

So, we end up with (4.75) or from the chain rule, we can easily see that

$$\left[\frac{dw^k(E)}{dE} \frac{dE}{d\nu} \right] \Big|_{E=-\nu^2} = \underbrace{\frac{dw^k(E)}{dE} \Big|_{E=-\nu^2}}_{<0} \underbrace{(-2\nu)}_{<0} > 0, \quad (4.82)$$

which means that (4.76). □

Corollary 4.5 *From Lemma 4.3, the number of bound states (negative eigenvalues) are at most N . This is the consequence of the fact that any $w^k(\nu)$ can intersect ν -axis only at once. In order to see this more clearly, suppose all the eigenvalues of Φ are non-degenerate, that is, we have $w_1(\nu) < w_2(\nu) < \dots < w_N(\nu)$. Due to (4.76), all the eigenvalues intersect ν -axis at once, we have N bound states. If there were degeneracies, some of the eigenvalues would be coincided, so that the number of bound states would be less than N . The graphs for $N = 2, 3, 4$ were given at the end of Chapter 3 in detail.*

Remark 4.3 *The integral given in (4.81) is convergent. In order to see this, we use the Cauchy-Schwarz inequality (Debnath & Mikusiński, 2005)*

$$\begin{aligned} \int_{\mathbb{R}^2} \left[\frac{\left| \sum_{i=1}^N A_i^*(-\nu^2) e^{\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}} \right|^2}{\left(\frac{\mathbf{p}^2}{2m} + \nu^2 \right)^2} \right] [d^2p] \\ \leq \int_{\mathbb{R}^2} \left[\frac{\sum_{j=1}^N |A_j^*(-\nu^2)|^2 \sum_{l=1}^N \left| e^{\frac{i\mathbf{p}\cdot\mathbf{a}_l}{\hbar}} \right|^2}{\left(\frac{\mathbf{p}^2}{2m} + \nu^2 \right)^2} \right] [d^2p]. \end{aligned} \quad (4.83)$$

Since A_j 's are normalized eigenvectors and from (4.80), we immediately obtain

$$\int_{\mathbb{R}^2} \left[\frac{\left| \sum_{i=1}^N A_i^*(-\nu^2) e^{\frac{i\mathbf{p}\cdot\mathbf{a}_i}{\hbar}} \right|^2}{\left(\frac{\mathbf{p}^2}{2m} + \nu^2 \right)^2} \right] [d^2p] \leq \frac{N^2 m}{2\pi \hbar^2 \nu^2}, \quad (4.84)$$

which is finite.

Definition 4.6 (Pazy, 1983)

Let Ω be a subset of the complex plane. A family $J(E)$, $E \in \Omega$, of bounded linear operators

on the Hilbert space \mathcal{H} under consideration which satisfies the resolvent identity

$$J(E_1) - J(E_2) = (E_1 - E_2)J(E_1)J(E_2), \quad (4.85)$$

for $E_1, E_2 \in \Omega$ is called a pseudo resolvent on Ω .

Theorem 4.13 (Pazy, 1983)

Let Ω be an unbounded subset of \mathbb{C} and $J(E)$ be a pseudo resolvent on Ω . If there is a sequence $E_k \in \Omega$ such that $|E_k| \rightarrow \infty$ as $k \rightarrow \infty$ and

$$\lim_{k \rightarrow \infty} -E_k J(E_k)x = x, \quad (4.86)$$

for all $x \in \mathcal{H}$, then $J(E)$ is the resolvent of a unique densely defined closed operator.

Theorem 4.14 (Kato, 1995)

If the family satisfies $J^\dagger(E) = J(E^*)$, it is a holomorphic family of type (A) in the sense of Kato. Hence, it defines a self-adjoint operator.

Corollary 4.6 After the renormalization procedure defined above, there exists a unique densely defined closed self-adjoint operator associated with the resolvent (4.52).

Proof Since the proof is very technical, we skip it and suggest the reader to read the reference (Dogan & Erman & Turgut, 2012). \square

Theorem 4.15 The bound state wave function $\psi_k(\mathbf{x})$ for the particle in the presence of N point interactions in two dimensions is given by

$$\begin{aligned} \psi_k(\mathbf{x}) &= \alpha \sum_{i=1}^N R_0(\mathbf{x}, \mathbf{a}_i; -\nu_k^2) A_i(-\nu_k^2) \\ &= \frac{m}{\pi \hbar^2} \alpha \sum_{i=1}^N K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{x} - \mathbf{a}_i|}{\hbar} \right) A_i(-\nu_k^2), \end{aligned} \quad (4.87)$$

where $\alpha = \left[- \left(\frac{dw^k(E)}{dE} \right) \Big|_{E=-\nu_k^2} \right]^{-\frac{1}{2}}$, A_i is the eigenvector of the renormalized principal matrix and $A_i(-\nu_k^2)$ is the eigenvector if the renormalized principal matrix associated with the eigenvalue $w(-\nu_k^2)$ such that $w(-\nu_k^2) = 0$.

Proof We had an eigenvalue problem given by (4.56). Since the renormalized principal matrix Φ given in (4.48) satisfies $\Phi_{ij}^\dagger(E) = \Phi_{ij}(E^*)$ on the complex plane, that means it is symmetric for real values of E : $\Phi_{ij}^\dagger(E) = \Phi_{ij}(E)$. Then, according to Theorem 4.11, there exists a holomorphic family of projection operators on the complex plane, so that we can apply the spectral theorem for $\Phi(E)$,

$$\Phi_{ij}(E) = \sum_k w^k(E) [\mathbb{P}_k(E)]_{ij} , \quad (4.88)$$

where $[\mathbb{P}_k(E)]_{ij} = A_i^k(E) [A^\dagger(E)]_j^k$ is the projection operator onto the eigenspace spanned by the eigenvectors A_i^k 's. Let Γ_k be a closed contour enclosing the bound state energy $E = -\nu_k^2$. We are going to apply Riesz integral (Definition 4.4) to find the wave function corresponding to the eigenvalue $-\nu_k^2$. Due to Theorem 4.11, the spectral resolution of the inverse renormalized principal matrix (4.48) is

$$[\Phi^{-1}(E)]_{ij} = \sum_k \frac{1}{w^k(E)} [\mathbb{P}_k(E)]_{ij} . \quad (4.89)$$

The residue can then be found from Eq. (4.52)

$$Res [R_0(\mathbf{x}, \mathbf{a}_i; E) [\Phi^{-1}(E)]_{ij} R_0(\mathbf{a}_j, \mathbf{y}; E), -\nu_k^2] , \quad (4.90)$$

since the free resolvent kernel has no poles on the negative real axis. Because $w^k(E)$ and $\mathbb{P}_k(E)$ are holomorphic on the negative E axis and due to Lemma 4.3,

$$Res \{ [\Phi^{-1}(E)]_{ij}, -\nu_k^2 \} = \left[\frac{dw^k(E)}{dE} \Big|_{E=-\nu_k^2} \right]^{-1} [\mathbb{P}_k(-\nu_k^2)]_{ij} , \quad (4.91)$$

where the only contribution to the k -sum is coming from the k -th term and we have used

$$w^k(E) = \underbrace{w^k(E = -\nu_k^2)}_0 + (E + \nu_k^2) \underbrace{\frac{dw^k(E)}{dE} \Big|_{E=-\nu_k^2}}_{\neq 0} + \dots . \quad (4.92)$$

Also, from Eq. (4.12),

$$2\pi i \text{Res} [R(\mathbf{x}, \mathbf{y}; E), -\nu_k^2] = \oint_{\Gamma_k} R(\mathbf{x}, \mathbf{y}; E) dE = -2\pi i \psi_k(\mathbf{x})\psi_k^*(\mathbf{y}), \quad (4.93)$$

so that

$$\psi_k(\mathbf{x})\psi_k^*(\mathbf{y}) = - \sum_{i,j=1}^N \frac{R_0(\mathbf{x}, \mathbf{a}_i; -\nu_k^2) A_i(-\nu_k^2) A_j^*(-\nu_k^2) R_0(\mathbf{a}_j, \mathbf{y}; -\nu_k^2)}{\left(\frac{dw^k(E)}{dE} \right) \Big|_{E=-\nu_k^2}}. \quad (4.94)$$

From Eq. (4.20) and using the relation between (4.44) and (4.48), we obtain

$$R_0(\mathbf{x}, \mathbf{a}_i; -\nu_k^2) = \frac{m}{\pi \hbar^2} K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{x} - \mathbf{a}_i|}{\hbar} \right) = R_0^*(\mathbf{x}, \mathbf{a}_i; -\nu_k^2), \quad (4.95)$$

where we have also used the fact that ν_k is real and positive. Hence, we end up with

$$\psi_k(\mathbf{x})\psi_k^*(\mathbf{y}) = - \frac{m^2}{\pi^2 \hbar^4} \sum_{i,j=1}^N \frac{K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{x} - \mathbf{a}_i|}{\hbar} \right) A_i(-\nu_k^2) A_j^*(-\nu_k^2) K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{y} - \mathbf{a}_j|}{\hbar} \right)}{\left(\frac{dw^k(E)}{dE} \right) \Big|_{E=-\nu_k^2}} \quad (4.96)$$

from which the wave function $\psi_k(\mathbf{x})$ in (4.87) is found. \square

Corollary 4.7 *The number of degeneracy of $-\nu_k^2$ equals to the number of degeneracy of the zero eigenvalue of the renormalized principal matrix (Albeverio & Gesztesy & Høegh-Krohn & Holden & Exner, 1988).*

Corollary 4.8 *The bound state wave function (4.87) does not belong to the domain of H_0 , i.e., $\psi_k(\mathbf{x}) \notin \mathcal{D}(H_0)$.*

Proof By taking the average value of H_0 ,

$$\begin{aligned} \langle \psi_k | H_0 | \psi_k \rangle &= - \frac{\hbar^2 |\alpha|^2}{2m} \int_{\mathbb{R}^2} \left[\sum_{i=1}^N R_0^*(\mathbf{x}, \mathbf{a}_i; -\nu_k^2) A_i^*(-\nu_k^2) \right. \\ &\quad \left. \times \sum_{j=1}^N \Delta R_0(\mathbf{x}, \mathbf{a}_j; -\nu_k^2) A_j(-\nu_k^2) \right] d^2x. \end{aligned} \quad (4.97)$$

From Eq. (4.95), the above equation becomes for the $i = j$ term:

$$\begin{aligned} \langle \psi_k | H_0 | \psi_k \rangle &= -\frac{m|\alpha|^2}{2\pi^2\hbar^2} |A_i(-\nu_k^2)|^2 \int_{\mathbb{R}^2} \left[K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{x} - \mathbf{a}_i|}{\hbar} \right) \right. \\ &\quad \left. \times \Delta K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{x} - \mathbf{a}_i|}{\hbar} \right) \right] d^2x . \end{aligned} \quad (4.98)$$

We use polar coordinates; $|\mathbf{x} - \mathbf{a}_i| = r$ and $d^2x = r dr d\theta$, then

$$\langle \psi_k | H_0 | \psi_k \rangle = -\frac{m|\alpha|^2}{\pi\hbar^2} |A_i(-\nu_k^2)|^2 \int_0^\infty K_0(ar) \frac{d^2 K_0(ar)}{dr^2} r dr , \quad (4.99)$$

where $a = \frac{\nu_k \sqrt{2m}}{\hbar}$. The integral in the above equation is

$$\int_0^\infty K_0(ar) \frac{d^2 K_0(ar)}{dr^2} r dr = \int_0^\infty K_0(ar) \left[a^2 K_0(ar) + \frac{a}{r} K_1(ar) \right] r dr , \quad (4.100)$$

where we have used recurrence relations of Bessel functions given in (3.135). But, it has already been proved in (3.137) that this integral is divergent, that is

$$\langle \psi_k | H_0 | \psi_k \rangle = \infty . \quad (4.101)$$

This means that $\psi_k(\mathbf{x}) \notin \mathcal{D}(H_0)$. □

We have found that the bound state wave function (4.87) in $L^2(\mathbb{R}^2)$ (see Remark 4.5) is not contained in the domain of H_0 although it belongs to the domain of the Hamiltonian, say H (its formal expression is not constructed in this approach), after the renormalization procedure. Renormalization procedure only provides us the resolvent formula. Pictorially,

It is well-known that Hamiltonian with point interaction can be described as a free Hamiltonian H_0 on a space with one point (center of the Dirac delta potential, say origin) deleted ($\mathbb{R}^2 \setminus \{0\}$) and a boundary condition which specifies the behavior of the wave function at the origin (Jackiw, 1995) (Albeverio & Kurasov, 2000).

Remark 4.4 *As a consequence of Corollary 4.6 and the above observation, we may think of our problem as a kind of self-adjoint extension since $\psi_k \in \mathcal{D}(H)$ whereas $\psi_k \notin \mathcal{D}(H_0)$ which means that the domain of H_0 is extended such that the bound state wave functions $\psi_k(\mathbf{x})$ are included so that $D(H) = D(H^\dagger)$.*

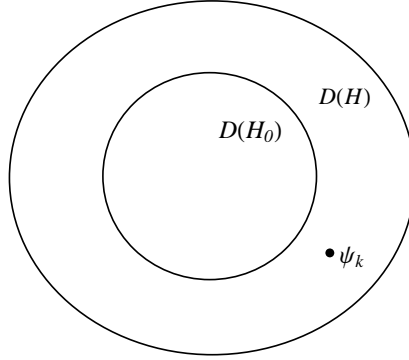


Figure 4.5. Domain of H and H_0

Remark 4.5 We will show that $\psi_k(\mathbf{x}) \in L^2(\mathbb{R}^2)$. From (4.87), we have

$$\begin{aligned} \int_{\mathbb{R}^2} |\psi_k(\mathbf{x})|^2 dx dy &= \frac{m^2 |\alpha|^2}{\pi^2 \hbar^4} \int_{\mathbb{R}^2} \left| \sum_{i=1}^N K_0 \left(\frac{\nu_k \sqrt{2m} |\mathbf{r} - \mathbf{a}_i|}{\hbar} \right) A_i(-\nu_k^2) \right|^2 dx dy \\ &\leq \frac{m^2 |\alpha|^2}{\pi^2 \hbar^4} \int_{\mathbb{R}^2} \sum_{i=1}^N K_0^2 \left(\frac{\nu_k \sqrt{2m} |\mathbf{r} - \mathbf{a}_i|}{\hbar} \right) dx dy, \end{aligned} \quad (4.102)$$

where $\mathbf{r} = (x, y)$. If we use polar coordinates, we find

$$\int_{\mathbb{R}^2} K_0^2 \left(\frac{\nu_k \sqrt{2m} |\mathbf{r} - \mathbf{a}_i|}{\hbar} \right) dx dy = \int_0^{2\pi} \int_0^\infty K_0^2 \left(\frac{\nu_k \sqrt{2m} r_i}{\hbar} \right) r_i dr_i d\theta, \quad (4.103)$$

where $r_i = |\mathbf{r} - \mathbf{a}_i|$. By using a sharp bound for K_0 (Erman, 2010):

$$K_0(x) \leq e^{-\frac{x}{2}} \left[\frac{2}{1+x} + \ln \left(1 + \frac{1}{x} \right) \right], \quad (4.104)$$

we obtain

$$\int_{\mathbb{R}^2} K_0^2 \left(\frac{\nu_k \sqrt{2m} |\mathbf{r} - \mathbf{a}_i|}{\hbar} \right) dx dy \leq 2\pi \int_0^\infty e^{-\frac{\nu_k \sqrt{2m} r_i}{\hbar}} \left[\frac{2\hbar}{\hbar + \nu_k \sqrt{2m} r_i} + \ln \left(1 + \frac{\hbar}{\nu_k \sqrt{2m} r_i} \right) \right]^2 r_i dr_i. \quad (4.105)$$

One can solve this integral and find out that it is finite for all $i = 1, \dots, N$, then $\psi_k(\mathbf{x}) \in L^2(\mathbb{R}^2)$.

4.4.3. Positivity and Non-degeneracy of the Ground State

The Perron-Frobenius theorem for positive symmetric matrices is going to provide us to determine that the ground state wave function is positive and non-degenerate. Firstly, let us state the Perron-Frobenius theorem for symmetric and positive matrices.

Theorem 4.16 (Perron-Frobenius Theorem) (Ninio, 1976)

Let $A = (a_{ij})$ be an $n \times n$ symmetric matrix with elements $a_{ij} > 0$ and let λ be the largest eigenvalue. Then,

1. $\lambda > 0$.
2. There exists a corresponding eigenvector (X_j) with every entry $X_j > 0$.
3. λ is non-degenerate.
4. If μ is any other eigenvalue, $\lambda > |\mu|$.

(For the proof, one can consult on Appendix E.)

Theorem 4.17 The ground state wave function corresponding to the finitely many point interactions in \mathbb{R}^2 can be chosen strictly positive and it is non-degenerate.

Proof The renormalized principal matrix given in Eq. (4.48) neither is symmetric nor positive. However, if we restrict E to be real, then we have a symmetric matrix. From the explicit expression of the renormalized principal matrix (3.145), we have $\Phi_{ii}(\nu) > 0$ for $\nu > \nu_{gr} > \mu_i$. The inequality $\nu_{gr} > \mu_i$ or $E_{gr} \leq -\mu_i^2$ is physically expected since when we add attractive potentials, the ground state is lower. However, $\Phi_{ij}(\nu) < 0$ for all

ν . Nevertheless, we can make the renormalized principal matrix positive by subtracting a constant diagonal matrix. First, consider the eigenvalue problem $\Phi A = wA$:

$$\sum_{j=1}^N \Phi_{ij}(\nu) A_j(\nu) = \Phi_{ii}(\nu) A_i(\nu) + \sum_{\substack{j=1 \\ j \neq i}}^N \Phi_{ij}(\nu) A_j(\nu) = w(\nu) A_i(\nu) . \quad (4.106)$$

In order to make Φ positive, we subtract $(1 + \epsilon) \max_{\nu} \Phi_{ii}(\nu)$ from $\Phi_{ij}(\nu)$ where ϵ is a small positive number, and multiply by -1 :

$$\Phi'_{ij}(\nu) = - \left[\Phi_{ij}(\nu) - (1 + \epsilon) \max_{\nu} \Phi_{ii}(\nu) \right] . \quad (4.107)$$

Note that in this way, we have a new positive matrix whose eigenvectors are the same as the one for the original renormalized principal matrix. (We have just shifted diagonal matrix from the original renormalized principal matrix.) Since $\nu \leq \nu_{gr}$ from Eq. (4.71), $\max_{\nu} \Phi_{ii}(\nu) = \Phi_{ii}(\nu_{gr})$. Therefore,

$$\sum_{j=1}^N \Phi'_{ij}(\nu) A_j(\nu) = - [w(\nu) - (1 + \epsilon) \Phi_{ii}(\nu_{gr})] A_i(\nu) , \quad (4.108)$$

or

$$\Phi'(\nu) A(\nu) = - [w(\nu) - (1 + \epsilon) \Phi_{ii}(\nu_{gr})] A(\nu) = w'(\nu) A(\nu) , \quad (4.109)$$

where $\Phi'(\nu) > 0$ and $- [w(\nu) - (1 + \epsilon) \Phi_{ii}(\nu_{gr})] = w'(\nu)$ is our shifted eigenvalue corresponding to the same eigenvector $A(\nu)$ as before. From now on we have a symmetric and positive new matrix $\Phi'(\nu)$, then from the Perron-Frobenius theorem applied to $\Phi'(\nu)$:

1. Largest eigenvalue $w'_{max} > 0$.
2. There exists a corresponding eigenvector (A_j) with every entry $A_j > 0$.
3. w'_{max} is non-degenerate.
4. If Ω is any other eigenvalue, then $w'_{max} > |\Omega|$.

From the first case we have $w'_{max}(\nu) = - [w_{max}(\nu) - (1 + \epsilon) \Phi_{ii}(\nu_{gr})] > 0$. That means $w_{max}(\nu) < (1 + \epsilon) \Phi_{ii}(\nu_{gr})$. The third case means that we have one and only one eigenvector

$A^{max}(\nu)$ corresponding to the eigenvalue $w'_{max}(\nu)$. Then,

$$\begin{aligned}\Phi'(\nu)A^{max}(\nu) &= w'_{max}(\nu)A^{max}(\nu) \\ &= -[w_{max}(\nu) - (1 + \epsilon)\Phi_{ii}(\nu_{gr})]A^{max}(\nu),\end{aligned}\quad (4.110)$$

or it can be written as

$$\begin{aligned}\Phi'_{ii}(\nu)A_i^{max}(\nu) + \sum_{\substack{j=1 \\ j \neq i}}^N \Phi'_{ij}(\nu)A_j^{max}(\nu) &= -w_{max}(\nu)A_i^{max}(\nu) \\ &+ (1 + \epsilon)\Phi_{ii}(\nu_{gr})A_i^{max}(\nu).\end{aligned}\quad (4.111)$$

On the other hand, from Eq. (4.107), we have

$$\begin{aligned}\Phi'_{ii}(\nu)A_i^{max}(\nu) + \sum_{\substack{j=1 \\ j \neq i}}^N \Phi'_{ij}(\nu)A_j^{max}(\nu) &= -\sum_{j=1}^N \Phi_{ij}A_j^{max}(\nu) \\ &+ (1 + \epsilon)\Phi_{ii}(\nu_{gr})A_i^{max}(\nu).\end{aligned}\quad (4.112)$$

By comparing the above equations, we find

$$\Phi(\nu)A^{max}(\nu) = w_{max}(\nu)A^{max}(\nu), \quad (4.113)$$

which means that $A^{max}(\nu)$ is also an eigenvector of $\Phi(\nu)$. It is easy to see that for a given ν , only $w_{max}(\nu)$ flows to the point ν_{gr} (associated with E_{gr}). From Eq. (4.87), (4.20) and Lemma 4.3, we have

$$\psi_{gr}(\mathbf{x}) = \underbrace{\alpha}_{>0} \sum_{i=1}^N \underbrace{R_0(\mathbf{x}, \mathbf{a}_i; E_{gr})}_{>0} \underbrace{A_i^{max}(E_{gr})}_{>0} > 0, \quad (4.114)$$

which means that the ground state wave function corresponding finitely many point interactions can be chosen positive and from non-degeneracy of $A_i^{max}(E_{gr})$ and Corollary 4.7, it is non-degenerate. \square

CHAPTER 5

SIMPLE HARMONIC OSCILLATOR POTENTIAL SUPPORTED BY A POINT INTERACTION IN \mathbb{R} AND \mathbb{R}^2

One way to understand the spectrum of this problem in a better way is to use heat kernel which is very useful and elegant. Let us first define the heat kernel:

5.1. The Heat Equation and Heat Kernel

The solution to the initial value problem (IVP) of the heat equation in \mathbb{R}^D (Calin & Chang & Furutani & Iwasaki, 2011)

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \mathbb{L}u(\mathbf{x}, t), \quad (5.1)$$

$$u(\mathbf{x}, 0) = f(\mathbf{x}), \quad (5.2)$$

where \mathbb{L} is a second order linear self-adjoint elliptic operator (in particular, it could be Laplacian), is given by

$$u(\mathbf{x}, t) = \int_{\mathbb{R}^D} K_t(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) dy. \quad (5.3)$$

Here, $K_t(\mathbf{x}, \mathbf{y})$ is called the fundamental solution of the heat operator or heat kernel if it satisfies

1. $\frac{\partial}{\partial t} K_t(\mathbf{x}, \mathbf{y}) = \mathbb{L}K_t(\mathbf{x}, \mathbf{y})$,
2. $\lim_{t \rightarrow 0} K_t(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y})$ in the sense of distributions.

Lemma 5.1 *The solution to the above initial value problem for $\mathbb{L} = \Delta$ in one dimension is given by*

$$u(x, t) = \int_{\mathbb{R}} \frac{e^{-\frac{(x-y)^2}{4t}}}{\sqrt{4\pi t}} f(y) dy . \quad (5.4)$$

Proof Consider the Fourier integral transform of $\phi(k, t)$ with respect to the variable k :

$$u(x, t) = \int_{\mathbb{R}} e^{ikx} \phi(k, t) [dk] , \quad (5.5)$$

where $[dk] = \frac{dk}{2\pi}$. When $t = 0$,

$$u(x, 0) = \int_{\mathbb{R}} e^{ikx} \phi(k, 0) [dk] = f(x) . \quad (5.6)$$

By the inverse Fourier transform,

$$\phi(k, 0) = \int_{\mathbb{R}} e^{-ikx} f(x) dx . \quad (5.7)$$

The goal is to find $u(x, t)$ in terms of $f(x)$. Let us write $u_t = \Delta u$ explicitly in Eq. (5.5),

$$\int_{\mathbb{R}} \left[\frac{\partial \phi(k, t)}{\partial t} + k^2 \phi(k, t) \right] e^{ikx} [dk] = 0 , \quad (5.8)$$

then $\frac{\partial \phi(k, t)}{\partial t} = -k^2 \phi(k, t)$. Separation of variables, $\phi(k, t) = \phi_1(k) \phi_2(t)$, yields $\phi_2(t) = A e^{-k^2 t}$ where A is some constant and since $\phi(k, 0) = A \phi_1(k)$, we have

$$\phi(k, t) = \phi(k, 0) e^{-k^2 t} . \quad (5.9)$$

From Eq. (5.7), the above equation becomes

$$\phi(k, t) = e^{-k^2 t} \int_{\mathbb{R}} e^{-iky} f(y) dy . \quad (5.10)$$

By substituting the above equation into (5.5), we obtain

$$u(x, t) = \frac{1}{2\pi} \int_{\mathbb{R}} \left[\int_{\mathbb{R}} e^{ik(x-y)} e^{-k^2 t} dk \right] f(y) dy . \quad (5.11)$$

The second integral looks like Gaussian integral. Let us write $k = k' + c$ where c is some constant and try to find this c in order to make the integral Gaussian. Then,

$$u(x, t) = \frac{1}{2\pi} \int_{\mathbb{R}} \left[e^{ic(x-y)-c^2 t} \int_{\mathbb{R}} e^{ik(x-y+2ict)} e^{-k^2 t} dk \right] f(y) dy . \quad (5.12)$$

To make the interior integral Gaussian, $x - y + 2ict$ should be zero. Hence, one can immediately obtain the result (5.4). \square

Corollary 5.1 *From Lemma 5.1, the heat kernel in one dimension is given by*

$$K_t(x, y) = \frac{e^{-\frac{(x-y)^2}{4t}}}{\sqrt{4\pi t}} , \quad (5.13)$$

due to Eq. (5.3).

Lemma 5.2 *The solution to the initial value problem for $\mathbb{L} = \Delta$ in two dimensions is given by*

$$u(\mathbf{x}, t) = \int_{\mathbb{R}^2} \frac{e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}}}{4\pi t} f(\mathbf{y}) d^2 y . \quad (5.14)$$

Proof We are now going to consider the Fourier integral transform in two dimensions:

$$u(\mathbf{x}, t) = \int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{k}, t) [d^2 k] , \quad (5.15)$$

where $[d^2 k] = \frac{d^2 k}{(2\pi)^2}$. When $t = 0$,

$$u(\mathbf{x}, 0) = \int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{k}, 0) [d^2 k] = f(\mathbf{x}) . \quad (5.16)$$

After applying the same procedure as we did for one dimension, we obtain

$$u(\mathbf{x}, t) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-k^2 t} d^2 k \right] f(\mathbf{y}) d^2 y . \quad (5.17)$$

We use polar coordinates for the interior integral, then

$$\int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-k^2 t} d^2 k = \int_0^\infty \int_0^{2\pi} k e^{-k^2 t} e^{ik|\mathbf{x}-\mathbf{y}|\cos\theta} dk d\theta , \quad (5.18)$$

and using the Bessel function of the first kind as we did for Eq. (3.129), we have

$$\begin{aligned} \int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-k^2 t} d^2 k &= 2\pi \int_0^\infty k e^{-k^2 t} J_0(k|\mathbf{x}-\mathbf{y}|) dk \\ &= \frac{\pi e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}}}{t} , \end{aligned} \quad (5.19)$$

where we have used the formula given by (Gradshteyn & Ryzhik, 2000)

$$\begin{aligned} \int_0^\infty x^\mu e^{-\alpha x^2} J_\nu(\beta x) dx &= \frac{\beta^\nu \Gamma\left(\frac{1}{2}\nu + \frac{1}{2}\mu + \frac{1}{2}\right)}{2^{\nu+1} \alpha^{\frac{1}{2}(\nu+\mu+1)} \Gamma(\nu+1)} \\ &\times {}_1F_1\left(\frac{\nu+\mu+1}{2}; \nu+1; -\frac{\beta^2}{4\alpha}\right) . \end{aligned} \quad (5.20)$$

Here, functions of the form ${}_1F_1(a; b; c)$ are called the confluent hypergeometric functions of the first kind and introduced by (Gradshteyn & Ryzhik, 2000)

$${}_1F_1(a; b; c) = \sum_{k=0}^{\infty} \frac{(a)_k c^k}{(b)_k k!} , \quad (5.21)$$

where

$$(a)_k = \begin{cases} 1 & \text{if } k = 0 , \\ a(a+1) \dots (a+k-1) & \text{if } k > 0 . \end{cases} \quad (5.22)$$

By inserting (5.19) into (5.17), we obtain (5.14). □

Corollary 5.2 *Due to Lemma 5.2, the heat kernel in two dimensions reads*

$$K_t(\mathbf{x}, \mathbf{y}) = \frac{e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}}}{4\pi t} . \quad (5.23)$$

Also, the heat kernel in D dimensions satisfies the following property (Calin & Chang & Furutani & Iwasaki, 2011):

$$\int_{\mathbb{R}^D} K_t(\mathbf{x}, \mathbf{y}) d^D x = 1 , \quad (5.24)$$

for all $\mathbf{y} \in \mathbb{R}^D$.

5.2. Eigenfunction Expansion of Heat Kernel and Mehler's Formula

Consider the self-adjoint differential operator \mathbb{L} defined on the interval I and let f_i be its eigenfunctions (Calin & Chang & Furutani & Iwasaki, 2011)

$$\mathbb{L}f_i = \lambda_i f_i , \quad (5.25)$$

where $i = 0, 1, \dots$ and $\lambda_i \in \mathbb{R}$ are eigenvalues of \mathbb{L} . We are going to assume that $\{f_i\}_{i \geq 0}$ is a complete orthogonal system of $L^2(I) = \{f : I \rightarrow \mathbb{C}; \int_I |f|^2 < \infty\}$. Then, for any function $\varphi \in L^2(I)$ we have

$$\varphi(x) = \sum_{i \geq 0} \langle f_i, \varphi \rangle f_i(x) , \quad (5.26)$$

where $\langle f_i, \varphi \rangle = \int_I f_i(x) \varphi(x) dx$. The next result provides a formal expansion for the heat kernel.

Proposition 5.1 (Calin & Chang & Furutani & Iwasaki, 2011) *Let $\{f_i\}_{i \geq 0}$ be a complete orthogonal system of $L^2(I)$ of real eigenfunctions of operator \mathbb{L} . Then, the heat kernel of \mathbb{L} is*

given by

$$K_t(x_0, x) = \sum_{i \geq 0} e^{\lambda_i t} f_i(x_0) f_i(x) . \quad (5.27)$$

In general, there is a complex conjugate of $f_i(x)$.

Proof The proof is trivial by checking whether it satisfies the definition of the heat kernel given above. \square

Lemma 5.3 (Calin & Chang & Furutani & Iwasaki, 2011) If $H_n(x)$ is the n -th Hermite polynomial, then Mehler's formula is given by

$$e^{-(x^2+y^2)} \sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) = \frac{e^{-\frac{(x^2+y^2-2xyz)}{1-z^2}}}{\sqrt{1-z^2}} , \quad (5.28)$$

where x, y, z are dimensionless variables.

Proof There are many different ways to prove this formula. One simple way is given in Appendix F.1. \square

Theorem 5.1 The heat kernel associated with the simple harmonic oscillator Hamiltonian in one dimension is given by

$$K_t(x, y) = \sqrt{\frac{m\omega}{\pi \hbar}} \frac{e^{-\frac{m\omega}{2\hbar} \coth(\omega t)(x^2+y^2) + \frac{m\omega}{\hbar \sinh(\omega t)} xy}}{\sqrt{2 \sinh(\omega t)}} . \quad (5.29)$$

Proof We have the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \Delta + \frac{1}{2} m \omega^2 x^2 , \quad (5.30)$$

then the heat equation for simple harmonic oscillator Hamiltonian given above is

$$\frac{\partial}{\partial t} u(x, t) = \mathbb{L}u(x, t) = -Hu(x, t) . \quad (5.31)$$

Since the eigenfunctions of simple harmonic oscillator in one dimension are given by (Merzbacher, 1961)

$$f_n(x) = \phi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-\frac{m\omega}{2\hbar} x^2}, \quad (5.32)$$

where H_n is the n -th Hermite polynomial and eigenvalues are

$$\lambda_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad (5.33)$$

by Proposition 5.1 and scaling $t \rightarrow \frac{t}{\hbar}$ because of the dimensional consistency, the heat kernel reads

$$K_t(x, y) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{\omega t}{2}} e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} \sum_{n=0}^{\infty} \frac{(e^{-\omega t})^n}{2^n n!} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x\right) H_n \left(\sqrt{\frac{m\omega}{\hbar}} y\right). \quad (5.34)$$

(For finding the eigenfunctions and eigenvalues of simple harmonic oscillator in one dimension, one can also consult on Appendix G.) Due to Lemma 5.3, the above equation becomes

$$K_t(x, y) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{\omega t}{2}} e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} \left[e^{\frac{m\omega}{\hbar}(x^2+y^2)} \frac{e^{-\frac{m\omega}{\hbar}(x^2+y^2 - 2xye^{-\omega t})}}{1 - e^{-2\omega t}} \right] \frac{1}{\sqrt{1 - e^{-2\omega t}}}. \quad (5.35)$$

By arranging this equation, we obtain the desired result (5.29). □

Corollary 5.3 *In particular, if we choose $x, y = 0$ in (5.29), we obtain*

$$K_t(0, 0) = \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2 \sinh(\omega t)}}, \quad (5.36)$$

which is going to be very useful for our calculations later on.

5.3. Spectrum of Isotropic Simple Harmonic Oscillator Supported by A Point Interaction in One Dimension

Theorem 5.2 *Consider the Hamiltonian*

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 - \lambda\delta(x) . \quad (5.37)$$

Then, the simple harmonic oscillator's odd-parity eigenfunctions $\phi_{2n+1}(x)$ are eigenfunctions of H with eigenvalues $E_{2n+1} = (2n + 1 + \frac{1}{2}) \hbar\omega$ for $n = 0, 1, \dots$. The eigenvalues corresponding to even-parity eigenfunctions are the solutions of the below transcendental equation:

$$\frac{1}{\lambda} = \frac{1}{2\hbar^{\frac{3}{2}}} \sqrt{\frac{m}{\omega}} \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega}\right)} . \quad (5.38)$$

Proof The time-independent Schrödinger equation in one dimension with a point interaction (formally), centered at the origin, and a simple harmonic oscillator potential is given by

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) - \lambda\delta(x)\psi(x) = E\psi(x) . \quad (5.39)$$

Also, due to the parity invariance of the Hamiltonian of simple Harmonic oscillator, the eigenfunctions $\psi(x)$ are even function if n is even and odd function if n is odd from Eq. (5.32). (Due to $H_n(-x) = (-1)^n H_n(x)$.) For odd-parity solutions $\psi_o(x)$: $\psi_o(-x) = -\psi_o(x)$. Hence, when $x = 0$, $\psi_o(0) = 0$. Then, Eq. (5.39) becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_o(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi_o(x) = E\psi_o(x) , \quad (5.40)$$

because of the property: $\delta(x)\psi(x) = \delta(x)\psi(0)$ which was given in Eq. (2.27). Then, $\psi_o(x) = \phi_{2n+1}(x)$ and eigenvalues are $E_n = (2n + \frac{3}{2}) \hbar\omega$ from (5.32) and (5.33), respectively. That means adding a point interaction to the simple harmonic oscillator potential does not change odd-parity spectrum of the simple harmonic oscillator which should be intuitively clear. For

even-parity solutions, we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_e(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi_e(x) - \lambda\delta(x)\psi_e(x) = E\psi_e(x) . \quad (5.41)$$

Let us expand $\psi_e(x)$ in terms of the even-parity eigenfunctions $\phi_{2n}(x)$ of simple harmonic oscillator (complete orthonormal system)

$$\psi_e(x) = \sum_{n=0}^{\infty} C_n \phi_{2n}(x) . \quad (5.42)$$

By substituting this into Eq. (5.41) and using the property (2.27), we find

$$\sum_{n=0}^{\infty} C_n \left[-\frac{\hbar^2}{2m} \frac{d^2\phi_{2n}(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \phi_{2n}(x) - E\phi_{2n}(x) \right] = \lambda\delta(x) \sum_{n=0}^{\infty} C_n \phi_{2n}(0) . \quad (5.43)$$

Since

$$-\frac{\hbar^2}{2m} \frac{d^2\phi_{2n}(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \phi_{2n}(x) = \left(2n + \frac{1}{2}\right) \hbar\omega \phi_{2n}(x) , \quad (5.44)$$

where we have used the fact given in (5.33). Afterwards, Eq. (5.43) becomes

$$\sum_{n=0}^{\infty} C_n \left[\left(2n + \frac{1}{2}\right) \hbar\omega - E \right] \phi_{2n}(x) = \lambda\delta(x) \sum_{n=0}^{\infty} C_n \phi_{2n}(0) . \quad (5.45)$$

After multiplying both sides with $\phi_{2l}(x)$ and integrating over x , we obtain

$$C_l \left[\left(2l + \frac{1}{2}\right) \hbar\omega - E \right] = \lambda\phi_{2l}(0) \sum_{n=0}^{\infty} C_n \phi_{2n}(0) = \lambda\phi_{2l}(0)\psi_e(0) , \quad (5.46)$$

so that

$$C_n = \frac{\lambda\phi_{2n}(0)\psi_e(0)}{\left[\left(2n + \frac{1}{2}\right) \hbar\omega - E\right]} , \quad (5.47)$$

where we relabeled l with n . Let us insert this quantity into Eq. (5.42) and writing $x = 0$, we have

$$\frac{1}{\lambda} = \sum_{n=0}^{\infty} \frac{[\phi_{2n}(0)]^2}{[(2n + \frac{1}{2}) \hbar\omega - E]} . \quad (5.48)$$

From Eq. (5.32), we have

$$\phi_{2n}(0) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{2^n \sqrt{(2n)!}} H_{2n}(0) . \quad (5.49)$$

By using $H_{2n}(0) = \frac{(-1)^n (2n)!}{n!}$ (Byron & Fuller, 1992), the above equation becomes

$$\phi_{2n}(0) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} (-1)^n \frac{\sqrt{(2n)!}}{2^n n!} . \quad (5.50)$$

Let us substitute this into Eq. (5.48) to get

$$\frac{1}{\lambda} = \sqrt{\frac{m\omega}{\pi\hbar}} \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} \frac{1}{[(2n + \frac{1}{2}) \hbar\omega - E]} . \quad (5.51)$$

By using this formula (proof is given in Appendix F.2),

$$\sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} \frac{1}{(2n + 1 - x)} = -\frac{\sqrt{\pi}}{(x-1)} \frac{\Gamma\left(\frac{3}{2} - \frac{x}{2}\right)}{\Gamma\left(1 - \frac{x}{2}\right)} , \quad (5.52)$$

Eq. (5.51) becomes

$$\frac{1}{\lambda} = -2\sqrt{\frac{m\omega}{\hbar}} \frac{1}{(2E - \hbar\omega)} \frac{\Gamma\left(\frac{5}{4} - \frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega}\right)} . \quad (5.53)$$

Also, using the property $\Gamma(x+1) = x\Gamma(x)$ (Lebedev, 1965), we finally obtain (5.38). \square

Since this is a transcendental equation, it is not so easy to solve exactly. We are going to analyze the solution case by case graphically and asymptotically.

Case A: For $\lambda > 0$ (attractive point interaction):

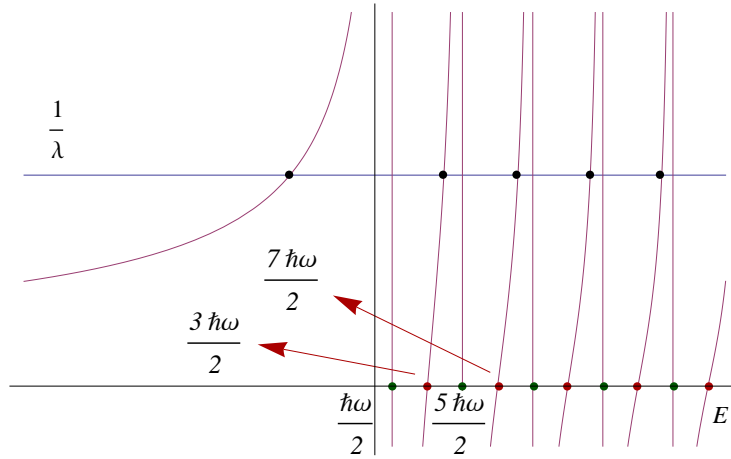


Figure 5.1. Attractive point interaction

Lemma 5.4 (Lebedev, 1965) *The Gamma function $\Gamma(z)$ has poles at negative integers.*

Due to Lemma 5.4, the right-hand side of Eq. (5.38) has poles at $\frac{1}{4} - \frac{E}{2\hbar\omega} = -n$, where $n = 0, 1, 2, \dots$, i.e., at $E = (2n + \frac{1}{2}) \hbar\omega$ and has zeros at $\frac{3}{4} - \frac{E}{2\hbar\omega} = -n$, where $n = 0, 1, 2, \dots$, i.e., at $E = (2n + \frac{3}{2}) \hbar\omega$ which correspond to the even and odd-parity solutions of the simple harmonic oscillator, respectively.

As can be seen from Figure 5.1, all the eigenvalues corresponding to the even states are lowered than the even-parity eigenvalues of the simple harmonic oscillator (even eigenvalues of simple harmonic oscillator are shifted backward). Also, all the even-parity eigenvalues are sandwiched between adjacent poles of the right-hand side of Eq. (5.38) except ground state energy.

- From Figure 5.1, as λ increases ($\frac{1}{\lambda}$ decreases), the root associated with the minimum eigenvalue (ground state) appears in the negative E axis so we have negative ground state energy. The critical value for λ in order to have a negative ground state energy can be found from the transcendental equation (5.38) for $E = 0$. This gives us

$$\lambda_{critical} = 2\hbar^{\frac{3}{2}} \sqrt{\frac{\omega}{m}} \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}. \quad (5.54)$$

If $\lambda > \lambda_{critical}$, then we have a negative ground state energy.

- As $\lambda \rightarrow \infty$, the roots of Eq. (5.38) approach to the eigenvalues of the odd-parity solutions of simple harmonic oscillator, so that the spectrum is going to become doubly degenerate.
- As $\lambda \rightarrow 0$, the roots of Eq. (5.38) approach to the eigenvalues of even-parity solutions of

simple harmonic oscillator. This means that the spectrum of simple harmonic oscillator supported by an attractive point interaction coincides with the spectrum of the simple harmonic oscillator Hamiltonian, which is physically expected because if we take the limit $\lambda \rightarrow 0$ in Eq. (5.39), we would have just simple harmonic oscillator Hamiltonian.

• Let us consider the situation as $\omega \rightarrow 0$. Therefore, we have a negative ground state energy, $E = -|E|$. Then, Eq. (5.38) becomes

$$\frac{1}{\lambda} = \frac{\sqrt{m}}{2\hbar^{\frac{3}{2}}} \lim_{\omega \rightarrow 0} \left[\frac{1}{\sqrt{\omega}} \frac{\Gamma\left(\frac{1}{4} + \frac{|E|}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4} + \frac{|E|}{2\hbar\omega}\right)} \right]. \quad (5.55)$$

Due to the asymptotic expansion of the ratios of Gamma functions (Lebedev, 1965),

$$\frac{\Gamma(\alpha + z)}{\Gamma(\beta + z)} = z^{\alpha-\beta} \left[1 + \frac{(\alpha - \beta)(\alpha + \beta - 1)}{2z} + \mathcal{O}(|z|^{-2}) \right], \quad (5.56)$$

where $|\arg(z)| \leq \pi - \delta$, we have

$$\frac{\Gamma\left(\frac{1}{4} + \frac{|E|}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4} + \frac{|E|}{2\hbar\omega}\right)} = \sqrt{\frac{2\hbar\omega}{|E|}}, \quad (5.57)$$

as $\omega \rightarrow 0$. Hence, Eq. (5.38) in the asymptotic limit $\omega \rightarrow 0$ gives (3.7) which is also an expected result. Because, if we consider the limit $\omega \rightarrow 0$ in Eq. (5.39), we would have not a simple harmonic oscillator, instead have just a point interaction and this is nothing but the ground state energy of point interaction.

Case B: For $\lambda < 0$ (repulsive point interaction):

It is clear from Figure 5.2 that the ground state energy $> \frac{\hbar\omega}{2}$. Similar to the case A, we have the following results:

- Even-parity eigenvalues of simple harmonic oscillator are shifted forward.
- There are no negative energy eigenvalues.
- As $\lambda \rightarrow 0$, energy eigenvalues approach to the even-parity eigenvalues of simple harmonic oscillator and spectrum coincides with the simple harmonic oscillator's spectrum.
- As $\lambda \rightarrow \infty$, energy eigenvalues approach to the odd-parity eigenvalues of simple harmonic oscillator. The spectrum becomes doubly degenerate.

- As $\omega \rightarrow 0$, there is no bound state energy which can be easily seen from the graph, as expected.

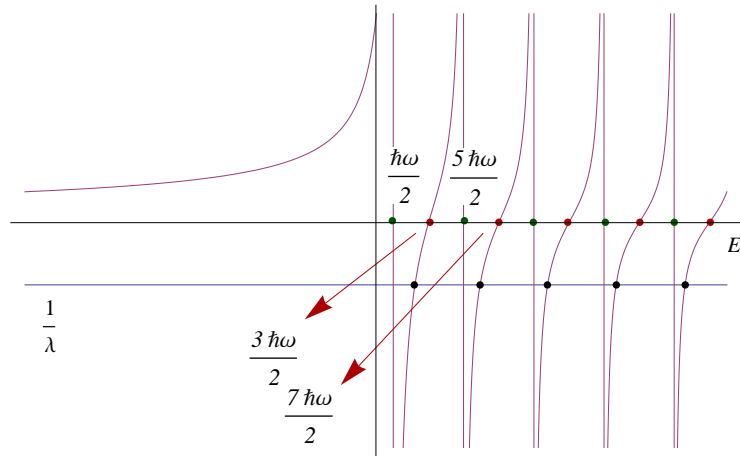


Figure 5.2. Repulsive point interaction

5.3.1. Resolvent and Heat Kernel

The point interaction term in one dimension can be written as

$$\delta(x - a)\psi(x) = \delta(x - a)\psi(a) , \quad (5.58)$$

from the property given in (2.27). If we take the point interaction centered at the origin, the above equation reads

$$\delta(x)\psi(x) = \langle x, 0 \rangle \langle 0, \psi \rangle , \quad (5.59)$$

where $|0\rangle\langle 0|$ is the Dirac delta representation as a projection operator point of view. As a consequence of this, the Hamiltonian of Eq. (5.39) can be written in terms of operators:

$$H_0 - \lambda|0\rangle\langle 0| = H , \quad (5.60)$$

where $H_0 = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$ and $|0\rangle = |x = 0\rangle$. By doing the same procedure as we did in the Section 4.2,

$$(H_0 - E)|\psi\rangle - \lambda|0\rangle\langle 0|\psi\rangle = |\rho\rangle . \quad (5.61)$$

By multiplying both sides with $(H_0 - E)^{-1}$ from left, we obtain

$$|\psi\rangle - \lambda(H_0 - E)^{-1}|0\rangle\psi(0) = (H_0 - E)^{-1}|\rho\rangle , \quad (5.62)$$

and also multiplying both sides with $\langle 0|$ from left yields

$$\psi(0) - \lambda\langle 0|(H_0 - E)^{-1}|0\rangle\psi(0) = \langle 0|(H_0 - E)^{-1}|\rho\rangle . \quad (5.63)$$

Hence,

$$\psi(0) = \frac{\langle 0|(H_0 - E)^{-1}|\rho\rangle}{1 - \lambda\langle 0|(H_0 - E)^{-1}|0\rangle} , \quad (5.64)$$

and substituting this into Eq. (5.62), we obtain

$$|\psi\rangle - (H_0 - E)^{-1}|0\rangle \frac{\langle 0|(H_0 - E)^{-1}|\rho\rangle}{\left[\frac{1}{\lambda} - \langle 0|(H_0 - E)^{-1}|0\rangle\right]} = (H_0 - E)^{-1}|\rho\rangle . \quad (5.65)$$

Let us define

$$\Phi(E) = \frac{1}{\lambda} - \langle 0|(H_0 - E)^{-1}|0\rangle , \quad (5.66)$$

which is the principal function, then Eq. (5.65) becomes

$$|\psi\rangle = [(H_0 - E)^{-1} + (H_0 - E)^{-1}|0\rangle\Phi^{-1}(E)\langle 0|(H_0 - E)^{-1}]|\rho\rangle . \quad (5.67)$$

Since the expression inside of the bracket is equal to

$$R(E) = (H - E)^{-1} = (H_0 - E)^{-1} + (H_0 - E)^{-1}|0\rangle\Phi^{-1}(E)\langle 0|(H_0 - E)^{-1}, \quad (5.68)$$

this equation can be written in that form:

$$R(E) = R_0(E) + R_0(E)|0\rangle\Phi^{-1}(E)\langle 0|R_0(E), \quad (5.69)$$

and then

$$R(x, y; E) = R_0(x, y; E) + R_0(x, 0; E)\Phi^{-1}(E)R_0(0, y; E), \quad (5.70)$$

where

$$\Phi^{-1}(E) = \frac{1}{\frac{1}{\lambda} - R_0(0, 0; E)}. \quad (5.71)$$

Lemma 5.5 *The integral representation of the free resolvent kernel in coordinate representation is given by*

$$R_0(x, y; E) = \int_0^\infty K_t(x, y) e^{\frac{Et}{\hbar}} \frac{dt}{\hbar}. \quad (5.72)$$

Proof

$$\begin{aligned} R_0(x, y; E) &= \langle x|R_0(E)|y\rangle = \langle x|(H_0 - E)^{-1}|y\rangle \\ &= \left\langle x \left| \int_0^\infty e^{-\frac{(H_0 - E)t}{\hbar}} \frac{dt}{\hbar} \right| y \right\rangle \\ &= \int_0^\infty K_t(x, y) e^{\frac{Et}{\hbar}} \frac{dt}{\hbar}, \end{aligned} \quad (5.73)$$

where $K_t(x, y) = \langle x|e^{-\frac{H_0 t}{\hbar}}|y\rangle$ and $(H_0 - E)^{-1} = \int_0^\infty e^{-\frac{(H_0 - E)t}{\hbar}} \frac{dt}{\hbar}$ for $\text{Re}(E) < 0$ (Fock, 1937) (Schwinger, 1951). \square

Due to Lemma 5.5, we have

$$R_0(0, 0; E) = \int_0^\infty K_t(0, 0) e^{\frac{Et}{\hbar}} \frac{dt}{\hbar} . \quad (5.74)$$

By substituting Eq. (5.36) into the above equation, we obtain

$$R_0(0, 0; E) = \sqrt{\frac{m\omega}{2\pi\hbar^3}} \int_0^\infty \frac{e^{\frac{Et}{\hbar}}}{\sqrt{\sinh(\omega t)}} dt = \sqrt{\frac{m\omega}{\pi\hbar^3}} \int_0^\infty e^{\frac{Et}{\hbar} - \frac{\omega t}{2}} (1 - e^{-2\omega t})^{-\frac{1}{2}} dt . \quad (5.75)$$

By changing the variable $e^{-2\omega t} = u$ and using the integral representation of the beta function (Lebedev, 1965):

$$B(x, y) = \int_0^1 u^{x-1} (1-u)^{y-1} du , \quad (5.76)$$

where $Re(x), Re(y) > 0$, we obtain

$$R_0(0, 0; E) = \frac{1}{2\hbar^{\frac{3}{2}}} \sqrt{\frac{m}{\omega\pi}} B\left(\frac{1}{4} - \frac{E}{2\omega\hbar}, \frac{1}{2}\right) = \frac{1}{2\hbar^{\frac{3}{2}}} \sqrt{\frac{m}{\omega}} \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega}\right)} , \quad (5.77)$$

where the conditions are justified by $Re(y) = \frac{1}{2} > 0$ and $Re(x) = \frac{1}{4} - \frac{E}{2\omega\hbar} > 0$. (This condition holds true because $E < \frac{\hbar\omega}{2}$ should be satisfied to stay in the resolvent set.) We also used the fact that Beta function satisfies (Lebedev, 1965)

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} , \quad (5.78)$$

for $x, y > 0$.

Theorem 5.3 *The odd-parity eigenvalues only comes from the poles of the resolvent for the simple Harmonic oscillator whereas the even-parity eigenvalues comes from the zeros of the principal function given in (5.66).*

Proof If H_0 was the free Hamiltonian, then the poles would come from zeros of the principal function, as shown before. However, in this case we have poles coming from the resolvent for the simple harmonic oscillator so that the pole structure of the full resolvent (5.70) is

much more complicated. Let us use the Riesz integral by using the contour Γ_k enclosing the odd-parity eigenvalue, say E_k :

$$\psi_k(x)\psi_k^*(y) = -\frac{1}{2\pi i} \oint_{\Gamma_k} [R_0(x, y; E) + R_0(x, 0; E)\Phi^{-1}(E)R_0(0, y; E)] dE, \quad (5.79)$$

where $\Phi^{-1}(E)$ is given in (5.71). By choosing $x = y = 0$, we have

$$|\psi_k(0)|^2 = -\frac{1}{2\pi i} \oint_{\Gamma_k} \frac{1}{\left[\frac{1}{R_0(0,0;E)} - \lambda\right]} dE. \quad (5.80)$$

Since $\psi_k(x)$ is the odd-parity eigenfunction, above equation must vanish. This means that $\frac{1}{R_0(0,0;E)} - \lambda$ can not have zeros or $\frac{1}{\lambda} - R_0(0, 0; E) = \Phi(E) \neq 0$. Therefore, the poles of $R(x, y; E)$ corresponding to the odd-parity eigenstates must come from the poles of R_0 , not from $\Phi^{-1}(E)$.

Let us multiply the formal resolvent given in (5.68) with $\langle \phi_{2k} |$ from left and with $|\phi_{2k}\rangle$ from right where ϕ_{2k} are even eigenfunctions of simple harmonic oscillator. Then, we have

$$\begin{aligned} \langle \phi_{2k} | (H - E)^{-1} | \phi_{2k} \rangle &= \langle \phi_{2k} | (H_0 - E)^{-1} | \phi_{2k} \rangle + \langle \phi_{2k} | (H_0 - E)^{-1} | 0 \rangle \frac{\langle 0 | (H_0 - E)^{-1} | \phi_{2k} \rangle}{\Phi(E)} \\ &= \int_{\mathbb{R}^2} \phi_{2k}^*(x) R_0(x, y; E) \phi_{2k}(y) dx dy \\ &+ \frac{\int_{\mathbb{R}} \phi_{2k}^*(x) R_0(x, 0; E) dx \int_{\mathbb{R}} R_0(0, y; E) \phi_{2k}(y) dy}{\frac{1}{\lambda} - R_0(0, 0; E)}, \end{aligned} \quad (5.81)$$

where we have used completeness relations.

Theorem 5.4 *Let $\phi_n(x)$ be the eigenfunctions of simple harmonic oscillator, then*

$$R_0(x, y; E) = \sum_n \frac{\phi_n(x)\phi_n^*(y)}{E_n - E}, \quad (5.82)$$

where $E_n = (n + \frac{1}{2}) \hbar\omega$.

Due to above theorem, Eq. (5.81) turns out to be

$$\begin{aligned}
\langle \phi_{2k} | (H - E)^{-1} | \phi_{2k} \rangle &= \int_{\mathbb{R}^2} \phi_{2k}^*(x) \sum_n \frac{\phi_n(x) \phi_n^*(y)}{E_n - E} \phi_{2k}(y) dx dy \\
&+ \frac{\int_{\mathbb{R}} \phi_{2k}^*(x) \sum_n \frac{\phi_n(x) \phi_n^*(0)}{E_n - E} dx \int_{\mathbb{R}} \sum_n \frac{\phi_n(0) \phi_n^*(y)}{E_n - E} \phi_{2k}(y) dy}{\frac{1}{\lambda} - \sum_r \frac{|\phi_{2r}(0)|^2}{E_{2r} - E}} \\
&= \frac{1}{E_{2k} - E} + \frac{\frac{|\phi_{2k}(0)|^2}{(E_{2k} - E)^2}}{\frac{1}{\lambda} - \sum_r \frac{|\phi_{2r}(0)|^2}{E_{2r} - E}}. \tag{5.83}
\end{aligned}$$

Here, we used orthonormality conditions: $\int_{\mathbb{R}} \phi_n(x) \phi_m^*(y) dx = \delta_{nm}$ and $\int_{\mathbb{R}} |\phi_{2k}(x)|^2 dx = 1$. By arranging the above equation, we obtain

$$\begin{aligned}
\langle \phi_{2k} | (H - E)^{-1} | \phi_{2k} \rangle &= \frac{\frac{1}{\lambda} - \sum_r \frac{|\phi_{2r}(0)|^2}{E_{2r} - E} + \frac{|\phi_{2k}(0)|^2}{(E_{2k} - E)}}{(E_{2k} - E) \left[\frac{1}{\lambda} - \sum_r \frac{|\phi_{2r}(0)|^2}{E_{2r} - E} \right]} \\
&= \frac{\frac{1}{\lambda} - \sum_{r \neq k} \frac{|\phi_{2r}(0)|^2}{E_{2r} - E}}{\frac{E_{2k} - E}{\lambda} - (E_{2k} - E) \sum_{r \neq k} \frac{|\phi_{2r}(0)|^2}{E_{2r} - E} - |\phi_{2k}(0)|^2} \\
&= \frac{1}{E_{2k} - E - \frac{|\phi_{2k}(0)|^2}{\chi}}, \tag{5.84}
\end{aligned}$$

where we have denoted $\chi = \frac{1}{\lambda} - \sum_{r \neq k} \frac{|\phi_{2r}(0)|^2}{E_{2r} - E}$. Note that $E = E_{2k}$ is not a pole anymore. Poles are come from

$$\frac{1}{\lambda} - \sum_{r \neq k} \frac{|\phi_{2r}(0)|^2}{E_{2r} - E} = \frac{|\phi_{2k}(0)|^2}{E_{2k} - E}, \tag{5.85}$$

or it can be written

$$\frac{1}{\lambda} = \sum_r \frac{|\phi_{2r}(0)|^2}{E_{2r} - E} = R_0(0, 0; E). \tag{5.86}$$

Hence, for the even-parity eigenvalues, they must come from the poles of $\Phi^{-1}(E)$ which gives Eq. (5.38). From this approach, one can also see that

$$\langle \phi_{2k+1} | (H - E)^{-1} | \phi_{2k+1} \rangle = \frac{1}{E_{2k+1} - E} + \frac{\frac{|\phi_{2k+1}(0)|^2}{(E_{2k+1} - E)^2}}{\frac{1}{\lambda} - \sum_r \frac{|\phi_r(0)|^2}{E_r - E}}, \tag{5.87}$$

where ϕ_{2k+1} are odd eigenfunctions of simple harmonic oscillator. Since $\phi_{2k+1}(0) = 0$, we have poles only come from $E = E_{2k+1}$ which is the same result that we found before. \square

5.4. Spectrum of Isotropic Simple Harmonic Oscillator Supported by A Point Interaction in Two Dimensions

Lemma 5.6 (Merzbacher, 1961) *The two-dimensional simple harmonic oscillator potential*

$$-\frac{\hbar^2}{2m}\Delta\phi_n(\mathbf{x}) + \frac{1}{2}m\omega^2\mathbf{x}^2\phi_n(\mathbf{x}) = E_n\phi_n(\mathbf{x}) . \quad (5.88)$$

has the eigenvalues

$$E_n = (n + 1)\hbar\omega , \quad (5.89)$$

where $n = n_1 + n_2$ and $n_1, n_2 = 0, 1, \dots$ and the eigenfunctions

$$\phi_n(\mathbf{x}) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{m\omega}{2\hbar}|\mathbf{x}|^2} \prod_{j=1}^2 \frac{1}{\sqrt{2^{n_j} n_j!}} H_{n_j} \left(\sqrt{\frac{m\omega}{\hbar}} x_j \right) , \quad (5.90)$$

where $\mathbf{x} = (x_1, x_2)$, and the degeneracy of the n -th energy is $n + 1$.

Lemma 5.7 *The heat kernel of the two-dimensional simple harmonic oscillator is given by*

$$K_t(\mathbf{x}, \mathbf{y}) = \left(\frac{m\omega}{\pi\hbar} \right) \frac{e^{-\frac{m\omega}{2\hbar} \coth(\omega t)(|\mathbf{x}|^2 + |\mathbf{y}|^2) + \frac{m\omega}{\hbar \sinh(\omega t)}(\mathbf{x} \cdot \mathbf{y})}}{2 \sinh(\omega t)} . \quad (5.91)$$

Proof From Eq. (5.27) and writing $\frac{t}{\hbar}$ instead of t because of dimensional consistency, we find

$$K_t(\mathbf{x}, \mathbf{y}) = \sum_{n_1, n_2=0}^{\infty} e^{-(n_1+n_2+1)\omega t} \phi_{n_1, n_2}(\mathbf{x}) \phi_{n_1, n_2}(\mathbf{y}) . \quad (5.92)$$

Then, from Eq. (5.90), we obtain

$$K_t(\mathbf{x}, \mathbf{y}) = \left(\frac{m\omega}{\pi\hbar}\right) \prod_{j=1}^2 \left[\sum_{n_j=0}^{\infty} e^{-\frac{m\omega}{2\hbar}(x_j^2+x_j'^2)} e^{\omega t(n_j+\frac{1}{2})} \right. \\ \left. \times \frac{H_{n_j}\left(\sqrt{\frac{m\omega}{\hbar}}x_j\right) H_{n_j}\left(\sqrt{\frac{m\omega}{\hbar}}x_j'\right)}{2^{n_j}n_j!} \right], \quad (5.93)$$

where $\mathbf{y} = (x_1', x_2')$. By the help of Lemma 5.3, we obtain the desired result (5.91). \square

Corollary 5.4 *In particular, by choosing $\mathbf{x}, \mathbf{y} = \mathbf{0}$ in Eq. (5.91), we obtain*

$$K_t(\mathbf{0}, \mathbf{0}) = \left(\frac{m\omega}{\pi\hbar}\right) \frac{1}{2 \sinh(\omega t)}, \quad (5.94)$$

which is going to be very useful in our calculations later on.

Theorem 5.5 *Let H_0 be the Hamiltonian of the two-dimensional simple harmonic oscillator and $H = H_0 - \lambda\delta^{(2)}(\mathbf{x})$. Then, the resolvent of the formal operator H after the renormalization is given by*

$$R(\mathbf{x}, \mathbf{y}; E) = R_0(\mathbf{x}, \mathbf{y}; E) + R_0(\mathbf{x}, \mathbf{0}; E)\Phi^{-1}(E)R_0(\mathbf{0}, \mathbf{y}; E), \quad (5.95)$$

where

$$\Phi(E) = \frac{m}{2\pi\hbar^2} \left[\Psi\left(\frac{1}{2} - \frac{E}{2\hbar\omega}\right) - \Psi\left(\frac{1}{2} + \frac{\mu^2}{2\hbar\omega}\right) \right], \quad (5.96)$$

and $\Psi(x)$ is the digamma function and $-\mu^2$ is the experimentally measured bound state energy for the system.

Proof This problem is still divergent because divergence appears due to the singular behavior of the potential at $x = 0$. If we follow the same steps formally as we did in one-dimensional case, we end up with Eq. (5.95) where

$$\Phi(E) = \frac{1}{\lambda} - R_0(\mathbf{0}, \mathbf{0}; E). \quad (5.97)$$

But, now the free resolvent $R_0(\mathbf{0}, \mathbf{0}; E)$:

$$R_0(\mathbf{0}, \mathbf{0}; E) = \int_0^\infty K_t(\mathbf{0}, \mathbf{0}) e^{\frac{Et}{\hbar}} \frac{dt}{\hbar} = \frac{m\omega}{2\pi\hbar} \int_0^\infty \frac{e^{\frac{Et}{\hbar}}}{\sinh(\omega t)} \frac{dt}{\hbar}, \quad (5.98)$$

is divergent due to the short “time” behavior of the integrand, i.e., as $t \rightarrow 0^+$ the denominator behaves like t so that the integral blows up near $t = 0$. First, we regularize the integral by introducing a new cut-off parameter ϵ for “time”, namely

$$R_0^\epsilon(\mathbf{0}, \mathbf{0}; E) = \frac{m\omega}{2\pi\hbar} \int_\epsilon^\infty \frac{e^{\frac{Et}{\hbar}}}{\sinh(\omega t)} \frac{dt}{\hbar}, \quad (5.99)$$

then choosing

$$\frac{1}{\lambda(\epsilon)} = \frac{m\omega}{2\pi\hbar} \int_\epsilon^\infty \frac{e^{-\frac{\mu^2 t}{\hbar}}}{\sinh(\omega t)} \frac{dt}{\hbar}, \quad (5.100)$$

where $-\mu^2$ is the experimentally measured bound state energy, Eq. (5.97) becomes

$$\begin{aligned} \Phi(E) &= \frac{m\omega}{\pi\hbar^2} \int_0^\infty e^{-\omega t} \sum_{n=0}^\infty (e^{-2\omega t})^n \left[e^{-\frac{\mu^2 t}{\hbar}} - e^{\frac{Et}{\hbar}} \right] dt \\ &= \frac{m}{2\pi\hbar^2} \sum_{n=0}^\infty \left[\frac{1}{(n + \frac{1}{2}) + \frac{\mu^2}{2\hbar\omega}} - \frac{1}{(n + \frac{1}{2}) - \frac{E}{2\omega\hbar}} \right] \\ &= \frac{m}{2\pi\hbar^2} \left[\Psi\left(\frac{1}{2} - \frac{E}{2\hbar\omega}\right) - \Psi\left(\frac{1}{2} + \frac{\mu^2}{2\hbar\omega}\right) \right], \end{aligned} \quad (5.101)$$

where we have used the infinite series representation of the difference of the digamma functions given by (Gradshteyn & Ryzhik, 2000)

$$\Psi(x) - \Psi(y) = \sum_{k=0}^\infty \left[\frac{1}{y+k} - \frac{1}{x+k} \right]. \quad (5.102)$$

□

Due to the same reason with the discussion in one dimension, states belonging to odd-parity are not affected by the perturbation of Dirac delta potential. For the even states, the situation is more complicated (see the discussion in the three dimensions (Fassari & Inglese,

1996)). For this reason, let us discuss the particular case, where $n = n_1 + n_2 = 2$ (first excited even state) whose energy $E_2 = (2 + 1)\hbar\omega = 3\hbar\omega$. The degeneracy of this state is $2 + 1 = 3$. Hence the state $(1, 1)$ is not affected due to the same reason. However, the energies corresponding to the states $(2, 0)$ and $(0, 2)$ will be lowered according to zeros of the renormalized principal matrix (5.101).

CHAPTER 6

CONCLUSION

In this thesis, we have reviewed the basic results of the spectrum of point interactions in one dimension and two dimensions. It has been shown that two-dimensional problem requires a regularization and renormalization procedure. The bound state spectrum for finitely many point interactions is investigated in detail. In particular, we discussed the case when the centers of point interactions are located at the vertices of a regular polygon. The positivity and non-degeneracy of the ground state has been proved. Finally, the bound state spectrum of the point interaction with harmonic oscillator has been examined using heat kernel in one dimension and two dimensions.

REFERENCES

- Griffiths D. J. (1999) *Introduction to Electrodynamics* Prentice-Hall, INC.
- Balakrishnan V. (2003) All about the Dirac delta function *Resonance*
- Dirac P. A. M. (1958) *The Principles of Quantum Mechanics* Oxford University Press
- Gelfand I. M. & Shilov G. E. (1964) *Generalized Functions* Academic Press
- Gustafson S. J. & Sigal I. M. (2011) *Mathematical Concepts of Quantum Mechanics* Springer
- Erman F. (2010) Heat Kernel Methods In Many Body Problems, Ph.D. Thesis, Boğaziçi University.
- Rajeev, S. G. (1999) Bound States in Models of Asymptotic Freedom *The Royal Swedish Academy of Sciences, arXiv:hep-th/9902025 v1*.
- Griffiths D. J. (1995) *Introduction to Quantum Mechanics* Prentice-Hall, INC.
- Mead R. L. & Godines J. (1991) An analytical example of renormalization in two-dimensional quantum mechanics *Am. J. Phys.* 59 (10)39406-5046.
- Gradshteyn I. S. & Ryzhik I. M. (2000) *Table of Integrals, Series, and Products* Academic Press.
- Lebedev N. N. (1965) *Special Functions and Their Applications* Prentice-Hall, INC.
- Appel W. (2007) *Mathematics for Physics and Physicists* Princeton University Press
- Zeidler E. (2006) *Quantum Field Theory I: Basics in Mathematics and Physics* Springer.
- Hislop P. D. & Sigal I. M. (1996) *Introduction to Spectral Theory with Applications to Schrödinger Operators* Springer.
- Greene R. E. & Krantz S. G. (2006) *Function Theory of One Complex Variable* American Mathematical Society.
- Halmos P. R. (1974) *Finite-Dimensional Vector Spaces* Springer.
- Vatsya S. R. (2004) Comment on “Breakdown of the Hellmann-Feynman Theorem: Degeneracy is the Key” *Physical Review B* 69, 037102.
- Ninio F. (1976) A Simple Proof of the Perron-Frobenius Theorem for Positive Symmetric

Matrices *J. Phys. A: Math. Gen.*, Vol. 9, No. 8.

Calin O. & Chang D-C. & Furutani K. & Iwasaki C. (2011) *Heat Kernels for Elliptic and Sub-elliptic Operators Methods and Techniques* Birkhäuser.

Byron F. W., JR. & Fuller R. W. (1992) *Mathematics of Classical and Quantum Physics* Dover Publications, Inc., New York.

Debnath L. & Mikusiński P. (2005) *Hilbert Spaces with Applications* Elsevier

Kanwal R. P. (2004) *Generalized Functions Theory and Applications* Springer Science+Business Media, LLC

Feynman, R. P. (1939) "Forces in Molecules" *Physical Review*, Vol. 56, No. 4, pp. 340-343.

Hellmann H. (1937) *Einführung in die Quantenchemie* Franz Deuticke

Corless R. M. & Gonnet G. H. & Hare D. E. G. & Jeffrey D. J. & Knuth D. E. (1996) "On the Lambert W Function", *Advances in Computational Mathematics* Vol. 5, No. 1, pp. 329-359.

Meyer C. D. (2001) *Matrix Analysis and Applied Linear Algebra* Society for Industrial and Applied Mathematics

Schechter M. (1981) *Operator Methods in Quantum Mechanics* Elsevier North Holland, Inc.

Zee A. (2010) *Quantum Field Theory in a Nutshell* Princeton University Press

Kato T. (1995) *Perturbation Theory for Linear Operators* Springer

Arfken G. B. & Weber H. J. (2005) *Mathematical Methods For Physicists* Elsevier Academic Press

Reed M. & Simon B. (1980) *Methods of Modern Mathematical Physics Vol. 1: Functional Analysis* Academic Press, Inc.

Reed M. & Simon B. (1975) *Methods of Modern Mathematical Physics Vol. 2: Fourier Analysis, Self-Adjointness* Academic Press, Inc.

Reed M. & Simon B. (1978) *Methods of Modern Mathematical Physics Vol. 4: Analysis of Operators* Academic Press, Inc.

Abramowitz M. & Sitegun I. A. (1972) *Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables* Dover Publications

Esteve J. G. & Falceto F. & Canal C. G. (2009) Generalization of the Hellmann-Feynman

Theorem ArXiv:0912.4153 v1 [quant-ph].

- Cohen Tannoudji C. & Diu B. & Laloe F. (1996) *Quantum Mechanics Volume 1* Wiley
- Pazy A. (1983) *Semigroups of Linear Operator and Applications to Partial Differential Equations* Springer-Verlag New York, Inc.
- Merzbacher E. (1961) *Quantum Mechanics* John Wiley & Sons, Inc.
- Jackiw R. (1995) *Diverse Topics in Theoretical and Mathematical Physics* World Scientific
- Eisberg R. & Resnick R. (1985) *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles* John Wiley & Sons, Inc.
- Albeverio S. & Gesztesy F. & Høegh-Krohn R. & Holden H. & Exner P. (1988) *Solvable Models in Quantum Mechanics* American Mathematical Society
- Valluri S. R. & Jeffrey D. J. & Corless R. M. (1988) Some Applications of the Lambert W Function to Physics
- Mitra I. & DasGupta A. & Dutta-Roy B. (1998) Regularization and renormalization in scattering from Dirac delta potentials *Am. J. Phys.*, Vol. 66, No. (12).
- Fock V. A. (1937) "Proper Time in Classical and Quantum Mechanics" *Izvestiya Akademii Nauk Seriya Fizicheskaya, USSR*, Vol. 4, No. 5, pp. 551.
- Schwinger J. (1951) "On Gauge Invariance and Vacuum Polarization" *Physical Review*, Vol. 82, No. 5, pp. 664-679.
- Olver F. W. (1974) *Asymptotics and Special Functions* Academic Press
- Roger A. H. & Charles R. J. (1992) *Matrix Analysis* Cambridge University Press
- Aldrovandi R. (2001) *Special Matrices of Mathematical Physics* World Scientific
- Kronig R. L. & Penney W. G. (1931) "Quantum Mechanics of Electrons in Crystal Lattices" *Proceedings of Royal Society, London A*, Vol. 130, No.814, pp. 499-513, 1931.
- Kittel C. (2005) *Introduction to Solid State Physics* John Wiley
- Maleev S. V. (1966) *Fiz. Tverd. Tela (Leningrad)* 7, 2990 (1965) (*Sov. Phys. - Solid State* 7, 2423 1966).
- Berezin A. A. (1986) Two and three dimensional Kronig-Penney model with δ function potential wells of zero binding energy *Phys. Rev. B*, 33 4 (1986).
- Fermi E. (1962) Sul moto dei neutroni nelle sostanze idrogenate *E. Fermi Collected Papers*,

Vol I, Italy, pp 980-1016.

Bethe H. & Peierls R. (1935) “Quantum Theory of the Dipion” *Proceedings of Royal Society, London A, Vol. 148, No. 1, pp. 146-156, 1935.*

Thomas L. H. (1935) “The Interaction Between a Neutron and a Proton and the Structure of H^3 ” *Physical Review, Vol. 47, No. 12, pp. 903-909, 1935.*

Thorn C. (1979) “Quark Confinement in the Infinite-Momentum Frame” *Physical Review D, Vol. 19, No. 2, pp. 639-651, 1979*

Demkov Yu. N. & Ostrovskii V. N. (1988) *Zero-Range Potentials and their applications in atomic physics* Plenum Press

Gosdzinsky P. & Tarrach R. (1991) “Learning Quantum Field Theory from Elementary Quantum Mechanics” *American Journal of Physics, Vol. 59, No. 1, pp. 70-74, 1991.*

Manuel C. & Tarrach R. (1994) “Perturbative Renormalization in Quantum Mechanics” *Physics Letters B, Vol. 328, No. 1-2, pp. 113-118, 1994.*

Perez J. F. & Coutinho F. A. B. (1991) “Schrödinger Equation in Two Dimensions for a Zero Range Potential and a Uniform Magnetic Field: Exactly Solvable Model” *American Journal of Physics, Vol. 59, No. 1, pp. 52-54, 1991.*

Huang K. (1982) *Quarks, Leptons and Gauge Fields* World Scientific

Jackiw R. (1991) *Delta Function Potentials in Two- and Three-Dimensional Quantum Mechanics* World Scientific

Philips D. R. & Beane S. R. & T. D. Cohen (1998) “Nonperturbative Regularization and Renormalization: Simple Examples from Nonrelativistic Quantum Mechanics” *Annals of Physics, Vol. 263, No. 2, pp. 255-275, 1998.*

Henderson R. J. & Rajeev S. G. (1998) “Renormalized Contact Potential in Two Dimensions” *Journal of Mathematical Physics, Vol. 39, No. 2, pp. 749-760, 1998.*

Nyeo S. L. (2000) “Regularization Methods for Delta-Function Potential in Two-dimensional Quantum Mechanics” *American Journal of Physics, Vol. 68, No. 6, pp. 571-576, 2000.*

Adhikari S. K. & Frederico T. (1995) “Renormalization Group in Potential Scattering” *Physical Review Letters, Vol. 74, No. 23, pp. 4572-4575, 1995.*

Kraus P. & Griffiths D. J. (1992) “Renormalization of a model quantum field theory” *American journal of physics, 60, 11 (1992).*

Camblong H. E. & Ordóñez C. R. (2002) “Renormalized Path Integral for the Two-

- Dimensional δ Function Interaction” *Physical Review A*, Vol. 65, No. 5, pp. 052123-1-052123-11, 2002.
- Holstein B. R. (1993) “Anomalies for Pedestrians” *American Journal of Physics*, Vol. 61, No. 2, pp. 142-147, 1993.
- Coleman S. & Weinberg E. (1973) “Radiative Corrections as the Origin of Spontaneous Symmetry Breaking” *Physical Review D*, Vol. 7, No. 6, pp. 1888-1910, 1973.
- Camblong H. E. & L. N. Epele & H. Fanchiotti & C. A. G. Canal (2001) “Dimensional Transmutation and Dimensional Regularization in Quantum Mechanics: I. General Theory” *Annals of Physics*, Vol. 287, No. 1, pp. 14-56, 2001.
- Camblong H. E. & L. N. Epele & H. Fanchiotti & C. A. G. Canal (2001) “Dimensional Transmutation and Dimensional Regularization in Quantum Mechanics: II. Rotational Invariance” *Annals of Physics*, Vol. 287, No. 1, pp. 57-100, 2001.
- Berezin F. A. & L. D. Faddeev (1961) “A Remark on Schrödinger’s Equation with a Singular Potential” *Soviet mathematics Doklady*, Vol. 2, pp. 372-375, 1961.
- Albeverio S. & P. Kurasov (2000) *Singular Perturbations of Differential Operators Solvable Schrödinger-type Operators* Cambridge University Press
- Gerbert P. & R. Jackiw (1989) “Classical and Quantum Scattering on a Spinning Cone” *Communications in Mathematical Physics*, Vol. 124, No. 2, pp. 229-260, 1989.
- Gerbert P. (1989) “Fermions in an Aharonov-Bohm Field and Cosmic Strings” *Physical Review D*, Vol. 40, No. 4, pp. 1346-1349, 1989.
- Dogan C. & Erman F. & Turgut O. T. (2012) Existence of Hamiltonians for some singular interactions on manifolds *Journal of Mathematical Physics*, 53, 043511.
- Schwartz L. (1966) *Mathematics for the Physical Sciences* Hermann
- Bohm A. (2001) *Quantum Mechanics: Foundations and Applications* Springer
- Fassari S. & Inglese G. (1996) Spectroscopy of a three dimensional isotropic harmonic oscillator with a δ -type perturbation *Helvetica Physica Acta*, Vol. 69, 1996.
- Ponomarenko S. A. (2004) Quantum harmonic oscillator revisited: A fourier space approach *American Journal of Physics*, Vol. 72, Issue 9, 2004.
- Uncu H. (2007) Solutions of the Schrödinger equation for Dirac delta decorated potentials, Ph.D. Thesis, Boğaziçi University.
- Cacciapuoti C. (2005) Point interactions in quantum mechanics and acoustics, Ph.D. Thesis, Università Degli Studi Di Napoli Federico II.

Altunkaynak I. B. (2002) Spectral and scattering properties of point interactions, M.Sc. Thesis, Boğaziçi University.

APPENDIX A

POINT INTERACTION IN THE COORDINATE REPRESENTATION IN ONE DIMENSION

We are going to consider three regions separately to solve Schrödinger equation given in (3.6) for bound state energies and bound state wave function (Griffiths, 1995). In the region $x < 0$, $-\lambda\delta(x) = V(x) = 0$. Hence,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x). \quad (\text{A.1})$$

Therefore, the general solution to this equation is

$$\psi(x) = Ae^{-kx} + Be^{kx}, \quad (\text{A.2})$$

where $k = \frac{\sqrt{-2mE}}{\hbar}$ and A, B are constants. Since E is real and negative, k is real and positive. Since we stay in the region $x < 0$, the first term blows up as $x \rightarrow \infty$ and we must take $A = 0$. Hence, the solution is $\psi(x) = Be^{kx}$ for $x < 0$. Similarly, it can be easily found that in the region $x > 0$, we have a solution $\psi(x) = Ce^{-kx}$ where C is a constant. It remains to examine the third region: $x = 0$. Since the wave function is always continuous, the boundary conditions yields us

$$\psi(x) = \begin{cases} Be^{kx} & \text{if } x \leq 0, \\ Ce^{-kx} & \text{if } x \geq 0. \end{cases} \quad (\text{A.3})$$

Because the derivative of the wave function is not continuous, we are going to search the solution in a different way. The idea is to integrate the Schrödinger equation given in (3.6) from $-\epsilon$ to $+\epsilon$, then

$$-\frac{\hbar^2}{2m} \left(\frac{d\psi(x)}{dx} \right) \Big|_{-\epsilon}^{+\epsilon} - \lambda \int_{-\epsilon}^{+\epsilon} \delta(x)\psi(x) dx = E \int_{-\epsilon}^{+\epsilon} \psi(x) dx, \quad (\text{A.4})$$

where we integrate both sides formally since $\psi(x)$ does not have to belong to the test space or Schwartz space. Now, using the property of the Dirac delta function given in (2.15), we obtain

$$-\frac{\hbar^2}{2m} \left(\frac{d\psi(x)}{dx} \right) \Big|_{-\epsilon}^{+\epsilon} - \lambda\psi(0) = E \int_{-\epsilon}^{+\epsilon} \psi(x) dx . \quad (\text{A.5})$$

If we take the limit as $\epsilon \rightarrow 0$, we obtain

$$k = \frac{m\lambda}{\hbar^2} . \quad (\text{A.6})$$

But, we had $E = -\frac{\hbar^2 k^2}{2m}$ at the beginning. Then, we obtain the same result which was given in (3.7) and from the normalization condition of the wave function, we have (3.8).

APPENDIX B

DIFFERENT REGULARIZATION SCHEMES

B.1. Dimensional Regularization

The integral given in Eq. (3.143) which is divergent can also be made sensible from another approach called the dimensional regularization (Mitra & DasGupta & Dutta-Roy, 1998). Let us consider that we have

$$\int_{\mathbb{R}^D} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{d^D p}{(2\pi\hbar)^D}. \quad (\text{B.1})$$

We give a formula now:

$$\int_{\mathbb{R}^D} \frac{1}{k^2 + a^2} \frac{d^D k}{(2\pi)^D} = \frac{\Gamma\left(1 - \frac{D}{2}\right)}{(4\pi)^{\frac{D}{2}}} \frac{1}{(a^2)^{1 - \frac{D}{2}}}. \quad (\text{B.2})$$

Therefore, our integral becomes

$$\int_{\mathbb{R}^D} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{d^D p}{(2\pi\hbar)^D} = \frac{\Gamma\left(1 - \frac{D}{2}\right)}{(4\pi\hbar^2)^{\frac{D}{2}}} \frac{2m}{(2m\nu^2)^{1 - \frac{D}{2}}}. \quad (\text{B.3})$$

Let us write $D = 2 - \epsilon$, where $\epsilon > 0$, into the above equation, then

$$\int_{\mathbb{R}^{2-\epsilon}} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{d^{2-\epsilon} p}{(2\pi\hbar)^{2-\epsilon}} = \frac{\Gamma\left(\frac{\epsilon}{2}\right)}{(4\pi\hbar^2)^{1 - \frac{\epsilon}{2}}} \frac{2m}{(2m\nu^2)^{\frac{\epsilon}{2}}}. \quad (\text{B.4})$$

We use this formula now:

$$\Gamma(-n + \epsilon) = \frac{(-1)^n}{n!} \left[\frac{1}{\epsilon} + \Psi(n + 1) + \mathcal{O}(\epsilon) \right], \quad (\text{B.5})$$

and also the Taylor expansion of A^ϵ (treating ϵ is a variable)

$$A^\epsilon = 1 + \epsilon \ln A + \mathcal{O}(\epsilon^2) . \quad (\text{B.6})$$

Therefore, Eq. (B.4) becomes

$$\int_{\mathbb{R}^{2-\epsilon}} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{d^{2-\epsilon}p}{(2\pi\hbar)^{2-\epsilon}} = \frac{m}{2\pi\hbar^2} \left[\frac{2}{\epsilon} + \Psi(1) + \ln \left(\frac{2\pi\hbar^2}{m\nu^2} \right) + \mathcal{O}(\epsilon) \right] . \quad (\text{B.7})$$

Also, we write

$$\frac{1}{\lambda_i} = \int_{\mathbb{R}^D} \frac{\mu^{2-D}}{\frac{p^2}{2m} + \mu_i^2} \frac{d^D p}{(2\pi\hbar)^D} , \quad (\text{B.8})$$

where μ^{2-D} was chosen because of dimensional reasons. By using the same formulae for $D = 2 - \epsilon$, we obtain

$$\frac{1}{\lambda_i(\epsilon)} = \frac{m}{2\pi\hbar^2} \left[\frac{2}{\epsilon} + \Psi(1) + \ln \left(\frac{2\pi\hbar^2}{m\mu_i^2} \right) + 2 \ln \mu + \mathcal{O}(\epsilon) \right] . \quad (\text{B.9})$$

As $\epsilon \rightarrow 0$, it is concluded that

$$\Phi_{ii}(\nu) = \frac{1}{\lambda_i} - \int_{\mathbb{R}^2} \frac{1}{\frac{p^2}{2m} + \nu^2} \frac{d^2 p}{(2\pi\hbar)^2} = \frac{m}{\pi\hbar^2} \ln \left(\frac{\mu\nu}{\mu_i} \right) , \quad (\text{B.10})$$

which is consistent with the result obtained from the cut-off regularization by redefining $\mu_i = \mu\mu_i$.

B.2. Pauli-Villars Regularization

We can replace (Mitra & DasGupta & Dutta-Roy, 1998)

$$\frac{1}{\frac{p^2}{2m} + \nu^2} \longrightarrow \frac{1}{\frac{p^2}{2m} + \nu^2} - \frac{1}{\frac{p^2}{2m} + \xi^2} , \quad (\text{B.11})$$

as $\xi \rightarrow \infty$. Then, our integral turns out to be

$$\int_{\mathbb{R}^2} \left(\frac{1}{\frac{p^2}{2m} + \nu^2} - \frac{1}{\frac{p^2}{2m} + \xi^2} \right) \frac{d^2p}{(2\pi\hbar)^2} = \frac{m}{\pi\hbar^2} \ln \left(\frac{\xi}{\nu} \right), \quad (\text{B.12})$$

where we have used the polar coordinates. Also, we can write

$$\frac{1}{\lambda_i(\xi)} = \int_{\mathbb{R}^2} \left(\frac{1}{\frac{p^2}{2m} + \mu_i^2} - \frac{1}{\frac{p^2}{2m} + \xi^2} \right) \frac{d^2p}{(2\pi\hbar)^2} = \frac{m}{\pi\hbar^2} \ln \left(\frac{\xi}{\mu_i} \right), \quad (\text{B.13})$$

then, as $\xi \rightarrow \infty$, we find

$$\frac{1}{\lambda_i} - \int_{\mathbb{R}^2} \frac{1}{\frac{p^2}{2m} + \nu^2} [d^2p] = \frac{m}{\pi\hbar^2} \ln \left(\frac{\nu}{\mu_i} \right), \quad (\text{B.14})$$

which is consistent with the result obtained from the cut-off regularization and also from the dimensional regularization.

APPENDIX C

PROOFS OF IMPORTANT THEOREMS

C.1. Proof of Riesz Integral Representation Theorem

Proof For the first case, let Γ_{z_0} and $\bar{\Gamma}_{z_0}$ be two admissible contours for defining \mathbb{P}_{z_0} . Suppose that Γ_{z_0} contains the region $\bar{\Gamma}_{z_0}$. Hence,

$$\mathbb{P}_{z_0}^2 = -\frac{1}{4\pi^2} \oint_{\Gamma_{z_0}} \left[\oint_{\bar{\Gamma}_{z_0}} R_H(E_1) R_H(E_2) dE_2 \right] dE_1 . \quad (\text{C.1})$$

We use the first resolvent identity which was given in Eq. (4.1). Then,

$$\begin{aligned} \mathbb{P}_{z_0}^2 &= -\frac{1}{4\pi^2} \left[\oint_{\Gamma_{z_0}} R(E_1) \left(\oint_{\bar{\Gamma}_{z_0}} \frac{1}{E_1 - E_2} dE_2 \right) dE_1 \right. \\ &\quad \left. - \oint_{\Gamma_{z_0}} \frac{1}{E_1 - E_2} dE_1 \oint_{\bar{\Gamma}_{z_0}} R(E_2) dE_2 \right] . \end{aligned} \quad (\text{C.2})$$

Without loss of the generality, we can choose $|E_1| > |E_2|$ that means $|E_1 - z_0| > |E_2 - z_0|$. Then, $\oint_{\bar{\Gamma}_{z_0}} \frac{1}{E_1 - E_2} dE_2 = 0$. Because, E_1 lies outside of the region $\bar{\Gamma}_{z_0}$. But, since E_2 lies inside of the region Γ_{z_0} , from the residue theorem, $\oint_{\Gamma_{z_0}} \frac{1}{E_1 - E_2} dE_1 = 2\pi i$. Therefore, we obtain

$$\mathbb{P}_{z_0}^2 = -\frac{1}{2\pi i} \oint_{\bar{\Gamma}_{z_0}} R(E) dE . \quad (\text{C.3})$$

One can see that \mathbb{P}_{z_0} is independent of the contour provided that the contour is admissible for z_0 and H . Hence,

$$\mathbb{P}_{z_0}^2 = -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} R(E) dE = \mathbb{P}_{z_0} . \quad (\text{C.4})$$

For the second case, we need to show that if $f \in Ker(H - z_0)$ then $f \in Ran(\mathbb{P}_{z_0})$. Let us assume that $f \in Ker(H - z_0)$. Then, for $E \neq z_0$,

$$(H - E)f = (z_0 - E)f \Rightarrow (z_0 - E)^{-1}f = (H - E)^{-1}f . \quad (C.5)$$

So,

$$\mathbb{P}_{z_0}f = -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} R(E)f dE = -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} \frac{f(E)}{z_0 - E} dE , \quad (C.6)$$

and from the residue theorem,

$$\mathbb{P}_{z_0}f(E) = f(z_0) , \quad (C.7)$$

which means that $f \in Ran(\mathbb{P}_{z_0})$.

For the third case, let X be a Hilbert space and $H = H^\dagger$. Is \mathbb{P}_{z_0} self-adjoint? Let us write $z = re^{i\theta} + z_0$ in Eq. (4.4). Then,

$$\mathbb{P}_{z_0} = -\frac{r}{2\pi} \int_{-\pi}^{\pi} e^{i\theta} R(re^{i\theta} + z_0) d\theta . \quad (C.8)$$

Adjoint of this is

$$\mathbb{P}_{z_0}^\dagger = -\frac{r}{2\pi} \int_{-\pi}^{\pi} e^{-i\theta} R^\dagger(re^{i\theta} + z_0) d\theta . \quad (C.9)$$

We can show that $R^\dagger(E) = R(E^*)$. In order to do this,

$$\langle (H - E)f_1, f_2 \rangle = \langle f_1, (H - E^*)f_2 \rangle , \quad (C.10)$$

because of $H = H^\dagger$. Define $g_1 = (H - E)f_1$ and $g_2 = (H - E^*)f_2$. Therefore,

$$\langle g_1, (H - E^*)^{-1}g_2 \rangle = \langle (H - E)^{-1}g_1, g_2 \rangle . \quad (C.11)$$

That means

$$[(H - E)^{-1}]^\dagger = (H - E^*)^{-1} \Rightarrow R^\dagger(E) = R(E^*) . \quad (\text{C.12})$$

By substituting this into Eq. (C.9) and using the $z_0 = z_0^*$ because of $H = H^\dagger$, we find

$$\mathbb{P}_{z_0}^\dagger = -\frac{r}{2\pi} \int_{-\pi}^{\pi} e^{-i\theta} R(re^{-i\theta} + z_0) d\theta . \quad (\text{C.13})$$

If we write $-\theta$ instead of θ , we obtain

$$\mathbb{P}_{z_0}^\dagger = -\frac{r}{2\pi} \int_{-\pi}^{\pi} e^{i\theta} R(re^{i\theta} + z_0) d\theta = \mathbb{P}_{z_0} . \quad (\text{C.14})$$

Our next aim is to show that $\text{Ran}(\mathbb{P}_{z_0}) = \text{Ker}(H - z_0)$. We have already proved $\text{Ran}(\mathbb{P}_{z_0}) \supset \text{Ker}(H - z_0)$. If we can show that $\text{Ran}(\mathbb{P}_{z_0}) \subset \text{Ker}(H - z_0)$, then proof is going to be completed. So,

$$\begin{aligned} (H - z_0)\mathbb{P}_{z_0} &= -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} (H - z_0)(H - E)^{-1} dE \\ &= -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} [1 + (E - z_0)(H - E)^{-1}] dE , \end{aligned} \quad (\text{C.15})$$

because of $(H - z_0)(H - E)^{-1} = [(H - E) + (E - z_0)][(H - E)^{-1}] = 1 + (E - z_0)(H - E)^{-1}$. Therefore,

$$(H - z_0)\mathbb{P}_{z_0} = -\frac{1}{2\pi i} \left[\oint_{\Gamma_{z_0}} dE + \oint_{\Gamma_{z_0}} (E - z_0)(H - E)^{-1} dE \right] . \quad (\text{C.16})$$

Since the first integral is analytic in that domain, it is zero. Then, we have

$$(H - z_0)\mathbb{P}_{z_0} = -\frac{1}{2\pi i} \oint_{\Gamma_{z_0}} (E - z_0)(H - E)^{-1} dE . \quad (\text{C.17})$$

We are going to use the Riemann removable singularities theorem (Greene & Krantz, 2006).

Theorem C.1 Let $f : \mathcal{D}(P, r) \setminus \{P\} \rightarrow \mathbb{C}$ be holomorphic and bounded. Then,

1. $\lim_{z \rightarrow P} f(z)$ exists.
2. The function $\tilde{f} : \mathcal{D}(P, r) \rightarrow \mathbb{C}$ defined by

$$\tilde{f}(z) = \begin{cases} f(z) & \text{if } z \neq P, \\ \lim_{\xi \rightarrow P} f(\xi) & \text{if } z = P, \end{cases} \quad (\text{C.18})$$

is holomorphic on $\mathcal{D}(P, r)$.

In our case; for $U_{z_0} \setminus \{z_0\}$, the operator $(E - z_0)(H - E)^{-1}$ is holomorphic operator-valued function where U_{z_0} is the interior of the contour Γ_{z_0} and also uniformly bounded. Because,

$$\|(E - z_0)(H - E)^{-1}\| = |(E - z_0)| \|R(E)\| < \frac{|(E - z_0)|}{d(E, \xi)}, \quad (\text{C.19})$$

where $\xi \in \sigma(H)$. Also, since it is allowed to choose Γ_{z_0} arbitrarily, we can take $|(E - z_0)| < d(z, \xi)$. Hence,

$$\|(E - z_0)(H - E)^{-1}\| < 1. \quad (\text{C.20})$$

Then, from the theorem we have $\tilde{f} : U_{z_0} \rightarrow \mathbb{C}$ defined by

$$\tilde{f}(E) = \begin{cases} (E - z_0)(H - E)^{-1} & \text{if } E \neq z_0, \\ \lim_{\xi \rightarrow z_0} (\xi - z_0)(H - \xi)^{-1} & \text{if } E = z_0, \end{cases} \quad (\text{C.21})$$

is holomorphic on U_{z_0} . By Cauchy's theorem, $\oint_{U_{z_0}} \tilde{f}(E) dE = 0$. Therefore,

$$(H - z_0)\mathbb{P}_{z_0} = 0. \quad (\text{C.22})$$

If $y = \mathbb{P}_{z_0}x$, then $y \in \text{Ran}(\mathbb{P}_{z_0})$. However, from the above equation, we have $y \in \text{Ker}(H - z_0)$. So, it is concluded that $\text{Ran}(\mathbb{P}_{z_0}) \subset \text{Ker}(H - z_0)$. \square

C.2. Proof of Geršgorin Theorem

Proof Let w be an eigenvalue of Φ , then suppose $\Phi \mathbf{x} = w\mathbf{x}$ where \mathbf{x} is a column vector and Φ is a $N \times N$ matrix. There is an element of \mathbf{x} that has largest absolute value, say $|x_p| \geq |x_i|$ for all $i = 1, 2, \dots, N$ and $x_p \neq 0$. Then,

$$wx_p = (w\mathbf{x})_p = (\Phi\mathbf{x})_p = \sum_{j=1}^N \Phi_{pj}x_j = \Phi_{pp}x_p + \sum_{\substack{i,j=1 \\ j \neq p}}^N \Phi_{pj}x_j, \quad (\text{C.23})$$

and by taking the absolute value of both sides and from the triangle inequality, we obtain

$$|w - \Phi_{pp}||x_p| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}||x_j|. \quad (\text{C.24})$$

Since $|x_p| \geq |x_j|$, it can be written

$$|w - \Phi_{pp}||x_p| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}||x_p|, \quad (\text{C.25})$$

and then we conclude that

$$|w - \Phi_{pp}| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}|. \quad (\text{C.26})$$

\square

C.3. Proof of Hellmann-Feynman Theorem

Proof It can be written that $E(\nu) = \langle \psi(\nu) | H(\nu) | \psi(\nu) \rangle$. Then, (Erman, 2010)

$$\begin{aligned} \frac{\partial E(\nu)}{\partial \nu} &= \frac{\partial}{\partial \nu} \int_{\mathbb{R}} \psi^*(\nu) H(\nu) \psi(\nu) d\nu = \int_{\mathbb{R}} \frac{\partial \psi^*(\nu)}{\partial \nu} H(\nu) \psi(\nu) d\nu \\ &+ \int_{\mathbb{R}} \psi^*(\nu) \frac{\partial H(\nu)}{\partial \nu} \psi(\nu) d\nu \\ &+ \int_{\mathbb{R}} \psi^*(\nu) H(\nu) \frac{\partial \psi(\nu)}{\partial \nu} d\nu . \end{aligned} \quad (\text{C.27})$$

Therefore,

$$\begin{aligned} \frac{\partial E(\nu)}{\partial \nu} &= \int_{\mathbb{R}} \left[\frac{\partial \psi^*(\nu)}{\partial \nu} \psi(\nu) + \psi^*(\nu) \frac{\partial \psi(\nu)}{\partial \nu} \right] H(\nu) d\nu \\ &+ \int_{\mathbb{R}} \psi^*(\nu) \frac{\partial H(\nu)}{\partial \nu} \psi(\nu) d\nu , \end{aligned} \quad (\text{C.28})$$

and since $\psi(\nu)$ is a normalized eigenfunction, $\frac{\partial}{\partial \nu} \langle \psi(\nu) | \psi(\nu) \rangle = 0$, the first integral is zero.

Hence,

$$\frac{\partial E(\nu)}{\partial \nu} = \int_{\mathbb{R}} \psi^*(\nu) \frac{\partial H(\nu)}{\partial \nu} \psi(\nu) d\nu = \left\langle \psi(\nu) \left| \frac{\partial H(\nu)}{\partial \nu} \psi(\nu) \right. \right\rangle . \quad (\text{C.29})$$

□

APPENDIX D

DEGENERATE CASE

Let us now examine the degenerate case. Let $E(\nu_0)$ be a N -fold degenerate eigenvalue. The non-degenerate case was given by $N = 1$. In a small neighborhood of ν_0 , the eigenvalue equation which is given in (4.73) can be written as (Vatsya, 2004)

$$H(\nu_0 + \epsilon)\phi_n(\nu_0 + \epsilon) = E_n(\nu_0 + \epsilon)\phi_n(\nu_0 + \epsilon) , \quad (\text{D.1})$$

where $n = 1, \dots, N$ and ϵ is a small parameter or it can be written in that form

$$H(\nu)\phi_n(\nu) = E_n(\nu)\phi_n(\nu) , \quad (\text{D.2})$$

where $\nu = \nu_0 + \epsilon$. As $E_n(\nu_0) = E(\nu_0)$ for each n , some of the eigenvalues $E_n(\nu_0 + \epsilon)$ may be distinct for all non-zero values of ϵ close to zero, which is the only case of interest here. For convenience, it is going to be assumed that each of $E_n(\nu_0 + \epsilon)$ is an isolated, non-degenerate eigenvalue, except for $\epsilon = 0$, and therefore all the corresponding normalized eigenvectors $\phi_n(\nu_0 + \epsilon)$ are uniquely defined. If some of $E_n(\nu_0 + \epsilon)$ are identical, we can approach it similarly. For a continuously differentiable $H(\nu)$, each of $E_n(\nu)$ defines a continuously differentiable curve. For a N -fold degenerate eigenvalue $E(\nu_0)$, N of the curves cross at ν_0 .

For $\phi_n(\nu)$ to be differentiable at $\nu = \nu_0$, it is necessary that $\phi_n(\nu_0 + \epsilon) \rightarrow \phi_n(\nu_0)$ as $\epsilon \rightarrow 0$. For a differentiable $H(\nu)$, this is also sufficient. The eigenvectors $\phi_n(\nu_0)$ can be calculated by the method of degenerate perturbation theory, which is indicated in the sequel below. So, it follows from Eq. (D.1) that

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \left[\frac{H(\nu_0 + \epsilon)\phi_n(\nu_0 + \epsilon) - H(\nu_0)\phi_n(\nu_0)}{\epsilon} \right] \\ = \lim_{\epsilon \rightarrow 0} \left[\frac{E_n(\nu_0 + \epsilon)\phi_n(\nu_0 + \epsilon) - E_n(\nu_0)\phi_n(\nu_0)}{\epsilon} \right] , \end{aligned} \quad (\text{D.3})$$

where limit operation is taken with respect to the norm in Hilbert space. Then, the left-hand

side can be written as

$$\lim_{\epsilon \rightarrow 0} \left[\frac{H(\nu_0 + \epsilon)[\phi_n(\nu_0 + \epsilon) - \phi_n(\nu_0)]}{\epsilon} + \frac{[H(\nu_0 + \epsilon) - H(\nu_0)]\phi_n(\nu_0)}{\epsilon} \right]. \quad (\text{D.4})$$

Since the limits exist, the above equation implies

$$H(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu} + \frac{\partial H(\nu)}{\partial \nu} \phi_n(\nu_0), \quad (\text{D.5})$$

for all the derivatives are evaluated at $\nu = \nu_0$ which is going to be assumed without further mention. After doing similar calculation for the right-hand side, we obtain

$$\frac{\partial H(\nu)}{\partial \nu} \phi_n(\nu_0) + H(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu} = \frac{\partial E_n(\nu)}{\partial \nu} \phi_n(\nu_0) + E_n(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu}. \quad (\text{D.6})$$

By taking the scalar product of this with $\phi_n(\nu_0)$ yields

$$\begin{aligned} \left\langle \phi_n(\nu_0) \left| \frac{\partial H(\nu)}{\partial \nu} \phi_n(\nu_0) \right. \right\rangle + \left\langle \phi_n(\nu_0) \left| H(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu} \right. \right\rangle &= \left\langle \phi_n(\nu_0) \left| \frac{\partial E_n(\nu)}{\partial \nu} \phi_n(\nu_0) \right. \right\rangle \\ &+ \left\langle \phi_n(\nu_0) \left| E_n(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu} \right. \right\rangle, \end{aligned}$$

Because of E is real and $H = H^\dagger$, the right-hand side becomes

$$\frac{\partial E_n(\nu)}{\partial \nu} + \left\langle \phi_n(\nu_0) \left| H(\nu_0) \frac{\partial \phi_n(\nu)}{\partial \nu} \right. \right\rangle.$$

Therefore,

$$\frac{\partial E_n(\nu)}{\partial \nu} = \left\langle \phi_n(\nu_0) \left| \frac{\partial H(\nu)}{\partial \nu} \right| \phi_n(\nu_0) \right\rangle, \quad (\text{D.7})$$

where $n = 1, \dots, N$.

Remark D.1 Note that $\phi_n(\nu_0)$ is not any normalized eigenvector. In the beginning, this rela-

tion was used in Eq. (4.72);

$$\frac{\partial E_n(\nu)}{\partial \nu} = \left\langle \psi(\nu_0) \left| \frac{\partial H(\nu)}{\partial \nu} \psi(\nu_0) \right. \right\rangle , \quad (\text{D.8})$$

where $\psi(\nu_0)$ is an arbitrary normalized vector in the N -dimensional eigenspace of $H(\nu_0)$. But, this result is invalid. Because, each such $\psi(\nu)$ is not differentiable except for $N = 1$.

We can also use the following form of the degenerate Hellmann-Feynman theorem from projections point of view which can be more convenient for some applications. Consider Eq. (D.2) in that way

$$H(\nu)|\phi_n(\nu)\rangle = E_n(\nu)|\phi_n(\nu)\rangle , \quad (\text{D.9})$$

with n solutions for the eigenvalues $E_n(\nu)$. By multiplying both sides of this with $\langle \phi_n(\nu)|$ from the right, we have

$$H(\nu)\mathbb{P}_N(\nu) = E_n(\nu)\mathbb{P}_N(\nu) , \quad (\text{D.10})$$

where $\mathbb{P}_N(\nu)$ is the orthoprojection on the respective eigenspace of $H(\nu)$ defined by

$$\mathbb{P}_N(\nu)u = \sum_{n=1}^N \phi_n(\nu)\langle \phi_n(\nu)|u\rangle , \quad (\text{D.11})$$

for each u in Hilbert space. If we take $\nu = \nu_0$, the above equation reduces to

$$\mathbb{P}_N(\nu_0)u = \sum_{n=1}^N \varphi_n(\nu_0)\langle \varphi_n(\nu_0)|u\rangle , \quad (\text{D.12})$$

where $\varphi_n(\nu_0)$ is an arbitrary orthonormal basis in the N -dimensional eigenspace of $H(\nu_0)$ corresponding to the degenerate eigenvalue. The projection $\mathbb{P}_N(\nu)$ admits the representation which we have already known

$$\mathbb{P}_N(\nu) = -\frac{1}{2\pi i} \oint_C [H(\nu) - E]^{-1} dE , \quad (\text{D.13})$$

where C is a positively oriented closed contour in the complex E -plane enclosing the N eigenvalues $E_n(\nu)$. With the help of this representation, it follows by direct differentiation that for a continuously differentiable $H(\nu)$, $\mathbb{P}_N(\nu)$ is also continuously differentiable with respect to ν . Let us differentiate Eq. (D.10) and operate with $\mathbb{P}_N(\nu_0)$ from left, we possess

$$\begin{aligned} \mathbb{P}_N(\nu_0) \frac{\partial H(\nu)}{\partial \nu} \mathbb{P}_N(\nu_0) &+ \mathbb{P}_N(\nu_0) H(\nu_0) \frac{\partial \mathbb{P}_N(\nu)}{\partial \nu} \\ &= \mathbb{P}_N(\nu_0) \frac{\partial E(\nu)}{\partial \nu} \mathbb{P}_N(\nu_0) \\ &+ \mathbb{P}_N(\nu_0) E(\nu_0) \frac{\partial \mathbb{P}_N(\nu)}{\partial \nu} . \end{aligned} \quad (\text{D.14})$$

The right-hand side of the above equation can be reduced to

$$\frac{\partial E(\nu)}{\partial \nu} \mathbb{P}_N(\nu_0) + \mathbb{P}_N(\nu_0) H(\nu_0) \frac{\partial \mathbb{P}_N(\nu)}{\partial \nu} , \quad (\text{D.15})$$

by means of $\mathbb{P}^2 = \mathbb{P}$ and $E(\nu_0) \mathbb{P}_N(\nu_0) = H(\nu_0) \mathbb{P}_N(\nu_0) = \mathbb{P}_N(\nu_0) H(\nu_0)$ because of $H = H^\dagger$. Therefore, Eq. (D.14) becomes

$$\mathcal{O}_N(\nu_0) = \mathbb{P}_N(\nu_0) \frac{\partial H(\nu)}{\partial \nu} \mathbb{P}_N(\nu_0) = \frac{\partial E(\nu)}{\partial \nu} \mathbb{P}_N(\nu_0) . \quad (\text{D.16})$$

It can be easily seen that if we apply $\langle \phi_n(\nu_0) |$ from left, we have Eq. (D.7).

In our problem, if we have a degeneracy, Eq. (4.4) can be written

$$\mathbb{P}_k = -\frac{1}{2\pi i} \oint_{\Gamma_k} R(E) dE , \quad (\text{D.17})$$

where $\mathbb{P}_k = \sum_{l=1}^{M_l} |\psi_{k,l}\rangle \langle \psi_{k,l}|$ and l is the label of the degeneracy. Also, in Eq. (4.89), we have degenerate projections such as

$$\mathbb{P}_k = \sum_{s=1}^{M_s} |A_i^{k,s}\rangle \langle A_j^{k,s}| . \quad (\text{D.18})$$

By applying the same procedure as in the non-degenerate case, we have

$$\sum_{l=1}^{M_l} \psi_{k,l}(x) \psi_{k,l}^*(y) = - \sum_{i,j=1}^N \sum_{s=1}^{M_s} \frac{R_0(\mathbf{x}, \mathbf{a}_i; -\nu_k^2) A_i^{s*}(-\nu_k^2) A_j^s(-\nu_k^2) R_0(\mathbf{a}_j, \mathbf{y}; -\nu_k^2)}{\left(\frac{\partial w^k(E)}{\partial E} \right) \Big|_{E=-\nu_k^2}} \quad (\text{D.19})$$

We cannot explicitly find the wave function from here. But, one can diagonalize the degenerate eigenstates and find the wave function by a unitary transformation and by doing same calculations, one can see that the non-degenerate case also satisfies Eq. (4.75).

APPENDIX E

PROOF OF PERRON-FROBENIUS THEOREM

Proof 1) Because the eigenvalues of A are real and their sum equals to the $TrA > 0$, it ensures $\lambda > 0$.

2) Let (U_j) be any real normalized eigenvector belonging to λ , then

$$AU_i = \lambda U_i = \sum_j a_{ij} U_j, \quad (\text{E.1})$$

for $i = 1, \dots, n$ and set $X_j = |U_j|$. Hence,

$$0 < \lambda = \sum_{ij} a_{ij} U_i U_j = \left| \sum_{ij} a_{ij} U_i U_j \right|, \quad (\text{E.2})$$

and

$$\lambda \leq \sum_{ij} |a_{ij}| |U_i| |U_j| = \sum_{ij} a_{ij} X_i X_j. \quad (\text{E.3})$$

By means of the variational theorem,

$$\lambda = \sum_{ij} a_{ij} X_i X_j, \quad (\text{E.4})$$

then,

$$\lambda X_i = \sum_j a_{ij} X_j, \quad (\text{E.5})$$

for $i = 1, \dots, n$ and that means (X_j) is an eigenvector belonging to λ . Therefore, if $X_i = 0$ for some i , then because of $a_{ij} > 0$ for all j , $X_j = 0$ which cannot be true. Thus, every $X_j > 0$.

3) Let us assume that λ is degenerate. Hence, we can find two real orthonormal eigenvectors (U_j) and (V_j) belonging to λ . Suppose that $U_i < 0$ for some i . From the addition of Eq. (E.1) and (E.5), we have

$$\lambda(U_i + X_i) = \sum_j a_{ij}(U_j + X_j) \Rightarrow \lambda(U_i + |U_i|) = \sum_j a_{ij}(U_j + |U_j|). \quad (\text{E.6})$$

Then, $U_j = -|U_j|$ for every j . If we assume that $U_i > 0$ for some i and subtracting Eq. (E.5) from (E.1), we obtain $U_j = |U_j|$. That means $U_j = \pm|U_j|$ and by applying the same procedure, we also have $V_j = \pm|V_j|$. Therefore,

$$\sum_j V_j U_j = \pm \sum_j |V_j U_j|. \quad (\text{E.7})$$

Since $|U_j|, |V_j| \neq 0$ for all j , $|V_j U_j| \neq 0$ which means that U and V cannot be orthogonal. Because of the contradiction with the first assumption, λ is non-degenerate.

4) Let (W_j) be a normalized eigenvector belonging to $\mu < \lambda$,

$$\sum_j a_{ij} W_j = \mu W_i. \quad (\text{E.8})$$

From the variational property, we have

$$\lambda = \sum_{ij} a_{ij} U_i U_j \geq \sum_{ij} a_{ij} Y_i Y_j. \quad (\text{E.9})$$

Let us choose $Y_i = |W_i|$ and from the non-degeneracy of λ ,

$$\lambda > \left| \sum_{ij} a_{ij} W_i W_j \right| = |\mu|. \quad (\text{E.10})$$

□

APPENDIX F

THE PROOF OF MEHLER'S FORMULA AND FORMULA (5.52)

F.1. Proof of Mehler's Formula: (5.28)

Let us substitute the integral representation of the Hermite polynomials (Lebedev, 1965):

$$H_n(x) = \frac{(-2i)^n e^{x^2}}{\sqrt{\pi}} \int_{\mathbb{R}} u^n e^{-u^2+2ixu} du, \quad (\text{F.1})$$

into the left-hand side of the Eq. (5.28) and try to find the right-hand side of this equation. So,

$$\begin{aligned} e^{-(x^2+y^2)} \sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) &= \frac{1}{\pi} \int_{\mathbb{R}^2} \left[\sum_{n=0}^{\infty} \frac{(-2zuv)^n}{n!} e^{-u^2-v^2+2ixu+2iyv} \right] du dv \\ &= \frac{1}{\pi} \int_{\mathbb{R}} e^{-v^2+2iyv} \left[\int_{\mathbb{R}} e^{-u^2+2iu(x-\frac{vz}{2})} du \right] dv. \end{aligned} \quad (\text{F.2})$$

From Eq. (G.10):

$$\int_{\mathbb{R}} e^{-u^2+2iu(x-\frac{vz}{2})} du = \sqrt{\pi} e^{-(x-\frac{vz}{2})^2}. \quad (\text{F.3})$$

Therefore, Eq. (F.2) turns out to be

$$e^{-(x^2+y^2)} \sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) = \frac{e^{-x^2}}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-v^2(1-z^2)+v(2iy-2ixz)} dv. \quad (\text{F.4})$$

Since the above integral is similar to the Gaussian integral, we can apply the same procedure as we did for (5.11), then

$$\frac{e^{-x^2}}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-v^2(1-z^2)+v(2iy-2ixz)} dv = \frac{e^{-\frac{(x^2+y^2-2xyz)}{1-z^2}}}{\sqrt{1-z^2}}, \quad (\text{F.5})$$

which is consistent with Eq. (5.28).

F.2. Proof of the Formula (5.52)

Proof Since $\sqrt{\pi} = \Gamma\left(\frac{1}{2}\right)$ and from the property $\Gamma(x+1) = x\Gamma(x)$,

$$\frac{\sqrt{\pi}}{(1-x)} \frac{\Gamma\left(\frac{3}{2} - \frac{x}{2}\right)}{\Gamma\left(1 - \frac{x}{2}\right)} = \frac{1}{2} \frac{\Gamma\left(\frac{1}{2}\right) \Gamma\left(\frac{1-x}{2}\right)}{\Gamma\left(1 - \frac{x}{2}\right)}. \quad (\text{F.6})$$

Also, from Eq. (5.78), the above equation becomes

$$\frac{\sqrt{\pi}}{(1-x)} \frac{\Gamma\left(\frac{3}{2} - \frac{x}{2}\right)}{\Gamma\left(1 - \frac{x}{2}\right)} = \frac{1}{2} B\left(\frac{1-x}{2}, \frac{1}{2}\right). \quad (\text{F.7})$$

There is a useful formula (Gradshteyn & Ryzhik, 2000):

$$B\left(z, \frac{1}{2}\right) = \sum_{k=1}^{\infty} \frac{(2k-1)!!}{2^k k!} \frac{1}{(z+k)} + \frac{1}{z}, \quad (\text{F.8})$$

and that is also satisfied:

$$B\left(z, \frac{1}{2}\right) = \sum_{k=1}^{\infty} \frac{(2k+1)!!}{(2k+1)2^k k!} \frac{1}{(z+k)} + \frac{1}{z}. \quad (\text{F.9})$$

Since $(2k+1)!! = \frac{(2k+1)!}{2^k k!}$ from (Gradshteyn & Ryzhik, 2000), the above equation holds

$$B\left(z, \frac{1}{2}\right) = \sum_{k=1}^{\infty} \frac{(2k)!}{4^k (k!)^2} \frac{1}{(z+k)} + \frac{1}{z}. \quad (\text{F.10})$$

By using this formula, Eq. (F.7) turns out to be

$$\frac{\sqrt{\pi}}{(1-x)} \frac{\Gamma\left(\frac{3}{2} - \frac{x}{2}\right)}{\Gamma\left(1 - \frac{x}{2}\right)} = \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} \frac{1}{(2n+1-x)}, \quad (\text{F.11})$$

where we have relabeled $k \rightarrow n$.

□

APPENDIX G

ONE-DIMENSIONAL SIMPLE HARMONIC OSCILLATOR IN FOURIER SPACE

The Fourier approach to quantum harmonic oscillator problem has been given in (Ponomarenko, 2004). The time-independent Schrödinger equation in one dimension with a simple harmonic oscillator is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x) . \quad (\text{G.1})$$

If we define dimensionless variables $y = \sqrt{\frac{m\omega}{\hbar}}x$ and $\epsilon = \frac{E}{\hbar\omega}$, the above equation turns out to be

$$\frac{d^2\psi}{dy^2} + (2\epsilon - y^2)\psi = 0 . \quad (\text{G.2})$$

If y is too large, then we expect $2\epsilon - y^2 \sim -y^2$ asymptotically. Hence,

$$\frac{d^2\psi}{dy^2} - y^2\psi = 0 , \quad (\text{G.3})$$

which has a solution $\psi(y) = \phi(y)e^{\frac{y^2}{2}}$. Let us substitute this into Eq. (G.2),

$$\phi''(y) + 2y\phi'(y) + (2\epsilon + 1)\phi(y) = 0 . \quad (\text{G.4})$$

By taking formal Fourier transform of both sides of the above equation, we obtain

$$\widehat{\phi}(k) = C e^{\frac{k^2}{4}} k^{-\frac{(2\epsilon+3)}{2}} \quad (\text{G.5})$$

where C is a constant. Then,

$$\psi(y) = C e^{\frac{y^2}{2}} \int_{\mathbb{R}} e^{iky} k^{\epsilon - \frac{1}{2}} e^{-\frac{k^2}{4}} \frac{dk}{2\pi}. \quad (\text{G.6})$$

This should be satisfied: $\psi(y) = \pm\psi(-y)$ because of the symmetry of the potential. After calculations, we find

$$(-1)^{\epsilon - \frac{1}{2}} = \pm 1, \quad (\text{G.7})$$

which means $\epsilon - \frac{1}{2} = n$ where n is an integer. So

$$E = \left(n + \frac{1}{2} \right) \hbar\omega. \quad (\text{G.8})$$

To find the wave function, we return to the Eq. (G.6):

$$\begin{aligned} \psi(y) &= C e^{\frac{y^2}{2}} \int_{\mathbb{R}} e^{iky} k^n e^{-\frac{k^2}{4}} \frac{dk}{2\pi} \\ &= C e^{\frac{y^2}{2}} \frac{d^n}{d(iy)^n} \int_{\mathbb{R}} e^{iky} e^{-\frac{k^2}{4}} \frac{dk}{2\pi}, \end{aligned} \quad (\text{G.9})$$

which looks like a Gaussian integral. We are going to apply the same procedure as we did for the integral given in (5.11). Then,

$$\int_{\mathbb{R}} e^{iky} e^{-\frac{k^2}{4}} \frac{dk}{2\pi} = \frac{e^{-y^2}}{\sqrt{\pi}}. \quad (\text{G.10})$$

So, Eq. (G.9) becomes

$$\psi_n(y) = D_n e^{-\frac{y^2}{2}} H_n(y), \quad (\text{G.11})$$

where D_n is a constant. By substituting $y = \sqrt{\frac{m\omega}{\hbar}}x$ and doing the normalization of the wave function, we obtain

$$\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right). \quad (\text{G.12})$$